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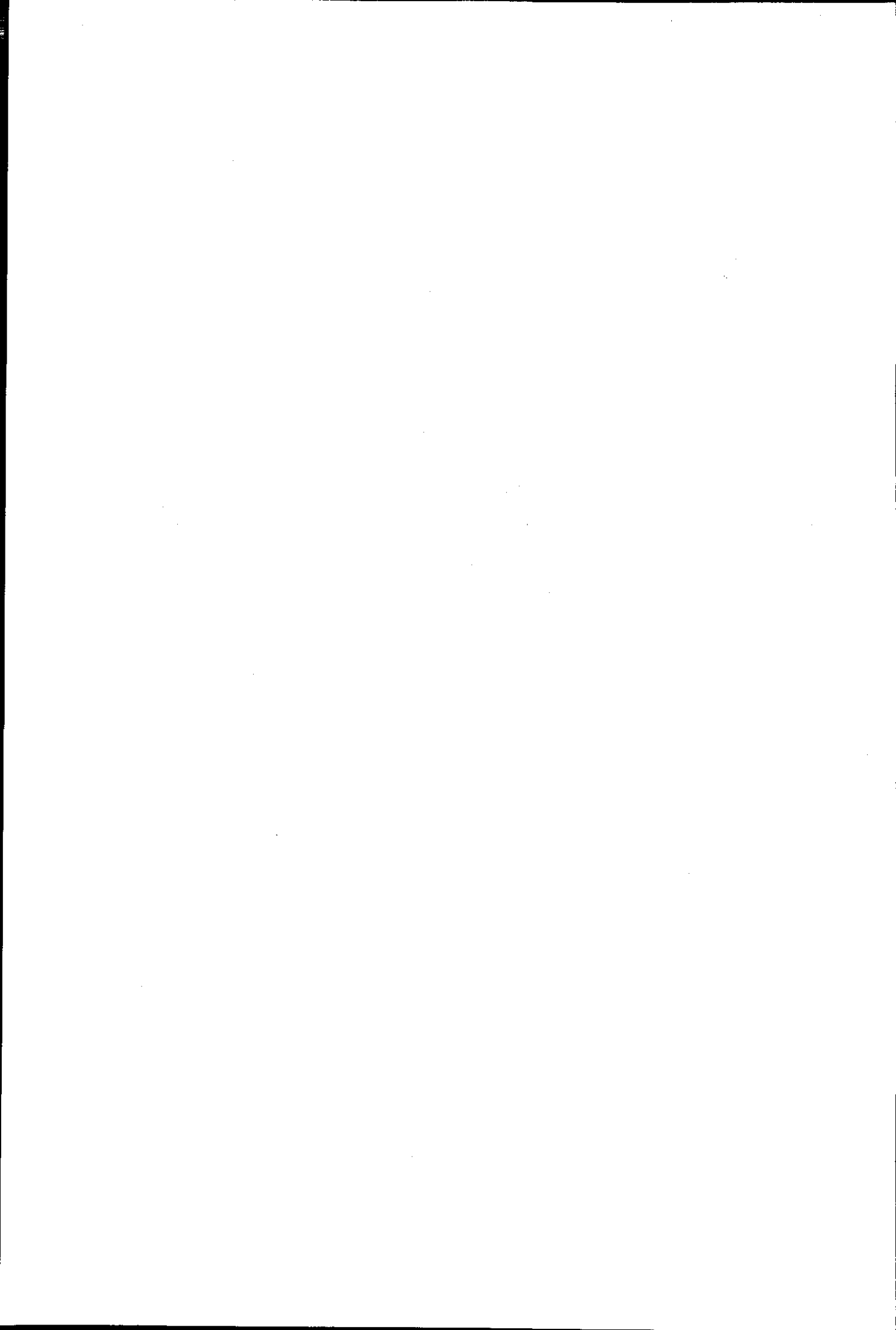
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**SPECTRAL ANALYSIS:
THEORY AND
NUMERICAL RESULTS**

by

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A Master's thesis
submitted in partial fulfilment of the
requirements for the award of Master of Philosophy
of Loughborough University

February 11, 2005

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Abstract

This paper explains how spectral theory characterises an operator, acting on a Banach or Hilbert space, and so helps to solve an equation of that operator, or characterise its solution. Sobolev spaces are discussed, and then Spectral theory is applied to a Laplace operator with Dirichlet boundary conditions, and the eigenvalues characterised. An adapted version of the Rayleigh-Ritz Approximation technique is then used to estimate the eigenvalues.

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Bob Marlow. 11th February, 2005.

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1 Introduction

We show here how spectral theory characterises an operator, acting on a Banach or Hilbert space, and so helps to solve an equation of that operator, or at least characterise its solution. We then apply spectral theory to a particular partial differential operator, namely the Laplace operator with Dirichlet boundary conditions, and so characterise its eigenvalues, and we then use numerical techniques to actually estimate those eigenvalues in an instance of a very general case.

Spectral theory is well-documented in works on functional analysis [Kolmogorov and Fomin] [Kreyszig] [Kirsch] [Meise and Vogt]. There is some difference in the definitions here, though this is only for the Banach space cases. We will detail these definitions and provide examples, and also introduce Sobolev spaces [Adams and Fournier] [Egorov and Kondratiev], which will be needed for our case study.

For our Laplace operator, we will show that, although it is unbounded, its inverse is compact and self-adjoint. Therefore spectral theory can be applied to it, and we can completely characterise its eigenvalues.

Solutions of partial differential equations, both analytic and numeric, are also well documented [Williams], as is the estimation of eigenvalues by trial functions [Kirsch] [Mitchell and Griffiths]. What we will do here is to show how to actually construct trial functions for a very general domain, for our operator, and then estimate the eigenvalues using the Mathematica package from Wolfram research [Pao].

Conventions and notations

"When I use a word, it means exactly what I want it to mean."

- Humpty Dumpty (Alice Through the Looking-Glass).

- 1) Inclusions are *strict*, so that $A \subset B$ follows the same sense as $a < b$, i.e., A is a strict subset of B , so that $B \setminus A \neq \emptyset$. If we are allowing $A = B$, then we will specifically write $A \subseteq B$ [Enderton].
- 2) Unless otherwise stated, spaces are assumed to be separable, as non-separable spaces are rather esoteric, needing the axiom of choice [Enderton] to deal with them, in the form of Zorn's lemma.
- 3) Unless otherwise stated, the underlying field of any Hilbert space is assumed to be \mathbb{C} .
- 4) We will usually write Δ , rather than the equivalent ∇^2 .
- 5) When referring to eigenvalues, ν (nu) refers to their multiplicity.
- 6) Unless otherwise stated, integrals are assumed to be Lebesgue integrals [Weir]. For convenience then, when looking at L^1, L^2 etc, we normally consider these to be 'partitioned' into equivalence classes, $\{\bar{f}_\alpha\}$ say, so that $f, g \in \bar{f}_\alpha$ iff $f = g$ a.e., so we don't need to actually write 'a.e.' on every line. Or, we can say it is taken as read that $f = g$ means a.e., and we then regard f and g as identical.
- 7) When discussing the Sobolev spaces $W^{m,p}(D)$ [Adams and Fournier], we may sometimes write, if D is clearly known, just $W^{m,p}$ (and $W_0^{m,p}$).

8) We use the standard analysis definitions for functions or operators, in that when we write:

$$f : X \mapsto Y$$

X is then referred to as the domain, and Y as the co-domain. The image of f is defined by $\{y \in Y \mid y = f(x), x \in X\}$, and is denoted by $Im(f)$. We do not require that f be defined on all of X ; it need only be defined on a *domain of definition*, which we write as $\mathfrak{D}(f)$, so that whenever we write $f : X \mapsto Y$, we implicitly mean $f : \mathfrak{D}(f) \mapsto Y$.

9) The adjoint of an operator \mathbf{A} will be written as \mathbf{A}^* , and the null space (kernel) of an operator \mathbf{A} as $\mathfrak{N}(\mathbf{A})$.

10) We write $[S]$ to mean closure of the set S .

11) The inner-product of two elements u, v of an inner-product space will be written (u, v) . In the product-space $Z = W \times W \times W \times \dots \times W$ (n times), an inner-product for $\underline{x} (= (x_1, x_2, \dots, x_n))$, $\underline{y} (= (y_1, y_2, \dots, y_n)) \in Z$ can be defined by:-

$$(\underline{x}, \underline{y}) = \sum_{i=1}^n (x_i, y_i)_W$$

and this shall always be the meaning of $(\underline{x}, \underline{y})$ in such a space.

2 Preliminaries

Spectral analysis is a method of finding the properties of an operator, which we here assume to be acting on a Banach or Hilbert space. It can be applied to many classes of operator: compact, bounded or unbounded, self-adjoint or non-self-adjoint [Kreyszig]. We will always assume here that the operator is linear. The spectrum of an operator can actually determine the form of the solution of an operator equation, but even if it cannot do that, it can provide information on the nature of the solution to the equation. In the former case, for example, suppose an operator A is actually compact and self-adjoint, acting on a Hilbert space H . Then spectral theory tells us that H has an orthogonal basis $\{e_n\}$, consisting of eigenvectors of A . So, for any $x \in H$, we can write $x = \sum x_n e_n$ [Kreyszig]. If we then wish to solve the operator equation:-

$$Ax = f$$

then, as

$$\begin{aligned}x &= \sum x_n e_n \\ \Rightarrow Ax &= \sum x_n \lambda_n e_n,\end{aligned}$$

λ_n being the corresponding eigenvalues. If we now write

$$f = \sum f_n e_n,$$

then

$$\sum x_n \lambda_n e_n = \sum f_n e_n.$$

Now suppose A has a trivial kernel. Then by Hilbert space theory [Kreyszig]:-

$$x_n = \frac{f_n}{\lambda_n}$$

and hence

$$x = \sum \frac{f_n}{\lambda_n} e_n$$

and the equation is solved.

2.1 Spectral theory - definitions and examples

The definitions for an operator's spectrum are different for Banach and Hilbert spaces. Firstly, for Hilbert space, let

$$T : H \mapsto H$$

be a linear operator. We define

$$T_\lambda = T - \lambda I, \quad \lambda \in \mathbb{C}.$$

We define the *resolvent set* $\rho(T)$ to be that subset of \mathbb{C} s.t. T_λ^{-1} ($= R_\lambda$) exists, by which we mean R_λ is a bounded operator, mapping H to H . The *point spectrum* $\sigma_p(T)$ consists of the eigenvalues, i.e.

$$\sigma_p(T) = \{\lambda \in \mathbb{C} \mid Tx = \lambda x, 0 \neq x \in H\}^1.$$

The *continuous spectrum* $\sigma_c(T)$ is defined as λ where we can define R_λ ($\mathcal{D}(R_\lambda) = \text{Im}(T_\lambda)$) as the inverse of T_λ , but R_λ is *not* bounded as a mapping from $H \mapsto H \setminus^2 \mathfrak{N}(T - \lambda I)^3$. Thus $\sigma_c(T)$ may coincide

¹We allow zero eigenvalues, though some authors do not.

²This " \setminus " means the orthogonal complement in H .

³By definition, this is the eigenspace of λ : for λ not an eigenvalue, the eigenspace is thus \emptyset .

with $\sigma_p(T)$, as we shall see shortly. Finally, if, *after* looking for $\sigma_p(T)$ and $\sigma_c(T)$, there are $\lambda \notin \sigma_p(T) \cup \sigma_c(T)$ s.t. $Im(T_\lambda) \neq H$, then such λ are in the *residual spectrum*, $\sigma_r(T)$. Illustrative examples are shown below.

2.1.1 Other definitions

The *essential spectrum* is the continuous spectrum, plus all eigenvalues of infinite multiplicity. Some authors refer to the *discrete spectrum* synonymously with the point spectrum, but we define the *discrete spectrum* as only those eigenvalues for which $\nu < \infty$ [Egorov and Kondratiev, p.141].

2.1.2 Banach space

As with Hilbert space, for a Banach space B , let

$$T : B \mapsto B$$

be a linear operator, and we define

$$T_\lambda = T - \lambda I, \quad \lambda \in \mathbb{C}.$$

Here though, as there is no concept of orthogonal complement, the definitions are slightly different. The definitions for resolvent set and eigenvalues (point spectrum) are the same; for the rest there are, unfortunately, various definitions. We will write one here, followed by an illustration.

So then, we define $\sigma_c(T)$, the *continuous spectrum*, as $\lambda \in \mathbb{C}$ s.t. λ is not an eigenvalue, and R_λ exists as a map from B to B ($\mathfrak{D}(R_\lambda) = Im(T_\lambda)$), but is not bounded. Then, just as in Hilbert space, *after* looking at

whether λ is in $\sigma_p(T)$ or $\sigma_c(T)$, if we then find that there are $\lambda \notin \sigma_p(T) \cup \sigma_c(T)$ s.t. R_λ exists, but $Im(T_\lambda)$ is not the whole of the co-domain, then λ is in the *residual spectrum*, $\sigma_r(T)$.

2.1.3 Illustrations of spectral definitions

First consider $T : L^2[0, 1] \mapsto L^2[0, 1]$, defined by $Tx = \mu(t)x(t)$, $\mu(t)$ being some bounded function on $[0, 1]$. Let's say μ has the shape shown in Figure 1.

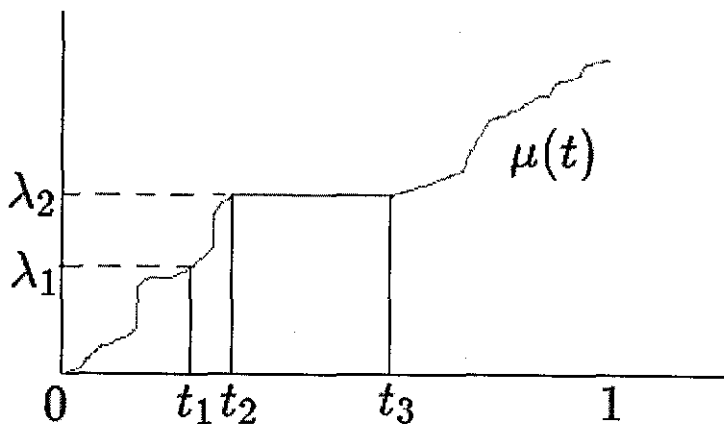


Figure 1: $\mu(t)$

We define $R_\lambda y(t)$ as $\frac{y(t)}{\mu(t) - \lambda}$, except where the denominator is zero, then we define it as zero, where $y(t) = Tx(t) - \lambda x(t)$. This returns us to the same $x(t)$, except possibly at points where the denominator above was zero. First of all then, if $\lambda \notin Im(\mu)$, then, as $\frac{1}{\mu(t) - \lambda}$ is bounded, $\Rightarrow \lambda \in \rho(T)$. Now looking for eigenvalues - these are points in $Im(\mu)$

where $\mu(t)$ is realised over a set of non-zero measure in $[0, 1]$.

The value λ_2 in Figure 1, being held over t_2 to t_3 , is clearly such a value; an example of an eigenfunction is shown in Figure 2.

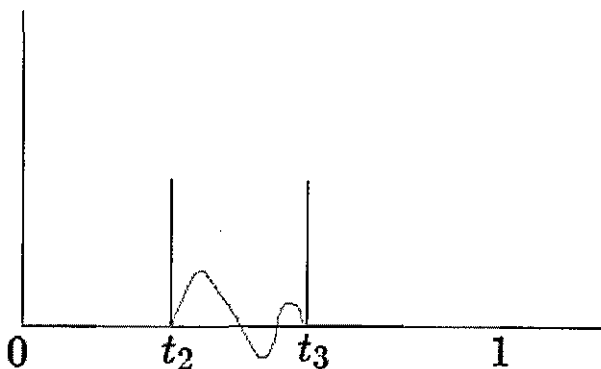


Figure 2: Example eigenfunction

Now suppose we are looking at the value $\lambda = \lambda_1$ in Figure 1 (or any non-eigenvalue point in $Im(\mu)$). Then R_{λ_1} maps $y(t)$ to $\tilde{x}(t)$, where $\tilde{x}(t)$ can differ from $x(t)$ only at the point t_1 . Consider a sequence of functions y_n , which are equivalent to 1, except at intervals centred on t_1 , the length of these intervals tending to zero from above. Each y_n is zero on the finite interval, and so $\|y_n\|_{L^2} < 1$. As the interval round t_1 is not zero, $y_n \in Im(T_{\lambda_1})$, but $\|R_{\lambda_1} y_n\|_{L^2} \rightarrow \infty$, so R_{λ_1} is not bounded, hence $\lambda_1 \in \sigma_c(T)$. For λ_2 , the same is true: if we remove the eigenspace (see Figure 2), we are left in the same situation as λ_1 , because the asymptotic

behaviour is still there, so λ_2 is in $\sigma_p(T)$ and $\sigma_c(T)$. In summary then:-

$$\rho(T) = \mathbb{C} \setminus \text{Im}(\mu).$$

$$\sigma_p(T) = \{\lambda \in \text{Im}(\mu) \text{ and constant on a set of non-zero measure}\}.$$

$$\sigma_c(T) = \text{Im}(\mu).$$

$$\sigma_r(T) = \emptyset.$$

Now suppose μ has a different form, as shown in Figure 3. μ is now discontinuous; in particular, it is only near λ_2 when it is λ_2 .

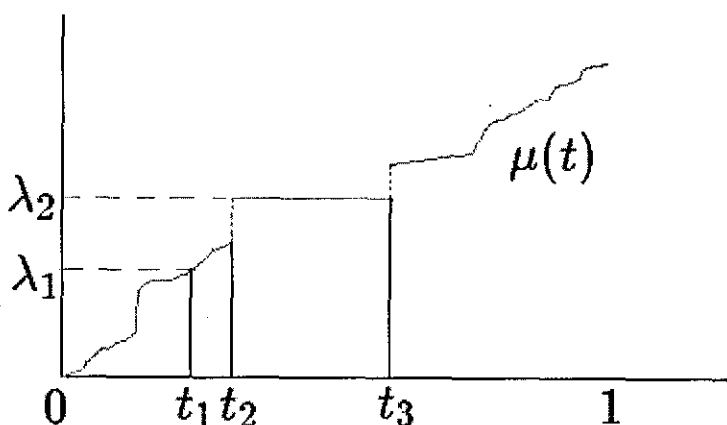


Figure 3: $\mu(t)$ with discontinuities

So now, $\mu(t) \not\rightarrow \lambda_2$ at t_2 from the left, and $\mu(t) \not\rightarrow \lambda_2$ at t_3 from the right. In this case, R_λ can be defined as a bounded operator on H to $H \setminus \mathfrak{N}(T - \lambda_2 I)$ ($\mathfrak{D}(R_\lambda) = \text{Im}(T - \lambda_2 I)$), as there is now no asymptote at λ_2 , hence $\lambda_2 \notin \sigma_c(T)$. The rest of the spectrum is the same.

For Banach space, we take the same operator and definitions as above,

except that we now map $C[0,1]$ to $C[0,1]$, and therefore μ must be continuous. $\rho(T)$ and $\sigma_p(T)$ are the same as in the Hilbert case. $\sigma_c(T)$ is slightly different, but it turns out this is only because we have excluded eigenvalues from it by definition. Referring to Figure 1, λ_2 is still an eigenvalue, but by our definition, it is not in the continuous spectrum. For λ_1 , or indeed any $\lambda \in Im(\mu) \setminus \{\lambda_2\}$, R_λ is unbounded, as it was in the Hilbert case, and we can prove this using almost the same construction:-

Consider the point t_1 (see Figure 1) and consider a sequence of functions y_n , which are equivalent to 1, except at intervals centred on t_1 , the length of these intervals tending to zero from above. Each y_n is zero on the middle third of this finite interval, and in the first third, slopes linearly to zero, whilst on the last third, slopes linearly back to 1. Thus each y_n is a continuous function, and by our definition of inverse (same as in the Hilbert case), $R_{\lambda_1} y_n$ exists. However, $\|y_n\|_{C[0,1]} = 1$, but $\|R_{\lambda_1} y_n\|_{C[0,1]} \rightarrow \infty$, because of the asymptote at t_1 , so R_{λ_1} is not bounded, hence $\lambda_1 \in \sigma_c(T)$. In summary then:-

$$\rho(T) = \mathbb{C} \setminus Im(\mu).$$

$$\sigma_p(T) = \{\lambda \in Im(\mu) \text{ and constant on a set of non-zero measure}\}.$$

$$\sigma_c(T) = Im(\mu) \setminus \sigma_p(T).$$

$$\sigma_r(T) = \emptyset.$$

2.2 Sobolev spaces

Note: In all the remaining sections of this paper, we assume D to be a bounded domain in \mathbb{R}^n , having a piecewise smooth boundary with no cusps.

We define the Sobolev ("Weak" space) $W^{m,p}(D)$ for $m \in \mathbb{Z}_+$, $1 \leq p < \infty$ and some region D in \mathbb{R}^n as [Adams and Fournier] [Weir]:-

$$W^{m,p}(D) = \{u \in L^p(D) : \partial^\alpha u \in L^p(D) : 0 \leq |\alpha| \leq m\}$$

where $\partial^\alpha u$ is the distributional ("weak") derivative of u . The norm on u is defined by:-

$$\|u\|_{W^{m,p}} = \left(\sum_{0 \leq |\alpha| \leq m} \|\partial^\alpha u\|^p \right)^{\frac{1}{p}}.$$

In addition, we define $W^{0,p}(D)$ to be $L^p(D)$.

The Sobolev space $W_0^{m,p}(D)$ is defined as the closure of $C_0^\infty(D)$ under $W^{m,p}$ norm - and having the same norm as that of $W^{m,p}(D)$.

The *trace* of a function u in a Sobolev space, for a bounded domain D , can be thought of as the limit of u approaching the boundary [Egorov and Kondratiev] where this limit exists, but can also be defined in terms of projections and transformations to map ∂D to a co-ordinate surface [Renardy and Rogers]. In the sections that follow, $u \Big|_{\partial D}$ will refer to this trace. If $m \geq 1$ and $p = 2$, with our conditions on D , the traces of functions in $W^{m,p}(D)$ exist and form a space in their own right, namely $W^{m-1,p}(\partial D)$. Furthermore, there is a *trace mapping* mapping functions in $W^{m,p}(D)$ to their traces [Adams and Fournier] [Renardy and Rogers].

As a simple example of a Sobolev space, if we look at the mod ($u = |x|$) function on $[-1,1]$:-

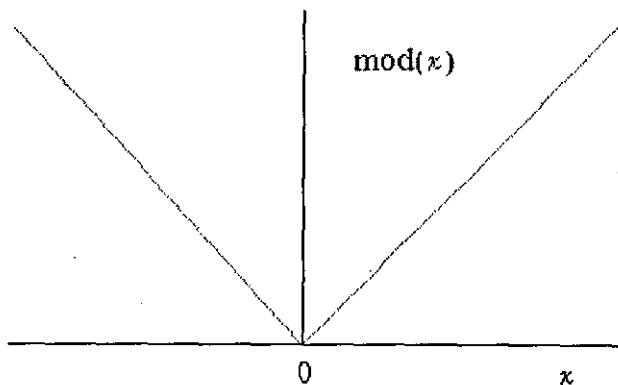


Figure 4: $\text{mod}(x)$

then, clearly u' does not exist in the classical (C) sense, and yet we can say u' does exist as an integrable function. So, in this case, we can say $u \in W^{1,1}([-1, 1])$. The Sobolev space definition arose from considering what space u belongs to in the PDE $-\Delta u = f$ when $f \in L^p(D)$. If f is in $L^2(D)$ for example, which is equivalent to $W^{0,2}(D)$, the definition above leads us to u being in $W^{2,2}(D)$, hence we see the value of m in $W^{m,p}(D)$ reduced by the order of the differential operator.

$W^{2,2}$ is one of two special Sobolev spaces we will use in the numeric work to follow. The second is the space $W_0^{1,2}$, which we defined as the closure of C_0^∞ under the norm of $W^{1,2}$ (and having that norm). (C_0^∞ , or rather, $C_0^\infty(D)$, is the set of functions in C^∞ that are zero near the boundary of D .) We can write that definition as $W_0^{1,2} = [C_0^\infty]_{W^{1,2}}$.

Both these spaces are actually Hilbert spaces. In fact, for any m , $W^{m,2}$ is a Hilbert space, with the inner-product:-

$$(f, g) = \sum_{|\alpha| \leq m} (\partial^\alpha f, \partial^\alpha g).$$

There are two theorems of Sobolev spaces that we will use in the sequel:-

1) The *Sobolev imbedding theorem* [Adams and Fournier] states that for integers $j \geq 0, m \geq 0, n \geq 1$ and for any numbers p, q, s such that $0 < s < \infty, 1 \leq q \leq \infty, 1 \leq p < \infty$, if $s < m$ and $m - 1 - j \leq n/p < s \leq m - j$, then the Besov space $B^{s,p,q}(D)$ is imbedded [Adams and Fournier] [Renardy and Rogers] in the generalised Hölder space $C^{j,\mu,q}(\overline{D})$ where $\mu = s - n/p$ and D is a domain in \mathbb{R}^n satisfying the strong Lipschitz condition (which our domain trivially does). Note that with these conditions, the Sobolev space $W^{m,p}(D)$ is imbedded in the Besov space $B^{s,p,\infty}(D)$. Furthermore, let $q = \infty$, and then the generalised Hölder space $C^{j,\mu,q}(\overline{D})$ is the standard Hölder space $C^{j,\mu}(\overline{D})$. We can combine these last two statements to produce a more tractable version of the theorem for our purposes, namely that $W^{m,p}(D)$ is imbedded in $C^{j,\mu}(\overline{D})$ where $s < m$ and $m - 1 - j \leq n/p < s \leq m - j$, with the same conditions as above. This theorem is illustrated in the following examples, where we are looking for the 'best possible' indices, typically the highest order of differentiability [Adams and Fournier] :-

i) $m = 2, p = 2, n = 1$. So $s < 2$ and $1 - j \leq 1/2 < s \leq 2 - j$, so then the best possible indices are $j = 1, s = 1 \Rightarrow \mu = 1/2$, hence $W^{2,2}(D)$ is imbedded in $C^{1,1/2}(D)$, and therefore, if u is in $W^{2,2}(D)$, $D \subseteq \mathbb{R}$, we can

say u is continuously differentiable, and its derivative satisfies the Hölder condition for $\mu = \frac{1}{2}$.

ii) $m = 2, p = 2, n = 2$. So $1 - j \leq 1 < s \leq 2 - j$. Hence j must be zero. But we need $s < m = 2$, so $s = m - \gamma$, for any γ in $(0, 1)$ and then $\mu = 1 - \gamma$, hence $W^{2,2}(D)$ is imbedded in $C^{0,\gamma}(D) \forall \gamma \in (0, 1)$ where $D \subseteq \mathbb{R}^2$.

2) *The trace imbedding theorem* [Adams and Fournier] [Renardy and Rogers] states that the trace mapping $W^{m,p}(D) \mapsto W^{m-1,p}(\partial D)$ (as defined above) is linear and continuous. An important corollary of this is that by our definition of $u \Big|_{\partial D}$, if $u_n \rightarrow u$ in $W^{2,2}(D)$, then:-

$$u_n \Big|_{\partial D} \rightarrow u \Big|_{\partial D} \quad \text{and} \quad \nabla u_n \Big|_{\partial D} \rightarrow \nabla u \Big|_{\partial D}.$$

3 Case study - theory

The operator we will analyse and estimate eigenvalues for is the one acting on u to produce this PDE :-

$$-\Delta u \Big|_D = f; \quad u \Big|_{\partial D} = 0. \quad (1)$$

Where $u \in W^{2,2}(D) \cap W_0^{1,2}(D)$, and D is some simply-connected bounded region [Apostol] in \mathbb{R}^2 :-



Figure 5: Example regions in \mathbb{R}^2

The value of u on the boundary refers to the trace of u , as defined in Section 2.2. And as we noted in that section, as $-\Delta$ is a second order differential operator, f is in $W^{0,2}(D)$, i.e., $L^2(D)$. We have chosen $W^{2,2}(D) \cap W_0^{1,2}(D)$ because of the comments above in Section 2.2, and also since, for the left-hand side, $W^{2,2}$ is a Hilbert space, making it easier to work with, and, for the right-hand side, if we used $W_0^{2,2}$ (meaning closure of C_0^∞ under $W^{2,2}$ norm), then we would actually over-specify

the problem. In fact, by the trace imbedding theorem in Section 2.2, if $u \in W_0^{2,2}(D)$,

then $u = \lim_{n \rightarrow \infty} u_n$ in $W^{2,2}$ norm, where $u_n \in C_0^\infty(D)$,

so u_n is zero near ∂D , hence $\nabla u_n \Big|_{\partial D} = 0$,

and so $u \Big|_{\partial D} = 0$, and $\nabla u \Big|_{\partial D} = 0$, but we have not specified this latter condition.

We refer to this operator ($-\Delta$ acting on u) and its boundary conditions as \mathbf{A} , and we write the domain of \mathbf{A} as $\mathfrak{D}(\mathbf{A}) = W^{2,2}(D) \cap W_0^{1,2}(D)$. We assume ∂D to be piecewise smooth (C^∞) with no cusps.

Let us now define $\mathfrak{D}(\mathbf{A})$ more precisely. We would normally use the norm of $W^{2,2}$ for the space $W^{2,2} \cap W_0^{1,2}$. However, we actually regard $\mathfrak{D}(\mathbf{A})$ as being the *domain of definition* of an operator acting on L^2 as discussed in the Introduction (Conventions), so we actually use the norm and inner-product of the space $L^2(D)$. Hence, the inner-product and norm are defined by:-

$$(u, v) = \int_D u \bar{v} dx \quad (2)$$

$$\|u\| = \left(\int_D |u|^2 dx \right)^{1/2}. \quad (3)$$

The image of u , f , is implicitly in L^2 , and has the same norm as (3). It's clear from the above definitions that the meaning of (1) is also not that of the conventional equation. In fact, we can say, and we can say only that $-\Delta u = f$ is in the L^2 sense, i.e. :-

$$\int_D (-\Delta u - f)^2 dx = 0 \quad (4)$$

and consequently:-

$$-\Delta u = f \text{ a.e.} \quad (5)$$

Note though, that even if we regard u as a function well-defined point-wise, $-\Delta u$ may exist only as a distribution. In fact, as we are working in \mathbb{R}^2 , the Sobolev imbedding theorem (see Section 2.2) actually shows us that u is continuous in D .

Continuing the analysis, we see $-\Delta$ is not bounded, by considering the sequence $u_n(x, y) = e^{-n(x^2+y^2)}\phi(x, y)$, where ϕ is a 'cut-off mollifier' function, used to give us $u_n \Big|_{\partial D} = 0$ (these are discussed further in Section 3.2.1). For then $\frac{\|-\Delta u_n\|}{\|u_n\|} \rightarrow \infty$ as $n \rightarrow \infty$. At first sight then, this appears to limit the theorems we can apply to \mathbf{A} . We will, however, now show that \mathbf{A} is closed and *an operator with compact resolvent* so therefore we can apply quite a substantial amount of spectral theory to it. We first prove it is closed:-

Theorem 3.1 *Let $u_n \rightarrow u$ and $Au_n \rightarrow v$ in L^2 norm, where $u_n \in \mathcal{D}(\mathbf{A})$, as defined above. Then $u \in \mathcal{D}(\mathbf{A})$ and $\mathbf{A}u = v$.*

Proof As \mathbf{A} is linear and always maps real-valued functions to real-valued functions, we need only prove this for such functions. First note that for f and g in $\mathcal{D}(\mathbf{A})$, Appendix 1 implies:-

$$(-\Delta f, g) = (f, -\Delta g). \quad (6)$$

Now as $\mathbf{A}u_n \rightarrow v$, and the inner-product preserves continuity, for any $\phi \in C_0^\infty(D)$:-

$$(-\Delta u_n, \phi) \rightarrow (v, \phi). \quad (7)$$

Similarly, we can say:-

$$(u_n, -\Delta\phi) \rightarrow (u, -\Delta\phi). \quad (8)$$

But from equation (6):-

$$(-\Delta u_n, \phi) = (u_n, -\Delta\phi). \quad (9)$$

So combining equations (7), (8) and (9), we have, for any $\phi \in C_0^\infty(D)$:-

$$(v, \phi) = (u, -\Delta\phi). \quad (10)$$

In the distribution sense [Kolmogorov and Fomin] [Kreyszig], the right-hand side of equation (10) actually defines $-\Delta u$, so in the distribution sense:-

$$(v, \phi) = (-\Delta u, \phi) \quad (11)$$

and again in that sense:-

$$v = -\Delta u. \quad (12)$$

By the elliptic regularity theorem [Folland] [Gilbarg and Trudinger], this implies $u \in W^{2,2}(D)$. Next then, we need to prove that $u \in W_0^{1,2}(D)$. As, by definition, $u_n \rightarrow u$ in L^2 norm, it remains to prove $\nabla u_n \rightarrow \nabla u$ in L^2 norm. From the definition in Section 2.2, this is equivalent to proving that $\forall \underline{\phi} \in C_0^\infty(D) \times C_0^\infty(D)$:-

$$(\nabla u_n, \underline{\phi}) \rightarrow (\nabla u, \underline{\phi}), \quad (13)$$

or equivalently, by definition of ∇u :-

$$(\nabla u_n, \underline{\phi}) \rightarrow (u, -\operatorname{div}\underline{\phi}). \quad (14)$$

Consider $(-\Delta u_n, u_n)$. From Appendix 1:-

$$(-\Delta u_n, u_n) = \int_D |\nabla u_n|^2. \quad (15)$$

But $(-\Delta u_n, u_n) \rightarrow (v, u)$, hence ∇u_n is a bounded (vector) sequence in $L^2 \times L^2$. But $L^2 \times L^2$ is weakly compact [Kreyszig], so ∇u_n has a weakly convergent sub-sequence, i.e., there is a $\underline{g} \in L^2 \times L^2$ and some sub-sequence u_n^k of u_n such that:-

$$(\nabla u_n^k, \underline{w}) \rightarrow (\underline{g}, \underline{w}) \quad (16)$$

for all $\underline{w} \in L^2 \times L^2$ as $k \rightarrow \infty$, this \underline{g} depending only on u_n , and in particular, for any $\underline{w} = \underline{\phi} \in C_0^\infty(D) \times C_0^\infty(D)$. As $u_n \in [C_0^\infty(D)]$ and $\underline{\phi} \in C_0^\infty(D) \times C_0^\infty(D)$:-

$$(\nabla u_n^k, \underline{\phi}) = (u_n^k, -\text{div} \underline{\phi}), \quad (17)$$

so as $(\nabla u_n^k, \underline{\phi}) \rightarrow (\underline{g}, \underline{\phi})$:-

$$(u_n^k, -\text{div} \underline{\phi}) \rightarrow (\underline{g}, \underline{\phi}). \quad (18)$$

By continuity of the inner-product:-

$$(u_n^k, -\text{div} \underline{\phi}) \rightarrow (u, -\text{div} \underline{\phi}), \quad (19)$$

so combining (18) and (19):-

$$(\underline{g}, \underline{\phi}) = (u, -\text{div} \underline{\phi}), \quad (20)$$

$\forall \underline{\phi} \in C_0^\infty(D) \times C_0^\infty(D)$, so by definition, $\underline{g} = \nabla u$. Looking at the complete sequence again:-

$$(\nabla u_n, \underline{\phi}) = (u_n, -\text{div} \underline{\phi}) \rightarrow (\underline{g}, \underline{\phi}) = (\nabla u, \underline{\phi}), \quad (21)$$

hence $\nabla u = \underline{g}$ and $\nabla u_n \rightarrow \nabla u$, as required. ■

Now we consider the resolvent at zero, i.e., :-

$$u = R_0 f \quad (22)$$

where we also regard R_0 as mapping L^2 to L^2 with the domain of definition being $Im(\mathbf{A})$. We need to first show that this is well-defined.

Suppose then, for $u, v \in \mathfrak{D}(\mathbf{A})$, that

$$-\Delta u = f \text{ and } -\Delta v = f. \quad (23)$$

So, putting $w = u - v$, (23) gives us:-

$$-\Delta w = 0 \text{ and } w \Big|_{\partial D} = 0. \quad (24)$$

By a variation of the uniqueness principle (see Appendix 1), applied to $\mathfrak{D}(\mathbf{A})$, we see $w = 0$, i.e., there is no zero eigenvalue and $u = R_0 f$ is well-defined. Furthermore, if $-\Delta u = f$ and $-\Delta v = g$, if we then write:-

$$w = R_0(f + g)$$

then

$$\begin{aligned} -\Delta w &= f + g \\ &= -\Delta u - \Delta v, \\ -\Delta w &= -\Delta(u + v). \end{aligned} \quad (25)$$

So from the zero eigenvalue property above, (25) \Rightarrow

$$w = u + v.$$

Hence $R_0(f + g) = R_0 f + R_0 g$, so R_0 is linear. We will now also show R_0 is bounded, self-adjoint and compact.

3.1 Boundedness of R_0

As $u \in W_0^{1,2}$, we can use Poincaré's inequality [Renardy and Rogers], that $\|u\| \leq C_D \|\nabla u\|$, the norms being in L^2 , as earlier indicated⁴. C_D is some positive constant, depending only on the domain D .

$$\begin{aligned} \text{Now, } \|\nabla u\|^2 &= \int_D |\nabla u|^2 dx \\ &= \int_D \nabla u \cdot \nabla u dx \end{aligned}$$

from Green's first theorem (see Appendix 1) on u , since $u|_{\partial D} = 0$:-

$$\begin{aligned} \|\nabla u\|^2 &= - \int_D u \Delta u dx \\ &= \int_D u f dx \Rightarrow \\ \|\nabla u\|^2 &\leq \|f\| \|u\|. \end{aligned} \tag{26}$$

Now, for any 2 real numbers a, b and any $\epsilon > 0$, we can write:-

$$ab \leq \epsilon^2 a^2 + \frac{b^2}{4\epsilon^2}.$$

Applying this to (26) :-

$$\|\nabla u\|^2 \leq \epsilon^2 \|u\|^2 + \frac{\|f\|^2}{4\epsilon^2}. \tag{27}$$

Writing Poincaré's inequality again:-

$$\|u\| \leq C_D \|\nabla u\|. \tag{28}$$

Now combining (27) and (28) :-

$$\begin{aligned} \|u\|^2 &\leq C_D^2 \|\nabla u\|^2 \\ &\leq C_D^2 (\epsilon^2 \|u\|^2 + \frac{\|f\|^2}{4\epsilon^2}) \\ \Rightarrow \|u\|^2 (1 - C_D^2 \epsilon^2) &\leq \frac{C_D^2}{4\epsilon^2} \|f\|^2. \end{aligned}$$

⁴we define $\|\nabla u\|$ as $(\int_D |\nabla u|^2 dx)^{\frac{1}{2}}$.

We choose ϵ so $1 - C_D^2 \epsilon^2 > 0$, so then:-

$$\|u\|^2 \leq \frac{C_D^2}{4\epsilon^2(1 - C_D^2 \epsilon^2)} \|f\|^2$$

and hence:-

$$\|u\| \leq \tilde{C}_D \|f\| \quad \forall u \in \mathfrak{D}(\mathbf{A})$$

hence R_0 is bounded.

3.2 Self-adjointness of R_0

Self-adjointness is normally defined for a bounded operator \mathbf{O} mapping all of a Hilbert space H to itself. For an unbounded operator, we can extend the definition [Meise and Vogt, p.211] to the case where we have only $\mathfrak{D}(\mathbf{O}) \subset H$, but for this to be valid, we require that $\mathfrak{D}(\mathbf{O})$ is actually dense in H , and the operator \mathbf{O} is then said to be *densely-defined*. In our case, as $\mathfrak{D}(R_0) = \text{Im}(\mathbf{A})$, we will prove the equivalent that $[\text{Im}(\mathbf{A})] = L^2(D)$. We will do this by actually considering the adjoint properties of \mathbf{A} . First then, we need to show $\mathfrak{D}(\mathbf{A})$ is dense in $L^2(D)$.

3.2.1 Density of \mathbf{A}

We use here a mollifier function ϕ [Adams and Fournier, p.36]:-

$$\phi(x) = \begin{cases} e^{-(|x|^2-1)^{-1}} & \text{if } |x| < 1 \\ 0 & \text{otherwise.} \end{cases}$$

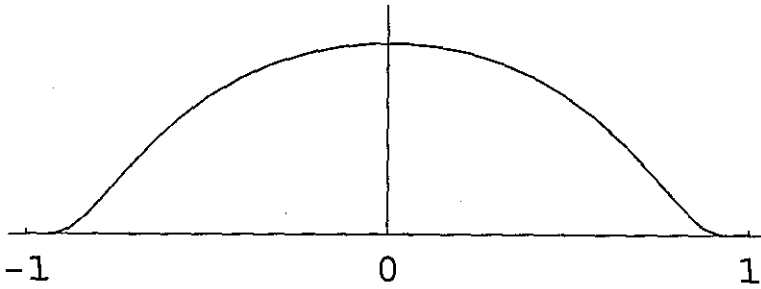


Figure 6: mollifier function

ϕ 's characteristic is that it has compact support, but is infinitely smooth everywhere, even at the 'cut-off' points. The function is shown above in its \mathbb{R} form. We now take $\chi(x) = \frac{1}{2}\phi(x)$, so that

$$\int_{\mathbb{R}^2} \chi(x) dx = 1$$

and then $\chi_k(x) = k^2\chi(kx)$ ($k > 0$), so that we also have

$$\int_{\mathbb{R}^2} \chi_k(x) dx = 1,$$

but the support of $\chi_k(x)$ is now reduced to a ball of diameter $\frac{1}{k}$. We will use the mollifier function to construct, by a convolution, an $f_k \in \mathcal{D}(\mathbf{A})$ that is arbitrarily close to any $f \in L^2(D)$. So, let $f \in L^2(D)$ and $\epsilon > 0$. Since $C_0^\infty(D) \subset W_0^{1,2}(D)$ and $C_0^\infty(D) \subset W^{2,2}(D)$, we need only find an f_k such that $\|f - f_k\|_{L^2} < \epsilon$, where $f_k \in C_0^\infty(D)$. In fact, we will actually

approximate an f_h which is itself arbitrarily close to f . We define a new domain D_h^- which is D except all points a distance h or less from ∂D , h chosen to be small enough for this to be a clear definition. (See Figure 7.) Now define f_h to be equal to f in D_h^- and zero elsewhere. Now choose a smaller h , if necessary, so that $\|f - f_h\|_{L^2} < \frac{\epsilon}{2}$. This is possible, simply by the Lebesgue definition of L^2 .

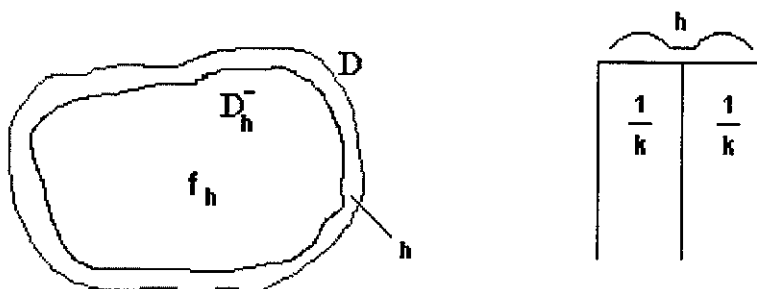


Figure 7: D less an "outer strip"

It is then only necessary to find an f_k such that $\|f_h - f_k\|_{L^2} < \frac{\epsilon}{2}$. So, for our $f_h \in L^2$, define:-

$$f_k(x) = \int_{\mathbb{R}^2} f_h(y) \chi_k(x - y) dy.$$

This is in $C^\infty(\mathbb{R}^2)$ [Weir, p.118]. Now consider how close we can get f_k to f_h :-

$$\|f_h - f_k\|^2 = \int_{\mathbb{R}^2} |f_h(x) - f_k(x)|^2 dx \quad (29)$$

$$\text{but since } \int_{\mathbb{R}^2} \chi_k(x - y) dy = 1$$

$$\begin{aligned} \text{we can write } f_h(x) &= f_h(x) \int_{\mathbb{R}^2} \chi_k(x - y) dy \\ &= \int_{\mathbb{R}^2} f_h(x) \chi_k(x - y) dy \end{aligned}$$

and so (29) becomes:-

$$\begin{aligned}\|f_h - f_k\|^2 &= \int_{\mathbb{R}^2} \left| \int_{\mathbb{R}^2} f_h(x) \chi_k(x-y) dy - \int_{\mathbb{R}^2} f_h(y) \chi_k(x-y) dy \right|^2 dx \\ &= \int_{\mathbb{R}^2} \left| \int_{\mathbb{R}^2} (f_h(x) - f_h(y)) \chi_k(x-y) dy \right|^2 dx.\end{aligned}\quad (30)$$

Now however, consider where $(f_h(x) - f_h(y)) \chi_k(x-y)$ can (possibly) be non-zero. $\chi_k(z)$ is only non-zero for $\|kz\| \leq 1$, or equivalently, $\|z\| < \frac{1}{k}$, so writing $z = y - x$, and noting that $\chi_k(z)$ is even, (30) becomes:-

$$\|f_h - f_k\|^2 = \int_{\mathbb{R}^2} \left| \int_{\|z\| < \frac{1}{k}} (f_h(x) - f_h(x+z)) \chi_k(z) dz \right|^2 dx. \quad (31)$$

But for any $f \in L^1$ and any $\epsilon > 0$, $\exists \delta = \delta(f, \epsilon) > 0$ such that if $\|v\| < \delta$, then $\|f - f_v\|_{L^1} < \epsilon$, where $f_v(x) = f(x-v)$ (this can be derived from Lebesgue's theorem [Egorov and Kondratiev].) In effect, we can 'shift' f by v , and if v is vanishingly small, then so is $\|f - f_v\|_{L^1}$. In particular, if $\|z\| < \delta$, then $\|f_h(x) - f_h(x+z)\|_{L^1} < \epsilon$. We can apply this to (31) after some manipulation. Firstly, as $\chi_k > 0$, we can write $\chi_k(z) = \chi_k(z)^{\frac{1}{2}} \chi_k(z)^{\frac{1}{2}}$, and so by the Schwarz inequality:-

$$\begin{aligned}\left| \int_{\|z\| < \frac{1}{k}} (f_h(x) - f_h(x+z)) \chi_k(z) dz \right|^2 &\leq \\ \int_{\|z\| < \frac{1}{k}} |f_h(x) - f_h(x+z)|^2 \chi_k(z) dz &\int_{\|z\| < \frac{1}{k}} \chi_k(z) dz.\end{aligned}\quad (32)$$

Using the fact that $\int_{\mathbb{R}^2} \chi_k(z) dz = 1$, we can combine (31) and (32) to give:-

$$\|f_h - f_k\|^2 \leq \int_{\mathbb{R}^2} \int_{\|z\| < \frac{1}{k}} |f_h(x+z) - f_h(x)|^2 \chi_k(z) dz dx.$$

By Fubini's theorem [Weir], the order of integration on the right-hand side can be reversed, so the above becomes:-

$$\|f_h - f_k\|^2 \leq \int_{\|z\| < \frac{1}{k}} \int_{\mathbb{R}^2} |f_h(x+z) - f_h(x)|^2 \chi_k(z) dx dz.$$

Now referring to the comments above on Lebesgue's theorem, we take suitably large k so that:-

$$\|f_h - f_k\|^2 < \frac{\epsilon^2}{4} \int_{\|z\| < \frac{1}{k}} \chi_k(z) dz,$$

but we also take k large enough, if necessary, in order that $\frac{1}{k} < \frac{h}{2}$ so that f_k is kept within D and is zero near ∂D , and hence $f_k \in C_0^\infty(D)$. (See Figure 7.) Now, since $\int_{\mathbb{R}^2} \chi_k(z) dz = 1$, we have:-

$$\|f_h - f_k\| < \frac{\epsilon}{2}$$

and the proof is complete. Now we can consider the adjoint properties of A .

3.2.2 Self-adjointness of A

For a densely-defined closed operator on L^2 , in our case A , the adjoint A^* is defined as follows [Meise and Vogt] :-

$$\mathfrak{D}(A^*) = \{v \in L^2; u \rightarrow (\overline{A}u, v) \text{ is a continuous function on } \mathfrak{D}(\overline{A})\} \quad (33)$$

where \overline{A} is the closure of the *graph* of A , and consequent to the above definition, that \exists a unique $A^*v \in L^2$ such that:-

$$(\overline{A}u, v) = (u, A^*v) \quad \forall u \in \mathfrak{D}(\overline{A}). \quad (34)$$

It is also a consequence of the above that A^* is linear, and that $\mathfrak{D}(A^*)$ is a linear subspace of L^2 . Note that the mapping $u \rightarrow (\overline{A}u, v)$ in (33) is a bounded functional on $\mathfrak{D}(\overline{A})$ with respect to the L^2 norm and can therefore be continued as a bounded functional on all of L^2 , by the Hahn-Banach theorem [Kreyszig], even though we know A is not bounded.

As $\mathfrak{D}(\bar{\mathbf{A}})$ is dense in L^2 and closed, we can quote the first Hilbert theorem (see Appendix 1):-

$$L^2 = [Im(\bar{\mathbf{A}})] \oplus \mathfrak{N}(\mathbf{A}^*). \quad (35)$$

So, if we can show $\mathfrak{N}(\mathbf{A}^*) = \{0\}$, then $Im(\mathbf{A})$ is dense in L^2 , and hence R_0 will also be densely-defined, and we can then speak of its adjoint. So we will now prove $\mathfrak{N}(\mathbf{A}^*) = \{0\}$. We do this by actually showing \mathbf{A} is self-adjoint. For then $\mathbf{A}^*u = 0 \Rightarrow \bar{\mathbf{A}}u = 0$. Now if $u \in \mathfrak{D}(\mathbf{A})$, then $-\Delta u \Big|_D = 0$ and $u \Big|_{\partial D} = 0$, but from our uniqueness principle (see Appendix 1), $u = 0$. If $u \in \mathfrak{D}(\bar{\mathbf{A}}) \setminus \mathfrak{D}(\mathbf{A})$, a limiting argument gives the same result, as ∇u will be vanishingly small. First then, we show $\bar{\mathbf{A}}$ is symmetric. Let $u, v \in \mathfrak{D}(\mathbf{A})$, then:-

$$(\mathbf{A}u, v) = - \int_D \Delta u \bar{v} dx = - \int_D \bar{v} \Delta u dx.$$

Applying Green's first theorem (see Appendix 1) to \bar{v} and u :-

$$(\mathbf{A}u, v) = - \int_{\partial D} \bar{v} \frac{\partial u}{\partial n} dS + \int_D \nabla \bar{v} \cdot \nabla u dx,$$

but as $v \in \mathfrak{D}(\mathbf{A})$, $v \Big|_{\partial D} = 0 \Rightarrow \bar{v} \Big|_{\partial D} = 0$, hence

$$(\mathbf{A}u, v) = \int_D \nabla \bar{v} \cdot \nabla u dx. \quad (36)$$

Similarly,

$$(u, \mathbf{A}v) = \int_D \nabla u \cdot \nabla \bar{v} dx \quad (37)$$

and so combining (36) and (37):-

$$(\mathbf{A}u, v) = (u, \mathbf{A}v).$$

so \mathbf{A} is symmetric, and continuity of the inner-product also proves this for $\overline{\mathbf{A}}$, therefore $\mathfrak{D}(\overline{\mathbf{A}}) \subseteq \mathfrak{D}(\mathbf{A}^*)$ follows immediately from the definition of adjoint in (33) and (34). So, to prove self-adjointness, it remains to prove $\mathfrak{D}(\mathbf{A}^*) \subseteq \mathfrak{D}(\overline{\mathbf{A}})$:-

Let $v \in \mathfrak{D}(\mathbf{A}^*)$. Then, by definition, $v \in L^2(D)$ and $(\overline{\mathbf{A}}u, v)$ is a continuous function on $\mathfrak{D}(\overline{\mathbf{A}})$ and \exists a unique $w = \mathbf{A}^*v \in L^2(D)$, such that $(\overline{\mathbf{A}}u, v) = (u, w) \forall u \in \mathfrak{D}(\overline{\mathbf{A}})$. But as $\mathfrak{D}(\mathbf{A}) \subseteq \mathfrak{D}(\overline{\mathbf{A}})$, then we can also say $v \in L^2(D)$ and $(\mathbf{A}u, v)$ is a continuous function on $\mathfrak{D}(\mathbf{A})$ and \exists a unique $w = \mathbf{A}^*v \in L^2(D)$, such that $(\mathbf{A}u, v) = (u, w) \forall u \in \mathfrak{D}(\mathbf{A})$. Let's look more closely at w :-

$$-\int_D \Delta u \bar{v} dx = \int_D u \bar{w} dx \quad \forall u \in \mathfrak{D}(\mathbf{A}).$$

But that is also true then, for any $\phi \in C_0^\infty(D)$:-

$$-\int_D \Delta \phi \bar{v} dx = \int_D \phi \bar{w} dx \quad \forall \phi \in C_0^\infty(D).$$

So in the distribution sense, $\bar{w} = -\Delta \bar{v}$ and therefore $w = -\Delta v$, and so Δv exists as an L^2 function. By the elliptic regularity theorem [Folland] [Gilbarg and Trudinger], this actually implies $v \in W^{2,2}(D)$. If we can now show v is zero on ∂D , we are done, for then $v \in W_0^{1,2}(D)$ (as $W^{1,2}(D) \subset W^{2,2}(D)$), hence $v \in \mathfrak{D}(\mathbf{A}) \Rightarrow v \in \mathfrak{D}(\overline{\mathbf{A}})$. Now from the definition, $(\mathbf{A}u, v) = (u, w) \forall u \in \mathfrak{D}(\mathbf{A})$,

$$\text{but } (\mathbf{A}u, v) = \int_D -\Delta u \bar{v} dx$$

and as $w = -\Delta v \Rightarrow w \in W^{2,2}(D)$, we can apply Green's first theorem (see Appendix 1),

$$= - \int_{\partial D} \bar{v} \frac{\partial u}{\partial n} dS + \int_D \nabla \bar{v} \cdot \nabla u dx \quad (38)$$

and similarly,

$$(u, w) = \int_D u \bar{w} dx = - \int_D u \Delta \bar{v} dx$$

and as both $v, w \in W^{2,2}(D)$, applying Green's first theorem again:-

$$= - \int_{\partial D} u \frac{\partial \bar{v}}{\partial n} dS + \int_D \nabla u \cdot \nabla \bar{v} dx. \quad (39)$$

So combining (38) and (39):-

$$\int_{\partial D} \left(u \frac{\partial \bar{v}}{\partial n} - \bar{v} \frac{\partial u}{\partial n} \right) dS = 0$$

but $u \Big|_{\partial D} = 0$,

$$\Rightarrow \int_{\partial D} \frac{\partial u}{\partial n} \bar{v} dS = 0 \quad \forall u \in \mathfrak{D}(\mathbf{A}).$$

Now, if we can show $\{\partial_n u (= \frac{\partial u}{\partial n}); u \in \mathfrak{D}(\mathbf{A})\}$ is dense in $L^2(\partial D)$, then that implies $\bar{v} \Big|_{\partial D} = 0$ (and hence $v \Big|_{\partial D} = 0$) as required. As $C^\infty(\partial D)$ is dense in $L^2(\partial D)$, it is enough to show that $\{\partial_n u; u \in \mathfrak{D}(\mathbf{A})\}$ is dense in $C^\infty(\partial D)$ with L^2 norm. We show the proof of this here. We assumed earlier that ∂D was piecewise smooth with no cusps and bounded in \mathbb{R}^2 . Without loss of generality, we look at one section of ∂D that is almost straight and parallel to the y -axis.

To illustrate the construction, consider a section that is actually straight and coincides with the y -axis. (See Figure (8).)

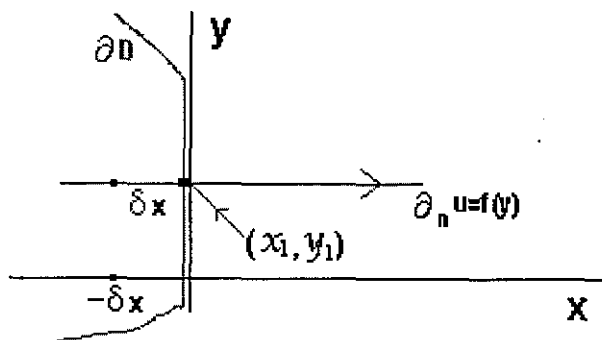


Figure 8: Straight section of ∂D

So, for some $f \in C^\infty(\partial D)$, we want to find a $u \in W^{2,2}(D) \cap W_0^{1,2}(D)$ such that $\|\partial_n u - f\|_{C^0(\partial D)} < \epsilon$ (as $C^0 \Rightarrow L^2$ norm), for any given $\epsilon > 0$. On the straight section, f is actually just $f(y)$. We can approximate f on this section by taking $u = xf(y)\chi(x)$, where $\chi(x)$ is a "cut-off" mollifier function, as defined above, but at some small distance from $x = 0$, we simply set $\chi(x) = 1$. Hence u is certainly $W^{2,2}(D)$ and $W^{1,2}(D)$, and it is zero on the boundary, so $u \in \mathcal{D}(A)$.

The normal derivative at the point (x_1, y_1) ($x_1 = 0$) is

$$-(0 - (\delta x f(y))) / \delta x = f(y),$$

as required, i.e., $\|\partial_n u - f\|_{C^0(\partial D)} < \epsilon$.

Now returning to the more general case, consider a section only slightly curved, so it is almost parallel to the y -axis, let us say it deviates by no more than a small angle α . (Drawn in exaggerated form in Figure (9).)

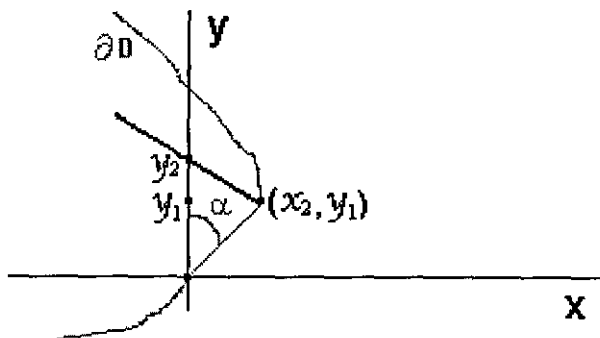


Figure 9: Curved section of ∂D

Now looking at the point (x_2, y_1) on the boundary, if we backward-project the normal at this point, we cross the y -axis at a point y_2 . The derivative at this point (in infinitesimal sense) is thus $f(y_2) \cos \alpha$. By choosing a suitably small section of ∂D , we can make $f(y_2)$ close to $f(y_1)$ and $\cos \alpha$ close to 1, as $f \in C^\infty(\partial D)$, so we achieve any desired closeness to $f(y_1)$ on a small enough section of ∂D . This can be done on a complete set of "small sections" of ∂D , and then a *partition of unity* [Spivak] pieces all these functions together to form one $u \in \mathcal{D}(\mathbf{A})$ such that $\|\partial_n u - f\|_{C^0(\partial D)} < \epsilon$. Now, 'rolling back' to where we started - we have just shown $\{\partial_n u\}$ is dense in $L^2(\partial D)$ for $u \in \mathcal{D}(\mathbf{A})$, and therefore $v|_{\partial D} = 0$, hence $v \in \mathcal{D}(\mathbf{A})$ and hence \mathbf{A} is self-adjoint. That however implies $v = 0$ and so $\mathfrak{N}(\mathbf{A}^*) = \{0\}$. Then the first Hilbert theorem (see Appendix 1) gives us that $Im(\mathbf{A})$ is dense in L^2 . ■

Hence $Im(\mathbf{A})$ is dense in L^2 , and hence R_0 is also densely-defined, and

so we may speak of its adjoint. The definitions are the same as for \mathbf{A} above in equations (33) and (34), as R_0 is also densely-defined in L^2 . The definition of self-adjoint [Meise and Vogt] is that the *closure* $\overline{R_0}$ of R_0 is self-adjoint, this closure being the closure of the *graph* of R_0 . But as R_0 is bounded and densely-defined, $\overline{R_0}$ is simply the extension of R_0 to the whole of L^2 . Now referring to equation (33), $u \rightarrow (\overline{R_0}u, v)$ is clearly continuous for any $v \in L^2$ as R_0 is bounded, so $\mathfrak{D}(\overline{R_0}^*) = L^2 = \mathfrak{D}(\overline{R_0})$. As the inner-product preserves continuity, it just remains to show symmetry for R_0 :-

For $f, g \in \text{Im}(\mathbf{A})$, using the definitions above, $f = -\Delta u$, $g = -\Delta v$,

$$\begin{aligned} (R_0 f, g) &= (u, -\Delta v) \\ &= \int_D u(-(\Delta v)) dx. \end{aligned}$$

Applying Green's first theorem (see Appendix 1) to u and $-\bar{v}$:-

$$-\int_D u \overline{\Delta v} dx = -\int_{\partial D} u \frac{\partial \bar{v}}{\partial n} dS + \int_D \nabla u \cdot \nabla \bar{v} dx. \quad (40)$$

By definition, $u \Big|_{\partial D} = 0$, so (40) becomes:-

$$(R_0 f, g) = \int_D \nabla u \cdot \nabla \bar{v} dx. \quad (41)$$

Similarly,

$$\begin{aligned} (f, R_0 g) &= (-\Delta u, v) = -\int_D \Delta u \bar{v} dx \\ &= -\int_D \bar{v} \Delta u dx \\ &= -\int_{\partial D} \bar{v} \frac{\partial u}{\partial n} dS + \int_D \nabla \bar{v} \cdot \nabla u dx \Rightarrow \\ (f, R_0 g) &= \int_D \nabla \bar{v} \cdot \nabla u dx. \end{aligned} \quad (42)$$

Combining (41) and (42):-

$$(R_0 f, g) = (f, R_0 g)$$

so R_0 is self-adjoint.

Since R_0 is bounded and self-adjoint, there is some spectral theory that can be applied to it. In particular, we can say all its eigenvalues are real, and there is a representation of R_0 in the form $\int_{m-0}^M \mu dE_\mu$, μ being the spectrum of R_0 [Kreyszig]. However, we need compactness to prove that the spectrum of R_0 consists *only* of eigenvalues.

3.3 Compactness of R_0

We prove this by expressing R_0 as $J\tilde{R}_0$, where \tilde{R}_0 is bounded and J is compact, so it then follows that R_0 is compact. Combining (27) and (28) again:-

$$\begin{aligned} \|\nabla u\|^2 &\leq \epsilon^2 C_D^2 \|\nabla u\|^2 + \frac{\|f\|^2}{4\epsilon^2} \\ \Rightarrow (1 - \epsilon^2 C_D^2) \|\nabla u\|^2 &\leq \frac{\|f\|^2}{4\epsilon^2}. \end{aligned}$$

We already chose ϵ so $1 - C_D^2 \epsilon^2 > 0$, so then:-

$$\|\nabla u\|^2 \leq \tilde{C}_D \|f\| \quad \forall u \in \mathcal{D}(\mathbf{A})$$

as well as

$$\|u\| \leq \tilde{C}_D \|f\| \quad \forall u \in \mathcal{D}(\mathbf{A}).$$

$$\begin{aligned} \text{Now, } \|u\|_{W^{1,2}}^2 &= \|u\|_{L^2}^2 + \left\| \frac{\partial u}{\partial x} \right\|_{L^2}^2 + \left\| \frac{\partial u}{\partial y} \right\|_{L^2}^2 \\ &= \|u\|_{L^2}^2 + \|\nabla u\|_{L^2}^2. \end{aligned}$$

Hence we can write $\|u\|_{W^{1,2}}^2 \leq \hat{C}_D \|f\|_{L^2}$, and so we define \tilde{R}_0 as mapping f to u , as R_0 does, but the co-domain is changed to $W^{1,2}$. The equation above proves \tilde{R}_0 is bounded. We now quote the Rellich-Kondrachov theorem [Adams and Fournier], which says that for a bounded domain D with sufficiently smooth boundary, the imbedding $J : W^{m,p}(D) \rightarrow W^{m-1,p}(D)$ is compact. Hence, the imbedding J taking u in $W^{1,2}(D)$ to u in $W^{0,2}(D) = L^2(D)$ is compact, and the compactness of R_0 is proved.

3.4 Characterising the eigenvalues

We now know that \mathbf{A} is an operator with compact resolvent, and we quote the result, as discussed above, that \mathbf{A} also has only a point spectrum, and that non-zero eigenvalues have only a finite multiplicity. Now let's relate the spectrum of R_0 to \mathbf{A} . As R_0 is compact, its eigenvalues are bounded, and if they proliferate, it is only towards the origin [Kolmogorov and Fomin]. Now, we proved above that there is no zero eigenvalue of \mathbf{A} . We can also prove this for R_0 , for if $\exists f \neq 0$ s.t. $-\Delta u = f$ and $u = 0$, then $f = 0$, which is a contradiction. We also saw the eigenvalues are all real, and as there are no zero eigenvalues, the eigenvalues λ_n of \mathbf{A} relate quite simply to the eigenvalues μ_n of R_0 by $\lambda_n = \frac{1}{\mu_n}$. As μ_n are bounded and can only proliferate at zero, that means there is a definite lowest eigenvalue λ_1 (with possible duplicates), though there may not be an upper limit. Now counting the values of λ_n according to their multiplicity, we can order these as a set of real numbers:-

$$\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots$$

Now, if u_n is an eigenvector, and we write $u_n = v + iw$, where v and w are real-valued, then from the definition of $\mathfrak{D}(\mathbf{A})$ we can see v and w are also in $W^{2,2}$ and $W_0^{1,2}$. As u_n is an eigenvector, v and w are not both zero. Without loss of generality, we take v to be non-zero, and we can then see v is an eigenvector in its own right. Then, as $v \Big|_{\partial D} = 0$, from the uniqueness principle (see Appendix 1),

$$\lambda_n \int_D v^2 dx = \int_D |\nabla v|^2 dx$$

and hence $\lambda_n > 0$. Thus the spectrum of \mathbf{A} is completely defined as a set of real numbers:-

$$0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots$$

4 Case study - numerical analysis

We will estimate the first 2 or more eigenvalues of equation (1) for a suitable domain, using a numerical technique which is a variant of the Rayleigh-Ritz Approximation (RRA) technique [Jeffreys and Jeffreys]. This is itself a special case of a Galerkin method to solve elliptic equations using sets of trial ("test") functions [Kirsch] [Mitchell and Griffiths], which we now define:-

Trial functions $f_i, i = 1, 2, 3 \dots$ are functions in a subset of our defined domain $\mathfrak{D}(\mathbf{A})$, in that they are actually C^∞ functions, or we can use any set of functions, provided their span is dense in $\mathfrak{D}(\mathbf{A})$ under $W^{1,2}$ norm. In our Dirichlet case, we also stipulate :-

$$f_i \Big|_{\partial D} = 0. \quad (43)$$

For a finite set Φ of trial functions $\{f_i\}, i = 1, 2, 3 \dots n$ we define:-

$$a_{jk} = (\nabla f_j, \nabla f_k), \quad j = 1, 2, 3 \dots n, \quad k = 1, 2, 3 \dots n \quad (44)$$

and

$$b_{jk} = (f_j, f_k), \quad j = 1, 2, 3 \dots n, \quad k = 1, 2, 3 \dots n. \quad (45)$$

As these are finite sets, we can denote $\{a_{jk}\}$ by the matrix A_Φ and $\{b_{jk}\}$ by the matrix B_Φ . RRA is actually a practical way of using *Courant's Minimax Principle* [Egorov, Komech and Shubin], which states that if λ_1 is the first eigenvalue, then:-

$$\lambda_1 = \min \frac{\|\nabla f_\alpha\|^2}{\|f_\alpha\|^2} ; \quad f \in C^\infty(D) ; \quad f_\alpha \Big|_{\partial D} = 0 \quad (46)$$

over all non-zero trial functions $\{f_\alpha\}$. Furthermore, if f_1 is the minimiser of (46), then f_1 is the first eigenfunction. Now, for a set Φ of trial functions $\{f_k\}$, as discussed above, define:-

$$\lambda_n^*(\Phi) = \max \left\{ \frac{\|\nabla f\|^2}{\|f\|^2} ; f \Big|_{\partial D} = 0; \right. \\ \left. f \neq 0 ; f = \sum_1^n c_k f_k, \text{ over all scalars } c_k \right\},$$

then the minimax principle is that, if λ_n is the n th. eigenvalue, then:-

$$\lambda_n = \min_{\Phi} \lambda_n^*(\Phi). \quad (47)$$

Hence λ_n is the *minimum* of a set of *maxima*. The RRA method finds the maximum $\lambda_n^*(\Phi)$ by solving the general eigenvalue problem for A_{Φ}, B_{Φ} [Maron] :-

$$A_{\Phi}x = \lambda B_{\Phi}x \quad (48)$$

with A_{Φ}, B_{Φ} as defined in equations (44) and (45) above, and then finding the highest of these roots. At this point, we refer to the arguments at the end of Section 3 proving the eigenvalues to be real. It is clear from that argument that we need consider henceforth only real-valued trial functions and likewise real-valued scalars.

Care is needed in adding more and more trial functions, as the eigenvalues may tend to infinity. We apply the RRA method then, as follows:-

Pick trial functions, and find the lowest two roots of (48) (or just the one root if we start with one trial function). Add another trial function, and keep adding until we see a 'convergence', in that λ_1 and λ_2 are not

getting significantly lower. Then these two values of λ are our estimates. Note the advantage of using a Hilbert space (Sobolev space) rather than Banach - the latter has no inner-product.

4.1 Classes of trial functions

We shall choose these to match what we expect of the *character* of our solution. In particular, in our Dirichlet case, we have a specific requirement of zero on the boundary. Apart from that, if we expect u to be smooth, for example, then our trial functions should be smooth.

4.2 Domain enlargement

If the domain of the Laplace operator with Dirichlet conditions is enlarged, each eigenvalue is decreased [Egorov, Komech and Shubin]. Enlargement is in terms of sets, so if D' is an enlargement of D , then as sets in \mathbb{R}^2 , $D \subset D'$. So if we surround our domain by a 'minimal surround' box, that gives us a useful lower bound.

4.3 Domains and trial functions: specifics

We want our domain to be computationally practical, but without a known analytic solution. We restrict ourselves then, to $D \subset \mathbb{R}^2$ such that ∂D is a finite curve in \mathbb{R}^2 which can be parameterised as polar coordinates $(s(\theta), \theta)$, where $s(\theta)$ is a strictly positive function in the range $0 \leq \theta \leq 2\pi$ ($s(0) = s(2\pi)$), $s(\theta)$ being at least a $C^{0,1}$ function on $[0, 2\pi]$ (see Section 2.2 for discussion of Hölder spaces $C^{j,\mu}$), and such that any

radial definitely touches ∂D , but only touches it once. We take ∂D to be always inside (including equal to) a bounding box of side 6, centred on the origin:-

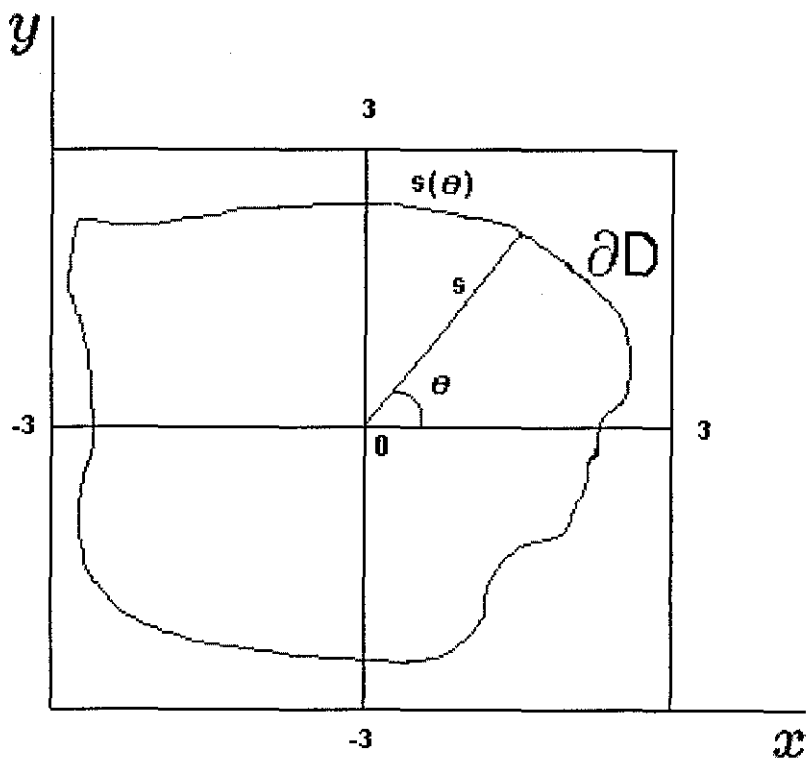


Figure 10: $s(\theta)$

This bounding box actually has a solution, i.e., the eigenfunctions are:-

$$\sin \frac{m\pi}{6}(x+3) \sin \frac{n\pi}{6}(y+3), \quad m = 1, 2, \dots, \quad n = 1, 2, \dots$$

so that the eigenvalues are $\frac{\pi^2}{36}(m^2 + n^2)$, $m = 1, 2, \dots$, $n = 1, 2, \dots$

$$= \frac{\pi^2}{36}(2, 5(\text{repeated}), 8, 10, \dots)$$

$$= 0.2742(2, 5, 5, 8, 10, \dots)$$

= 0.5484, 1.371(twice), 2.1936, 2.742...

and so these eigenvalues form our lower bounds, in light of section 4.2 above.

Now, for this Dirichlet problem, actually constructing a suitable C^∞ function that is zero on a given ∂D can be quite tricky, but what we will do instead is to describe a set of $C^{0,1}(D)$ functions to use as trial functions, and then we will prove below that these can be used instead of C^∞ functions. For a given $s(\theta)$ then, we first define this modifier function:-

$$\begin{aligned} T_1(r, \theta) &= 1 \text{ if } r = 0 \text{ else} \\ &= 1 - \frac{r}{s(\theta)} \text{ if } r \leq s(\theta) \text{ else} \\ &= 0 \text{ if } r > s. \end{aligned}$$

Essentially, T_1 is a cone, tapering to a point at the origin, where its value is 1. If $s(\theta)$ is a square, then T_1 is a pyramid, and if $s(\theta)$ is a circle, T_1 is a cone. Apart from potentially inheriting a $C^{0,1}(D)$ status from s (think of, for example, the pyramid edges), we can see T_1 is itself continuous, but will always have a discontinuous (though bounded) derivative at the origin, thus T_1 is always a $C^{0,1}(D)$ function. We now use this modifier function to multiply by sines to give our required set of trial functions - these will definitely be zero on ∂D . Now the minimax (RRA) methods rely on the fact that $W_0^{1,2}$ is the closure of C_0^∞ , but as our trial functions are clearly not C^∞ , we must now show that they do have a span that is dense in $W_0^{1,2}$. (See definition of minimax under equation (46).) We

define then:-

$$\chi_{m,n} = T_1(x, y) \sin \frac{m\pi}{8}(x + 4) \sin \frac{n\pi}{8}(y + 4),$$

$$m = 1, 2, \dots, \quad n = 1, 2, \dots,$$

and we then let $\chi = sp\{\chi_{m,n}\}$. We claim χ is dense in $W_0^{1,2}(D)$. It suffices to prove that χ is dense in $C_0^\infty(D)$, as that is dense in $W_0^{1,2}(D)$.

We prove this here:-

Theorem 4.3.1 *Let χ , T_1 and D be as defined above. Then χ is dense in $C_0^\infty(D)$.*

Proof Let $u \in C_0^\infty(D)$ and let $V = \frac{u}{T_1}$ if T_1 is not zero, else V is zero. As u is zero near ∂D and as it's a C^∞ function, V is well-defined, and in fact, we can see V is a $C^{0,1}(D)$ function, as T_1 is only zero on ∂D . Now extend V by zero to an 8×8 zero-centred square, so it is now a $C^{0,1}$ function on this square, and zero on its boundary. Let's call that $C_0^{0,1}(\text{square})$. But $C_0^{0,1}(\text{square}) \subset W_0^{1,2}(\text{square})$, so V has a Fourier expansion of the form:-

$$V = \sum_{m,n=1}^{\infty} \gamma_{mn} \sin \frac{m\pi}{8}(x + 4) \sin \frac{n\pi}{8}(y + 4)$$

(limits above and norms below are in the $W^{1,2}$ sense). So, for a given $\epsilon > 0$, $\|V - V_\epsilon\| < \epsilon$

$$\text{where } V_\epsilon = \sum_{m,n=1}^{N_\epsilon} \gamma_{mn} \sin \frac{m\pi}{8}(x + 4) \sin \frac{n\pi}{8}(y + 4).$$

$$\text{Now } \|u - T_1 V_\epsilon\| = \|T_1(V - V_\epsilon)\|,$$

so looking at the form of T_1 , it is clearly bounded as an operator on $W^{1,2}$, so we can write:-

$$\|u - T_1 V_\epsilon\| \leq \|T_1\| \|V - V_\epsilon\|.$$

By suitable choice of N_ϵ , we can arrive at:-

$$\|u - T_1 V_\epsilon\| < \epsilon$$

and $T_1 V_\epsilon$ is clearly in χ . ■

Note that we chose the 8 x 8 square to ensure we are not using trial functions that are close to zero on ∂D (as we are allowing ∂D to actually coincide with the 6 x 6 square). This could cause poor convergence due to over-specification of the problem, as discussed in Section 3.

$T_1(x, y) \rightarrow T_1(r, \theta)$ conversion

(From herein, we take "z = 0" to mean, in computing terms, $|z| \leq 1.0 \times 10^{-6}$, or whatever lower limit is required.)

$$r = \sqrt{x^2 + y^2}$$

$$\text{if } r = 0 \text{ then } \theta = 0$$

$$\text{else } \theta = \text{ArcTan}(x, y)^5$$

$$s = s(\theta)$$

$$\text{if } r \geq s \text{ then } T_1 = 0$$

$$\text{else } T_1 = 1 - \frac{r}{s}$$

⁵If this software function returns a value in the range $-\pi$ to π , then we add any -ve values to 2π to get our range.

Sample $s(\theta)$

(1) Square of side 3:-

(In this case, the eigenvalues *are* the lower bounds above.)

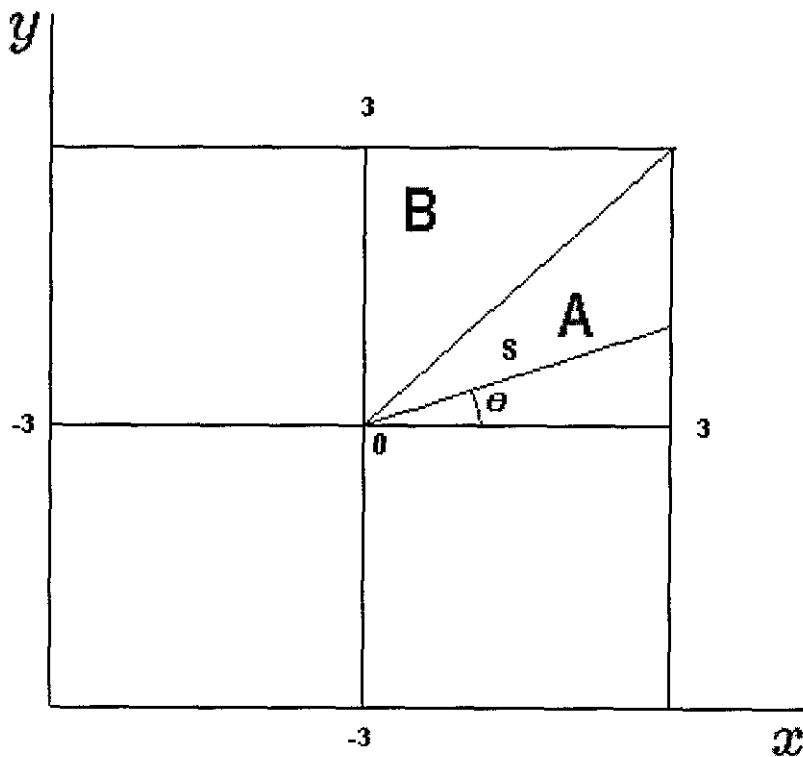


Figure 11: $s(\theta)$ for square

Referring to Figure (11), in A :-

$$\begin{aligned} s^2 &= 9 + s^2 \sin^2 \theta \\ \Rightarrow s^2(1 - \sin^2 \theta) &= 9 \\ \Rightarrow s &= \frac{3}{\cos \theta}. \end{aligned}$$

Similarly, in B :-

$$s = \frac{3}{\sin \theta}.$$

A similar logic applies in the 'mirror' segments, forcing a positive s , so we get:-

$$\begin{aligned} \text{if } & 0 \leq \theta < \frac{\pi}{4} \text{ or } \frac{3\pi}{4} \leq \theta < \frac{5\pi}{4} \text{ or } \frac{7\pi}{4} \leq \theta, \\ \text{then } & s = \frac{3}{|\cos \theta|} \\ \text{else } & s = \frac{3}{|\sin \theta|}. \end{aligned}$$

(2) General form:-

$$s(\theta) = 2 + \sum_1^k (\alpha_k \sin k\theta + \beta_k \cos k\theta) \quad (\alpha_k, \beta_k < 1 \text{ or } \ll 1).$$

The 2 is there so that s is always positive, and now we see the reason to have a square of side 3 in the introductory text above. $k = 2$ is probably high enough to get a suitable shape, but we will set $\beta_1 = 0$, so we don't just get an ellipse.

RRA algorithm

1. Define $s(\theta)$ and specify limits, i.e. $x \pm 3, y \pm 3$.
2. Now define $T_1(x, y)$.
3. Define trial functions of the form:-

$$f_i(x, y) = T_1(x, y) \sin \frac{m\pi}{8}(x + 4) \sin \frac{n\pi}{8}(y + 4)$$

where m and n increase symmetrically, so our functions are dimensionally unbiased.

4. We calculate a_{jk} and b_{jk} , as defined in equations (44) and (45) above.

5. Now find solutions $\{\lambda\}$ of the general eigenvalue problem [Maron] for A_Φ, B_Φ ($A_\Phi x = \lambda B_\Phi x$), where

$$\Phi = \{f_1\}.$$

Repeat for $\Phi = \{f_1, f_2\}$, and so on, until we see a 'convergence' in the lowest two or more values of λ - these will be our eigenvalue estimates.

4.4 Constructing the computational elements

The RRA algorithm was implemented using the software package *Mathematica* developed by Wolfram Research [Pao]. We describe here how this algorithm was built up, and the mathematical problems that the package itself presented (see Appendix 2 for the "notebook").

Firstly, the *ArcTan* function did operate as suggested in Section 4.3 and returned values in the range $-\pi$ to π , so if a negative value was returned, we brought it into our system by adding 2π to it. On a general point here, although functions can be defined in *Mathematica* using an "if-then-else" structure, they can then be difficult to actually utilise; in particular, graph plots and integration can fail. It is best therefore to define functions in terms of other known functions wherever possible. In this first case, *Mathematica* has a built-in function "Sign" which returns -1, 0, 1 depending on whether its argument is negative, zero or positive. We can thus define our $[-\pi, \pi] \rightarrow [0, 2\pi]$ conversion by:-

$$\text{To2pi}(\phi) = \phi + \pi \text{Sign}(\phi)(\text{Sign}(\phi) - 1). \quad (49)$$

A similar treatment was needed to define $s(\theta)$ for the square. Rather than an "if-then-else" structure, it can be realised as a sum of step functions on $[0, \frac{\pi}{4}), [\frac{\pi}{4}, \frac{3\pi}{4}), \dots$ multiplied by $\frac{3}{|\cos \theta|}, \frac{3}{|\sin \theta|} \dots$

Notice the intervals are open on the right, so they don't overlap, or we would get twice the required value at the crossover points. We needed then, a step function that is 1 on $[a, b)$ and zero elsewhere. The 'UnitStep' function that Mathematica provides is 0 for $x < 0$ and 1 for $x \geq 0$. So $\text{UnitStep}(z - a)$ gives us a function that is 0 for $z < a$ and 1 for $z \geq a$. We will always have $b > a$ in our definitions, so we then just need a 'modifier' that will set $\text{UnitStep}(z - a)$ to zero if $z \geq b$. Let $x = z - b$, then:-

$$x < 0 \Rightarrow z < b$$

$$x \geq 0 \Rightarrow z \geq b.$$

So the required modifier is $1 - \text{UnitStep}(z - b)$. Thus our required step function is:-

$$\text{Step}(z, a, b) = \text{UnitStep}(z - a)(1 - \text{UnitStep}(z - b)).$$

Since we are now *not* using "if-then-else" statements, but are using these step functions, we cannot guarantee to not divide by zero. For example, when evaluating:-

$$\text{Step}(\theta, 0, \frac{\pi}{4}) \frac{3}{|\cos \theta|}$$

at $\theta = \frac{\pi}{2}$, Mathematica actually evaluates both parts, and then multiplies them, resulting in an error. We avoided this by using a 'Notzero' function, which raises any zero values to a tiny non-zero amount, so making little

difference numerically:-

$$\text{Notzero}(\zeta) = \zeta + 2 \times 10^{-24} \text{Step}(\zeta, -10^{-24}, 10^{-24}).$$

It should be noted here that all of these functions were tested out in Mathematica itself by supplying a range of values, and checking the answer. In addition to this, for some functions, we drew plots in Mathematica for additional validation and also visualisation. The plot of 'Notzero' is shown below.

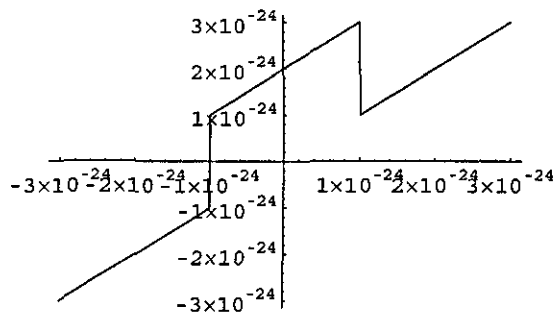


Figure 12: 'Notzero' function

Now even using known functions, Mathematica still failed to integrate some of our defined functions. *Extensive analysis and trials of Mathematica showed its built-in routines cannot always integrate functions that are not classically differentiable.* We therefore devised our own integration routines, using a simple quadrature method to expediate matters [Jacques and Judd]. Specifically, the integral of a function $f \in \mathbb{R}^2$ over the range $\{x_1 \rightarrow x_2, y_1 \rightarrow y_2\}$ can be approximated by:-

$$\text{Rintegrate2d}(f, x_1, x_2, y_1, y_2, n) = \delta x \delta y \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} f(x_1 + i\delta x, y_1 + j\delta y) \quad (50)$$

where $\delta x = \frac{(x_2-x_1)}{n}$ and $\delta y = \frac{(y_2-y_1)}{n}$, n being the number of sub-divisions of our x and y range. We have used the same n as we expect $x_2 - x_1$ to be in the order of $y_2 - y_1$. With just $n = 100$, tests in Mathematica showed this function was accurate to the true value to 4 significant digits. Another test involving our T_1 function will be shown in section 4.5 below.

For the factors a_{jk} defined in Equation (44) above, we have to go further and approximate ∇ , as at certain points it does not exist in the classical sense, and Mathematica is unable to evaluate it. In fact, it is simpler to approximate the whole term. So, for two trial functions u, v over the range $\{x_1 \rightarrow x_2, y_1 \rightarrow y_2\}$:-

$$\begin{aligned}
 (\nabla u, \nabla v) &= \int_{y_1}^{y_2} \int_{x_1}^{x_2} \nabla u \cdot \nabla v \, dx dy \\
 &= \int_{y_1}^{y_2} \int_{x_1}^{x_2} (u_x v_x + u_y v_y) dx dy \\
 &\approx \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} \left((u_x v_x)_{i,j} + (u_y v_y)_{i,j} \right) \delta x \delta y \quad (51)
 \end{aligned}$$

where $(u_x v_x)_{i,j} = \left(u(x_1 + (i+1)\delta x, y_1 + j\delta y) - u(x_1 + i\delta x, y_1 + j\delta y) \right) / \delta x$
 $\times \left(v(x_1 + (i+1)\delta x, y_1 + j\delta y) - v(x_1 + i\delta x, y_1 + j\delta y) \right) / \delta x$,
 $(u_y v_y)_{i,j} = \left(u(x_1 + i\delta x, y_1 + (j+1)\delta y) - u(x_1 + i\delta x, y_1 + j\delta y) \right) / \delta y$
 $\times \left(v(x_1 + i\delta x, y_1 + (j+1)\delta y) - v(x_1 + i\delta x, y_1 + j\delta y) \right) / \delta y$
and $\delta x = \frac{x_2-x_1}{n}$, $\delta y = \frac{y_2-y_1}{n}$.

n has the same definition as in our first approximation in (50), and we make a further simplification for our cases: as we will always be integrating over the 6×6 box shown in Figure (10), then $x_1 = y_1, x_2 = y_2$, hence

$\delta x = \delta y$ and so equation (51) simplifies to:-

$$\begin{aligned}
 (\nabla u, \nabla v) \approx \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} & \left(\left(u(x_1 + (i+1)\delta x, y_1 + j\delta y) - \right. \right. \\
 & \left. \left. u(x_1 + i\delta x, y_1 + j\delta y) \right) \right. \\
 & \times \left(v(x_1 + (i+1)\delta x, y_1 + j\delta y) - \right. \\
 & \left. \left. v(x_1 + i\delta x, y_1 + j\delta y) \right) \right. \\
 & + \left(u(x_1 + i\delta x, y_1 + (j+1)\delta y) - \right. \\
 & \left. \left. u(x_1 + i\delta x, y_1 + j\delta y) \right) \right. \\
 & \times \left(v(x_1 + i\delta x, y_1 + (j+1)\delta y) - \right. \\
 & \left. \left. v(x_1 + i\delta x, y_1 + j\delta y) \right) \right). \tag{52}
 \end{aligned}$$

The above equation therefore defines our approximation function $Dsum2D(u, v, x_1, x_2, n)$.

This was tested out over the range $\{-3 \rightarrow 3, -3 \rightarrow 3\}$ as follows:-

$$\begin{aligned}
 \text{Let } u = e^{xy}, v = e^{-xy}. \text{ Then } \nabla u \cdot \nabla v &= \begin{pmatrix} ye^{xy} \\ xe^{xy} \end{pmatrix} \cdot \begin{pmatrix} -ye^{-xy} \\ -xe^{-xy} \end{pmatrix} \\
 &= -x^2 - y^2 \\
 \Rightarrow (\nabla u, \nabla v) &= - \int_{-3}^3 \int_{-3}^3 (x^2 + y^2) dx dy \\
 &= - \int_{-3}^3 \left[\frac{x^3}{3} + xy^2 \right]_{-3}^3 dy \\
 &= - \int_{-3}^3 (18 + 6y^2) dy \\
 &= - [18y + 2y^3]_{-3}^3 \\
 &= -(6.18 + 2.2.27) \\
 &= -(6.2.9 + 4.3.9) \\
 &= -(12 + 12).9 \\
 &= -24.9 \\
 &= -216.
 \end{aligned}$$

With $n = 100$, Mathematica returned a value of -216.394, hence accurate to 3 significant digits. At $n = 1000$, the value was -216.004, clearly much better, but at this stage timing trials were done, and the $n = 1000$ case was prohibitive in timing terms. Further trials showed $n = 100$ was the best compromise.

4.5 Proving the algorithm

The algorithm was tested on the bounding box itself, as defined in Section 4.3, which is also referred to there as the first sample $s(\theta)$. Thus we know

exactly what the eigenvalues are for this case, i.e.,

$$0.5484, 1.371(\text{twice}), 2.1936, 2.742 \dots$$

A first test was done for the square with T_1 set to 1, so that we are actually using the known eigenfunctions. This was done to prove the RRA method itself. This first test estimated the eigenvalues to three significant digits. See Appendix 2 for the Mathematica notebook for the main test. $s(\theta)$ is defined as in Section 4.3 ('Mod' is Modulus, added here to be certain that s is only ever defined on the range $0 \leq \theta \leq 2\pi$ and that $s(0) = s(2\pi)$). We then plotted it to ensure it hadn't gone negative. We then drew the 'parametric' plot, which effectively means we were drawing ∂D . As Appendix 2 shows, both these results were satisfactory. Note also though, that as in the previous section, all these constructed functions were tested out successfully with a range of arguments, especially at the 'crossover' points.

The T_1 function was defined next. This follows the logic in Section 4.3. We have implemented T_1 being 1 at the origin by actually making it 1 near the origin, i.e., where $s(\theta) < 1 \times 10^{-24}$, hence the construction shown. This gives a better-defined value near the origin, because otherwise we would be using arctan with two zero, or very small values, and its result is not then reliable. The second step function ensures T_1 is zero outside ∂D . The plot shows the expected pyramid shape. We have done a further integration test on T_1 here, though it could be said it also tests out our integration function. As the area of the base of the pyramid is 36, and its height is 1, the volume is $\frac{36}{3} = 12$, so integrating T_1 over D should

give this value. As Appendix 2 shows, we actually get a value of 11.9988, which is sufficiently close for our calculations.

Next we defined the trial functions, and calculated the a_{jk} terms as defined in equation (44), and from these calculated the eigenvalues. As stated in Section 4.3, our generic function is:-

$$T_1(x, y) \sin \frac{m\pi}{8}(x + 4) \sin \frac{n\pi}{8}(y + 4)$$

and we want to let m, n increase symmetrically. Computer resources limited us to 20 trial functions, hence (m, n) were set to:-

(1, 1), (2, 1), (1, 2), (2, 2), (3, 1), (1, 3), (3, 2), (2, 3), (4, 1), (1, 4),

(3, 3), (2, 4), (4, 2), (3, 4), (4, 3), (1, 5), (5, 1), (2, 5), (5, 2), (4, 4).

Note we also want our sequence of trial functions to reflect increasing eigenvalues, so for example, for the 9th. trial function, (4, 1) is preferred over (3, 3) as $4^2 + 1^2 = 17 < 18 = 3^2 + 3^2$.

Appendix 2 shows the defined trial functions and calculation of the a_{jk} terms.

The "(* ... *)" expression in the notebook has the same meaning as " ... ", and is there for brevity. The "g" terms are there because if, for example, $f_1(x, y) * f_1(x, y)$ is input directly to the Rintegrate2D function, Mathematica sometimes attempts an algebraic expansion of Rintegrate2D, i.e., it doesn't recognise $f_1(x, y) * f_1(x, y)$ as a function of x and y . Only the first two eigenvalues calculated are shown here, but this notebook was used to calculate all twenty, and the results are shown in the table below.

i	λ_1	λ_2	λ_3	λ_4
1	0.703266			
2	0.703266	1.54616		
3	0.703266	1.54616	1.54616	
4	0.703266	1.54616	1.54616	2.45332
5	0.673223	1.54616	1.54616	2.45332
6	0.653316	1.54616	1.54616	2.45332
7	0.653316	1.546	1.54616	2.45332
8	0.653316	1.546	1.546	2.45332
9	0.653316	1.49926	1.546	2.45332
10	0.653316	1.49926	1.49926	2.45332
11	0.605768	1.49926	1.49926	2.45332
12	0.605768	1.49926	1.49926	2.45315
13	0.605768	1.49926	1.49926	2.45305
14	0.605768	1.44616	1.49926	2.45305
15	0.605768	1.44616	1.44616	2.45305
16	0.594974	1.44616	1.44616	2.45305
17	0.584985	1.44616	1.44616	2.45305
18	0.584985	1.42922	1.44616	2.45305
19	0.584985	1.42922	1.42922	2.45305
20	0.584985	1.42922	1.42922	2.33937

The results appear to show a slow convergence, and after our twenty trial functions, we have estimated the values for the first two eigenvalues to within 6.7%.

4.6 The general case

See Appendix 3 for the Mathematica notebook (the computational elements described in Section 4.4 have been omitted for brevity). As with the previous notebook, we define $s(\theta)$ and plot it, to ensure it hasn't gone negative, and then do a parametric plot so we see what ∂D actually looks like. We have chosen $s(\theta)$ as:-

$$s(\theta) = 2 + 0.5 \cos(\theta) + 0.2 \cos(2\theta) + 0.6 \sin(2\theta).$$

We also plotted it with the square, to ensure it is contained within it, which the plot shows it to be.

As with the square, T_1 was then defined and plotted. Then we estimated the eigenvalues in exactly the same manner as we did in the notebook for the square (proving the algorithm). The results are shown in the table below.

i	λ_1	λ_2	λ_3	λ_4
1	1.82487			
2	1.68987	3.57986		
3	1.68987	3.04364	5.37704	
4	1.67996	3.01403	4.89026	6.3531
5	1.62727	2.96241	4.8725	5.25733
6	1.59345	2.95739	4.78505	5.23078
7	1.58879	2.9535	4.74822	5.13835
8	1.58845	2.95074	4.73096	5.13457
9	1.58818	2.91826	4.7309	4.9784
10	1.58811	2.9142	4.73071	4.9784
11	1.58796	2.9135	4.73071	4.97674
12	1.58653	2.91348	4.7305	4.97671
13	1.58651	2.91336	4.72432	4.96338
14	1.5865	2.91133	4.72426	4.9627
15	1.58474	2.91021	4.72418	4.96187
16	1.58183	2.90859	4.72407	4.95951
17	1.57987	2.90747	4.71825	4.94918
18	1.57827	2.90368	4.71681	4.94884
19	1.57822	2.90367	4.71629	4.94811
20	1.5782	2.90332	4.71429	4.94736

Again, we can see a slow convergence in the first two eigenvalues, but we would need to see a lot more trial functions to give a confident estimate.

4.7 Conclusion

We have shown how the Rayleigh-Ritz Approximation method can be adapted to estimate eigenvalues for the Laplace operator with Dirichlet boundary conditions on an arbitrary finite domain in \mathbb{R}^2 with smooth boundary. The estimate for the first two eigenvalues was within 6.7% for the known case. For the general case, the method appears to be converging, but many more trial functions would be needed to give a confident estimate. In addition, the adaptation involving the T_1 function would probably be improved if T_1 was made smoother, perhaps having a polynomial form, rather than just linear.

Appendix 1: Green's first theorem, the uniqueness principle and the first Hilbert theorem

1) For $\phi \in C^1(D)$, $\psi \in C^2(D)$, D being a bounded region with smooth boundary in \mathbb{R}^n , Green's first theorem [Jeffreys and Jeffreys] states that if ϕ and $\partial\psi/\partial n$ both exist on the boundary of D , then they satisfy this identity:-

$$\int_D \phi \Delta \psi dx = \int_{\partial D} \phi \frac{\partial \psi}{\partial n} dS - \int_D \nabla \phi \cdot \nabla \psi dx.$$

This can be extended to Sobolev spaces. As any function in the Sobolev space $W^{m,p}(D)$ can be realised as a limit of $C^\infty(D)$ functions [Adams and Fournier], by applying Green's first theorem to such functions, and passing to the limit [Gel'fand and Shilov], we can get the same identity as above for $u \in W^{1,2}(D)$ and $v \in W^{2,2}(D)$:-

$$\int_D u \Delta v dx = \int_{\partial D} u \frac{\partial v}{\partial n} dS - \int_D \nabla u \cdot \nabla v dx,$$

where $u \Big|_{\partial D}$ is the *trace* of u , and $\partial v/\partial n$ is derived from the *trace* of ∇v , as defined in Section 2.2.

2) Uniqueness principle. Following on from above, if $u \in W^{2,2}(D)$ and $u \Big|_{\partial D} = 0$, and we put $u = v$:-

$$\int_D |\nabla u|^2 dx = - \int_D u \Delta u dx$$

and hence, if $\Delta u \Big|_D = 0$, then $\nabla u \Big|_D = 0$, so u is constant, but u is zero on the boundary of D , hence $u \Big|_D = 0$.

3) If M is a closed subspace of a Hilbert space H , then $H = M \oplus M^\perp$ [Kreyszig]. If A is a densely-defined operator on L^2 , then $\mathfrak{N}(A^*) = \text{Im}(A)^\perp$ [Meise and Vogt]. Combining these two, if A is closed, we get the first Hilbert theorem for a closed, densely-defined operator A on L^2 :-

$$L^2 = [\text{Im}(\overline{A})] \oplus \mathfrak{N}(A^*).$$

Appendix 2: Mathematica notebook - proving the method

To2pi[phi_] := phi + pi * Sign[phi] * (Sign[phi] - 1)

Step[z_, a_, b_] := UnitStep[z - a](1 - UnitStep[z - b])

Notzero[zeta_] := zeta + 2 * 10^24 * Step[zeta, -1 * 10^24, 1 * 10^24]

Rintegrate2D[f_, x1_, x2_, y1_, y2_, n_] := {dx = (x2 - x1)/n; dy = (y2 - y1)/n; Rvalue = 0; Do[Rvalue = Rvalue + f[x1 + i * dx, y1 + j * dy], {i, 0, n - 1}, {j, 0, n - 1}]; N[dx * dy * Rvalue]}[[1]]

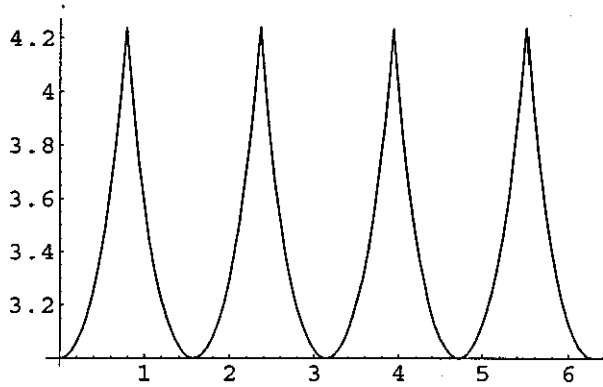
Dsum2D[u_, v_, x1_, x2_, n_] := {dx = (x2 - x1)/n; dy = dx; y1 = x1; Dxxx = 0; Do[Dxxx = N[Dxxx + (u[x1 + (i + 1) * dx, y1 + j * dy] - u[x1 + i * dx, y1 + j * dy]) * (v[x1 + (i + 1) * dx, y1 + j * dy] - v[x1 + i * dx, y1 + j * dy]) + (u[x1 + i * dx, y1 + (j + 1) * dy] - u[x1 + i * dx, y1 + j * dy]) * (v[x1 + i * dx, y1 + (j + 1) * dy] - v[x1 + i * dx, y1 + j * dy])], {i, 0, n - 1}, {j, 0, n - 1}]; N[Dxxx]}[[1]]

(* Define s(theta) for the square:- *)

s[theta_] := 3/Abs[Notzero[cos[Mod[theta, 2pi]]]] * (Step[Mod[theta, 2pi], 0, pi/4] + Step[Mod[theta, 2pi], 3pi/4, 5pi/4] + Step[Mod[theta, 2pi], 7pi/4, 2pi]) + 3/Abs[Notzero[sin[Mod[theta, 2pi]]]] * (Step[Mod[theta, 2pi], pi/4, 3pi/4] + Step[Mod[theta, 2pi], 5pi/4, 7pi/4])

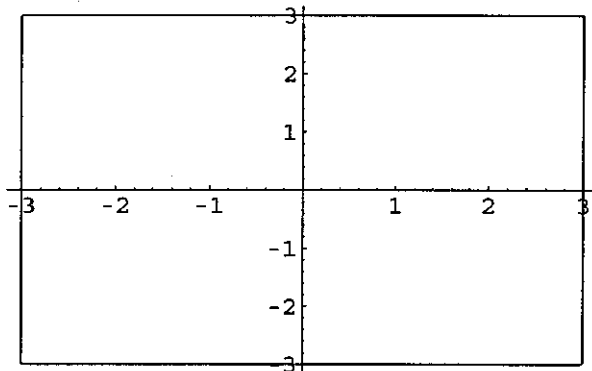
(* First, plot as a line function, so we can be sure it hasn't gone negative:- *)

```
Plot[s[θ], {θ, 0, 2π}]
```



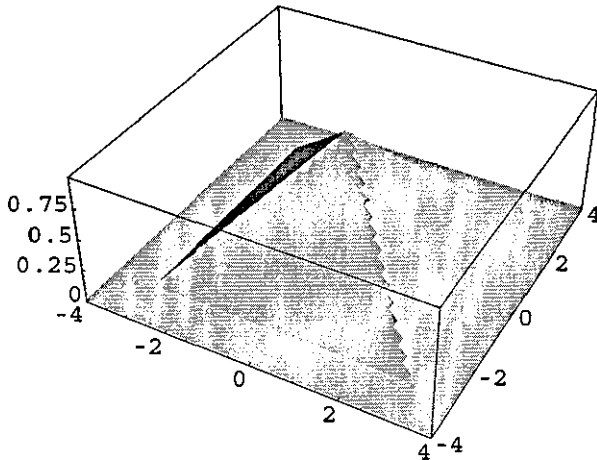
(* Now the 'Parametric' plot:- *)

```
ParametricPlot[{s[θ] cos[θ], s[θ] sin[θ]}, {θ, 0, 2π}]
```



(* Define and plot T1:- *)

```
T1[x_, y_] := Step[Sqrt[x*x+y*y], 0, 1.*10^-24] + (1 - Sqrt[x*x+y*y]/  
s[To2pi[arctan[Notzero[x], Notzero[y]]]])  
Step[Sqrt[x*x+y*y], 1.*10^-24, s[To2pi[arctan[Notzero[x],  
Notzero[y]]]]];  
Plot3D[T1[x, y], {x, -4, 4}, {y, -4, 4}, PlotPoints -> 40, Mesh -> False]
```



(* Integration test *)

```
Rintegrate2D[T1, -3, 3, -3, 3, 100]
```

11.9988

(* By calculus, $(V=1/3A=36/3)$ this is correct. *)

(* Define the functions, and derived ones to stop symbol expansion *)

```
f1[x_, y_] := T1[x, y] sin[( $\pi/8$ ) * (x + 4)] sin[( $\pi/8$ ) * (y + 4)]
```

```
g11[x_, y_] := f1[x, y] * f1[x, y]
```

$$f2[x_, y_] := T1[x, y] \sin[(\pi/4) * (x + 4)] \sin[(\pi/8) * (y + 4)]$$

$$g12[x_, y_] := f1[x, y] * f2[x, y]$$

$$g22[x_, y_] := f2[x, y] * f2[x, y]$$

(* ... *)

$$n = 100$$

$$a11 = Dsum2D[f1, f1, -3, 3, n]$$

$$3.01018$$

$$a12 = Dsum2D[f1, f2, -3, 3, n]; a21 = a12$$

$$-1.91714 \times 10^{-16}$$

$$a22 = Dsum2D[f2, f2, -3, 3, n]$$

$$3.1415$$

(* ... *)

$$b11 = Rintegrate2D[g11, -3, 3, -3, 3, n]$$

$$4.28029$$

$$b12 = Rintegrate2D[g12, -3, 3, -3, 3, n]; b21 = b12$$

$$-7.71714 \times 10^{-16}$$

$$b22 = Rintegrate2D[g22, -3, 3, -3, 3, n]$$

2.0318

(* ... *)

(* Now find eigenvalues *)

a_{11}/b_{11}

0.703266

$A2 = \{\{a_{11}, a_{12}\}, \{a_{21}, a_{22}\}\};$

$B2 = \{\{b_{11}, b_{12}\}, \{b_{21}, b_{22}\}\};$

Eigenvalues[$\{A2, B2\}$]

{1.54616, 0.703266}

(* ... *)

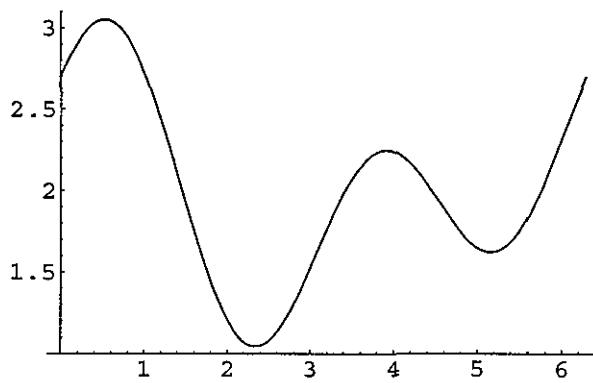
Appendix 3: Mathematica notebook - general case

(* Define $s(\theta)$ for the general case:- *)

$$s[\theta_] := 2 + 0.5 \cos[\theta] + 0.2 \cos[2\theta] + 0.6 \sin[2\theta]$$

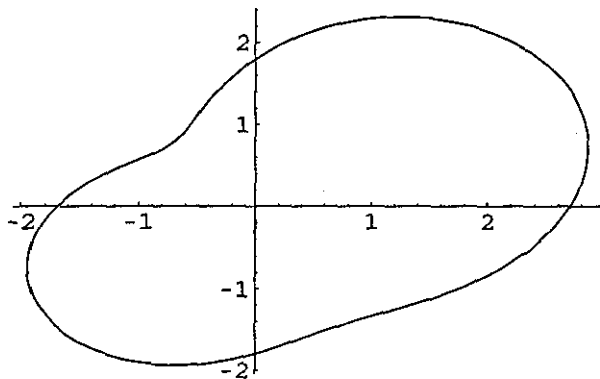
(* First, plot as a line function, so we can be sure it hasn't gone negative:- *)

Plot[s[θ], {θ, 0, 2π}]



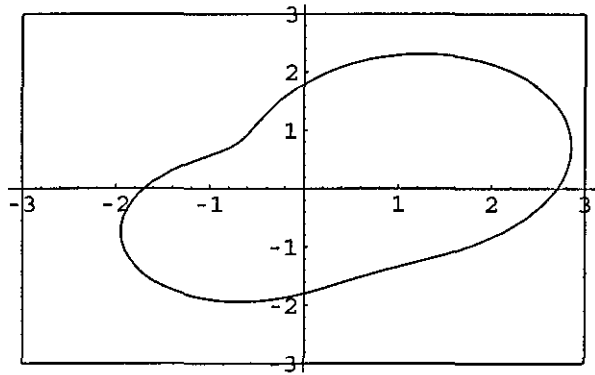
(* Now the actual ('Parametric') plot:- *)

```
ParametricPlot[{s[θ] cos[θ], s[θ] sin[θ]}, {θ, 0, 2π}]
```



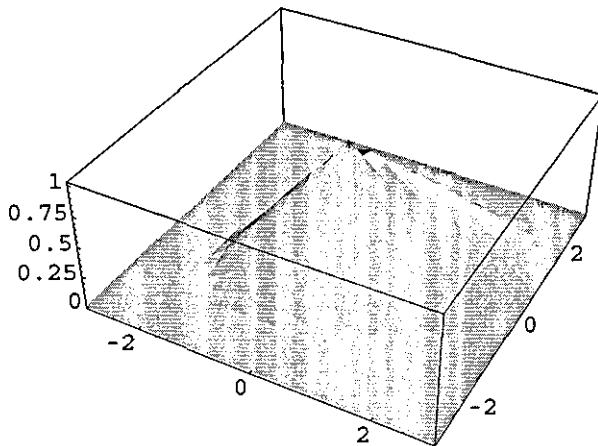
(* Also plot it with the -3 x 3 square, to ensure it is within it (t(θ) is square again) :- *)

```
t[θ_] := 3/Abs[Notzero[cos  
[Mod[θ, 2π]]]] * (Step[Mod[θ, 2π], 0, π/4] + Step[Mod[θ, 2π], 3π/4, 5π  
/4] + Step[Mod[θ, 2π], 7π/4, 2π]) + 3/Abs[Notzero[sin[Mod[θ, 2π]]]] *  
(Step[Mod[θ, 2π], π/4, 3π/4] + Step[Mod[θ, 2π], 5π/4, 7π/4])  
ParametricPlot[{ {s[θ] cos[θ],  
s[θ] sin[θ]}, {t[θ] cos[θ],  
t[θ] sin[θ]}}, {θ, 0, 2π}]
```



(* Define and plot T1:- *)

```
T1[x_, y_] := Step[Sqrt[x*x+y*y], 0, 1.*10^-24] + (1 - Sqrt[x*x+y*y]/
s[To2pi[arctan[Notzero[x], Notzero[y]]]])
Step[Sqrt[x * x + y * y], 1. * 10^ - 24, s[To2pi[arctan[Notzero[x],
Notzero[y]]]]];
Plot3D[T1[x, y], {x, -3, 3}, {y, -3, 3}, Mesh -> False]
```



(* Define the functions, and derived ones to stop symbol expansion *)

```
f1[x_, y_] := T1[x, y] sin[(pi/8) * (x + 4)] sin[(pi/8) * (y + 4)]
```

$$g11[x_, y_] := f1[x, y] * f1[x, y]$$

$$f2[x_, y_] := T1[x, y] \sin[(\pi/4) * (x + 4)] \sin[(\pi/8) * (y + 4)]$$

$$g12[x_, y_] := f1[x, y] * f2[x, y]$$

$$g22[x_, y_] := f2[x, y] * f2[x, y]$$

(* ... *)

$$n = 100$$

$$a11 = Dsum2D[f1, f1, -3, 3, n]$$

$$3.50643$$

$$a12 = Dsum2D[f1, f2, -3, 3, n]; a21 = a12$$

$$-0.179116$$

$$a22 = Dsum2D[f2, f2, -3, 3, n]$$

$$1.75644$$

(* ... *)

$$b11 = Rintegrate2D[g11, -3, 3, -3, 3, n]$$

$$1.92147$$

$$b12 = Rintegrate2D[g12, -3, 3, -3, 3, n]; b21 = b12$$

$$-0.366582$$

$b_{22} = \text{Rintegrate2D}[g_{22}, -3, 3, -3, 3, n]$

0.597019

(* ... *)

(* Now find eigenvalues *)

a_{11}/b_{11}

1.82487

$A2 = \{\{a_{11}, a_{12}\}, \{a_{21}, a_{22}\}\};$

$B2 = \{\{b_{11}, b_{12}\}, \{b_{21}, b_{22}\}\};$

$\text{Eigenvalues}\{A2, B2\}$

{3.57986, 1.68987}

(* ... *)

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