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Validated computations for fundamental solutions of linear elliptic operators

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Abstract—We present a method to enclose fundamental solutions of linear elliptic operators, especially for one dimensional Schrödinger operators which have periodic potentials. Our method is based on Floquet theory and Nakao's verification method for nonlinear equations. We show how to enclose fundamental solutions together with characteristic exponents and give a numerical example.

1. Introduction

We consider to compute fundamental solutions for the following equation

$$L\psi \equiv -\psi'' + q(x)\psi = 0, \quad x \in \mathbf{R}, \tag{1}$$

where we assume that $q(x) \in L^\infty(\mathbf{R})$ is a periodic function with a period r.

By Floquet Theory there exist fundamental solutions $\psi_1(x), \psi_2(x)$ of $L\psi = 0$ s.t.

$$\psi_1(x) = e^{\mu x}p_1(x), \quad \psi_2(x) = e^{-\mu x}p_2(x), \tag{2}$$

where μ is the characteristic exponent and $p_1(x), p_2(x)$ are periodic functions. Our aim is to compute $\psi_1(x), \psi_2(x)$ with guaranteed accuracy.

Once after we obtained such enclosed fundamental solutions, we may use them for another problem. For example, using those guaranteed fundamental solutions we define the Green's function $G(x,y,\lambda)$ [1] for $-\infty < x, y < \infty$ by

$$G(x,y,\lambda) = \begin{cases} \psi_1(x)\psi_2(y)/W(\psi_1,\psi_2)(x) & (x \le y) \\ \psi_2(x)\psi_1(y)/W(\psi_1,\psi_2)(x) & (x \ge y) \end{cases} \tag{3}$$

where $W(\psi_1,\psi_2)(x) \equiv \psi_1(x)\psi_2'(x) - \psi_1'(x)\psi_2(x)$ stands for the Wronskian. Then we have [1]

$$L^{-1}f = \int_{\mathbf{R}} G(x,y,\lambda)f(y)dy. \tag{4}$$

This kind of expression for L^{-1} is useful to execute another verification method related to the operator L.

2. Verification for fundamental solutions

In order to verify the fundamental solutions ψ_1 and ψ_2 in (1) satisfying (2), it is sufficient to enclose the functions ϕ_1 and ϕ_2 which are solutions for the following equations:

$$\begin{cases} -\phi_1'' + q\phi_1 = 0 & \text{in } [0,r] \\ \phi_1(0) = 1, \ \phi_1'(0) = 0 \end{cases} \tag{5}$$

$$\begin{cases} -\phi_2'' + q\phi_2 = 0 & \text{in } [0,r] \\ \phi_2(0) = 0, \ \phi_2'(0) = 1 \end{cases} \tag{6}$$

Let S_h denote the set of continuous and piecewise linear polynomials on $[0,r]$ with uniform mesh $0 = x_0 < x_1 < \cdots < x_N = r$ and mesh size h. We define a function space

$$V \equiv W^1_{\infty,0}(0,r) \cap \left(\bigwedge_{i=0}^{N} C^1[x_i, x_{i+1}] \right),$$

and we define the norm for $(w,\mu) \in V \times \mathbf{R}$ by

$$\|(w,\mu)\|_{V\times\mathbf{R}} \equiv \max\{\|w\|_{W^1_{\infty,0}}, \ |\mu|\},$$

where $W^1_{\infty,0}(0,r)$ is a usual Sobolev space defined by

$$W^1_{\infty,0}(0,r) \equiv \{\phi \in W^1_{\infty,0}(0,r) \mid \phi(0) = \phi(r) = 0\}$$

Setting $\phi_1(r) = \kappa$, $\phi_2(r) = \tau$ and transforming

$$\widetilde{\phi}_1(x) \equiv \phi_1(x) + \frac{1-\kappa}{r}x - 1, \ \widetilde{\phi}_2(x) \equiv \phi_2(x) - \frac{\tau}{r}x,$$

we consider the following problems:

Find $(\widetilde{\phi}_1, \kappa) \in V \times \mathbf{R}$ **s.t.**

$$\begin{cases} -\widetilde{\phi}_1'' + q\left(\widetilde{\phi}_1 + \dfrac{\kappa-1}{r}x + 1\right) = 0 \quad \text{in } [0,r] \\ \widetilde{\phi}_1(0) = \widetilde{\phi}_1(r) = 0 \\ \widetilde{\phi}_1'(0) = \dfrac{1-\kappa}{r} \end{cases} \tag{7}$$

Find $(\widetilde{\phi}_2, \tau) \in V \times \mathbf{R}$ **s.t.**

$$\begin{cases} -\widetilde{\phi}_2'' + q\left(\widetilde{\phi}_2 + \dfrac{\tau}{r}x\right) = 0 \quad \text{in } [0,r] \\ \widetilde{\phi}_2(0) = \widetilde{\phi}_2(r) = 0 \\ \widetilde{\phi}_2'(0) = 1 - \dfrac{\tau}{r} \end{cases} \tag{8}$$

Let $P_{h0} : V \to S_h$ denote the H_0^1-projection defined by

$$(\nabla(u - P_{h0}u), \nabla v)_{L^2} = 0 \ \text{ for all } v \in S_h,$$

and define the projection $P_h : V \times R \to S_h \times R$ by

$$P_h(u, \lambda) \equiv (P_{h0}u, \lambda).$$

In the below we describe how to enclose $(\widetilde{\phi}_1, \kappa) \in V \times \mathbf{R}$ in (7). The enclosure for $(\widetilde{\phi}_2, \tau) \in V \times \mathbf{R}$ is analogous.

Now, let $(\widetilde{\phi}_{1,h}, \kappa_h) \in S_h \times R$ be a finite element solution of (7). We will verify the solution $(\widetilde{\phi}_1, \kappa)$ in the neighborhood of $(\bar{\phi}_1, \kappa_h)$ satisfying

$$\begin{cases} -\bar{\phi}_1'' & = & -q\left(\widetilde{\phi}_{1,h} + \dfrac{\kappa - 1}{r}x + 1\right) & \text{in } (0, r), \\ \bar{\phi}_1(x) & = & 0 & \text{for } x = 0, r. \end{cases} \tag{9}$$

Notice that $\bar{\phi}_1 \in W^1_{\infty,0}(0, r) \bigcap W^2_{\infty,0}(0, r)$, and $\widetilde{\phi}_{1,h} = P_{h0}\bar{\phi}_1$. Defining $w = \widetilde{\phi}_1 - \bar{\phi}_1$, $v_0 = \bar{\phi}_1 - \widetilde{\phi}_{1,h}$, $\mu = \kappa - \kappa_h$, we have

$$\begin{cases} -w'' = -q\left(w + v_0 + \dfrac{\mu}{r}x\right) & \text{in } (0, r) \\ w(0) = w(r) = 0 & \\ w'(0) = \dfrac{1 - \mu - \kappa_h}{r} - v_0'(0) - \widetilde{\phi}'_{1,h}(0) & \end{cases} \tag{10}$$

Thus using the following compact map on $V \times R$

$$\begin{aligned} F(w, \mu) \ \equiv \ & \Big((-\Delta)^{-1}\Big\{-q\left(w + v_0 + \frac{\mu}{r}x\right), \\ & \mu + w'(0) - \frac{1 - \mu - \kappa_h}{r} \\ & + v_0'(0) + \widetilde{\phi}'_{1,h}(0)\Big), \end{aligned} \tag{11}$$

where $(-\Delta)^{-1}$ means the solution operator for Poisson equation with homogeneous boundary condition, we have the fixed point equation for $z = (w, \mu)$

$$z = F(z). \tag{12}$$

Now we decompose (12) into finite and infinite dimensional parts:

$$\begin{cases} P_h(z) & = & P_hF(z), \\ (I - P_h)(z) & = & (I - P_h)F(z). \end{cases} \tag{13}$$

And we use the Newton-like method only for the former part of (13), that is, we define the Newton-like operator

$$\begin{aligned} \mathcal{N}_h(z) \ \equiv \ & P_h(z) \\ & -[I - F'(-v_0, 0)]_h^{-1}(P_h(z) - P_hF(z)), \end{aligned}$$

where we assumed that the restriction to $S_h \times R$ of the operator $P_h[I - F'(-v_0, 0)] : V \times R \to S_h \times R$ has an inverse

$$[I - F'(-v_0, 0)]_h^{-1} : S_h \times R \to S_h \times R.$$

This assumption can be numerically checked in the actual computation.

We next define the operator $T : V \times R \to V \times R$ as

$$T(z) \equiv \mathcal{N}_h(z) + (I - P_h)F(z). \tag{14}$$

Then T becomes a compact map on $V \times R$, and

$$z = T(z) \Leftrightarrow z = F(z) \tag{15}$$

holds.

Our purpose is to find a fixed point of T in a certain set $Z \subset V \times \mathbf{R}$, which is called a 'candidate set'. Given positive real numbers α and γ we define the corresponding candidate set Z by

$$Z \equiv Z_h + [\alpha], \tag{16}$$

where

$$Z_h \equiv \{z_h \in S_h \times \mathbf{R} \mid \|z_h\|_V \le \gamma\}, \tag{17}$$

$$[\alpha] \equiv \{z_\perp \in S_h^\perp \times \{0\} \mid \|w_\perp\|_{W^1_{\infty,0}} \le \alpha\}. \tag{18}$$

Here $S_h^\perp$ denotes the orthogonal complement of S_h in V. If the relation

$$T(Z) \subset Z \tag{19}$$

holds, by Schauder's fixed point theorem, there exists a fixed point of T in Z. Decomposing $T(Z) \subset Z$ into finite and infinite dimensional parts we have a sufficient conditions for it as follows:

$$\begin{cases} \sup\limits_{z \in Z} \|\mathcal{N}_h(z)\|_V \le \gamma \\ \sup\limits_{z \in Z} \|(I - P_h)F(z)\|_{W^1_{\infty,0}} \le \alpha. \end{cases} \tag{20}$$

We find γ and α which satisfy the conditions (20) by iteration method.

After enclosing $\phi_1(x)$ and $\phi_2(x)$ by the method mentioned above, we evaluate $\phi_1(r)$ and $\phi_2'(r)$ rigorously. Then we can calculate the real values ρ_1 and ρ_2 which are solutions of the quadratic equation:

$$\rho^2 - \{\phi_1(r) + \phi_2'(r)\}\rho + 1 = 0. \tag{21}$$

Note that ρ_1 and ρ_2 are characteristic multipliers for $L\psi = 0$ and characteristic exponents μ_1 and μ_2 are calculated by the relation $e^{r\mu_i} = \rho_i \ \ (i = 1, 2)$. (Note that $\mu_1 + \mu_2 = 0$ holds.)

Here we mention about the relation between ϕ_1, ϕ_2 and ψ_1, ψ_2. We define the matrix A by

$$A = \begin{pmatrix} \phi_1(r) & \phi_1'(r) \\ \phi_2(r) & \phi_2'(r) \end{pmatrix}.$$

Since we enclose $\phi_1(r)$, $\phi_1'(r)$, $\phi_2(r)$ and $\phi_2'(r)$ by intervals, the matrix A is usually an interval matrix. Then clearly ρ_1 and ρ_2 are eigenvalues of A. Let v_1 and v_2 be the corresponding eigenvectors for ρ_1 and ρ_2, respectively. Then we can define ψ_1 and ψ_2 by

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \equiv \begin{pmatrix} v_1 & v_2 \end{pmatrix}^{-1} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}. \tag{22}$$

Now we define p_1 and p_2 by

$$\begin{pmatrix} p_1 \\ p_2 \end{pmatrix} \equiv \begin{pmatrix} e^{\mu x}\psi_1 \\ e^{-\mu x}\psi_2 \end{pmatrix}, \tag{23}$$

where $\mu \equiv |\mu_1| = |\mu_2|$ Then we can observe that $p_i(x+r) = p_1(x)$ $(i = 1, 2)$ and the ψ_1 and ψ_2 defined by (22) satisfy the relation (2).

3. Numerical examples

We consider the case that $q(x) = 5\cos 2\pi x - 9.0$, $r = 3$ and $N = 2000$ as an example.

The computations were carried out on the DELL Precision WorkStation 340 (Intel Pentium4 2.4GHz) using MATLAB (Ver. 7.0.1). The verification results for $\widetilde{\phi}_k$ $(k = 1, 2)$ are shown in Table 1 and 2, and the solutions $\widetilde{\phi}_k$ are enclosed as

$$\|\widetilde{\phi}_k - \widetilde{\phi}_{k,h}\|_V \le \|v_0\|_{W^1_{\infty,0}} + \alpha + \gamma \quad (k = 1, 2).$$

Table 1: Verification Results for $\widetilde{\phi}_1$

$\|v_0\|_{W^1_{\infty,0}}$	γ	α
0.1472	0.4842	0.0204

Table 2: Verification Results for $\widetilde{\phi}_2$

$\|v_0\|_{W^1_{\infty,0}}$	γ	α
0.0061	0.0037	1.5188×10^{-4}

From these verified results we could obtain

$$\begin{aligned} \kappa &\in [-9.4586 \times 10^{-6}, -9.0384 \times 10^{-6}] \\ \tau &\in [2.5080 \times 10^{-7}, 2.5392 \times 10^{-7}] \end{aligned}$$

and finally we obtain

$$\mu \in [0.73995\mathbf{353},\ 0.73995\mathbf{485}],$$

which derives the aimed fundamental solutions ψ_1 and ψ_2.

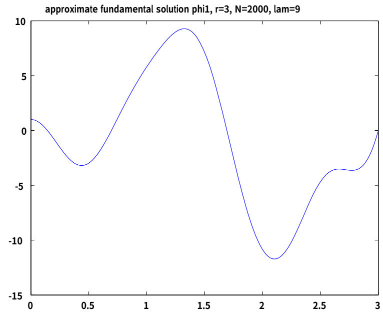

Figure 1: Approximate solution for ϕ_1

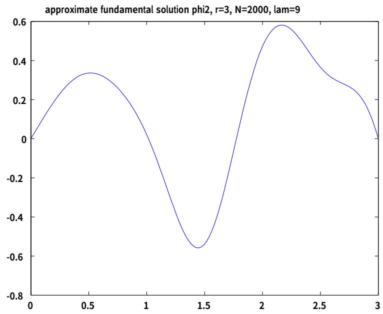

Figure 2: Approximate solution for ϕ_2

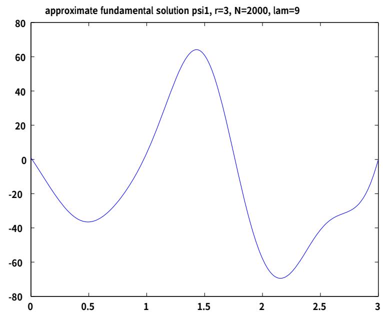

Figure 3: Approximate solution for ψ_1

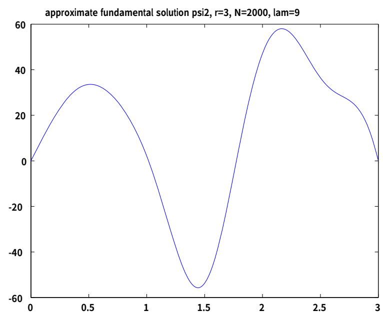

Figure 4: Approximate solution for ψ_2

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