Eigenvalues and eigenfunctions of the Laplacian via inverse iteration with shift

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ABSTRACT

In this paper we present an iterative method, inspired by the inverse iteration with shift technique of finite linear algebra, designed to find the eigenvalues and eigenfunctions of the Laplacian with homogeneous Dirichlet boundary condition for arbitrary bounded domains $\Omega \subset \mathbb{R}^N$. This method, which has a direct functional analysis approach, does not approximate the eigenvalues of the Laplacian as those of a finite linear operator. It is based on the uniform convergence away from nodal surfaces and can produce a simple and fast algorithm for computing the eigenvalues with minimal computational requirements, instead of using the ubiquitous Rayleigh quotient of finite linear algebra. Also, an alternative expression for the Rayleigh quotient in the associated infinite dimensional Sobolev space which avoids the integration of gradients is introduced and shown to be more efficient. The method can also be used in order to produce the spectral decomposition of any given function $u \in L^2(\Omega)$.

1. Introduction

In [1] we introduced an iterative method for computing the first eigenpair of the p-Laplacian operator $\Delta_p u := \operatorname{div}\left(|\nabla u|^{p-2} \nabla u\right)$, $p > 1$, with homogeneous Dirichlet boundary condition in a bounded domain $\Omega \subset \mathbb{R}^N$, $N \geqslant 1$. The technique was inspired by the inverse power method or inverse iteration of finite linear algebra.

In the present paper we concentrate in the special case $p = 2$, the Laplace operator Δ, which was superficially dealt with in [1]. Besides clarifying some of the arguments sketched in that paper for this case and providing some error estimates, our main purpose in this work is to show how inverse iteration with shift in the presence of uniform convergence can be used in order to obtain a fast and efficient method for computing the eigenvalues and eigenfunctions of the Laplacian operator with homogeneous Dirichlet boundary condition for any bounded domain Ω. If the eigenvalues or at least good estimates for them are *a priori* known, the method can produce the corresponding eigenfunctions with great speed and accuracy.

The technique can alternatively also be used as a fast process to obtain the spectral decomposition of any function $u \in L^2(\Omega)$ (in other words, the Fourier series of u).

We remark that the application of the method to the special case of the Laplacian operator is more natural since the Laplacian is a linear operator, $L^2(\Omega)$ is a Hilbert space and the inverse operator $-\Delta^{-1}$ is a self-adjoint and compact operator, therefore allowing the complete characterization of its spectral structure, as well as having the property that its eigenfunctions constitute a basis for $L^2(\Omega)$ (except for compactness, these properties are absent in the p-Laplacian when $p \neq 2$).

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Our approach of the inverse iteration with shift is based on the following iterative process started by a given function $u \in L^2(\Omega)$:

$$\phi_0 := u \quad \text{and} \quad \begin{cases} -\Delta_\sigma \phi_{n+1} = \phi_n & \text{in } \Omega, \\ \phi_{n+1} = 0 & \text{on } \partial\Omega, \end{cases} \tag{1}$$

where $\sigma > 0$ is a previously fixed *shift* and $\Delta_\sigma := \Delta + \sigma I$ is the corresponding *shifted operator*.

The sequence $\{\phi_n\}$ is then handled in order to produce approximations for the pair $(\lambda_u^\sigma, e_u^\sigma)$ where λ_u^σ denotes the eigenvalue of the Laplacian appearing in the spectral expansion of u which is closest to σ, and e_u^σ denotes the eigenfunction obtained as the projection of u on the λ_u^σ-eingenspace.

Inverse iteration with shift is used in finite linear algebra in order to find the eigenvalues and eigenfunctions of a finite-dimensional linear operator. As an eigenvalue-finding procedure it is not as efficient as other methods, such as the *QR* algorithm. However, if very good estimates of the eigenvalues are known in advance, its rate of convergence to both eigenvalues and eigenfunctions can be very fast (see [2], for instance).

This approach can be naturally extended to self-adjoint compact linear operators in infinite-dimensional Hilbert spaces such as the Laplacian and those arising in Sturm–Liouville problems. In spite of this, we have not been able to find any reference in the literature to this approach being used in the Laplacian context.

Since there is now a vast literature concerning the search for estimates for the eigenvalues of the Laplacian, as well as the gaps between eigenvalues (see, for instance, [3–6]; although particularly useful in our context would be lower bounds for the difference between consecutive eigenvalues), these results can be used in connection with the inverse iteration with shift algorithm to find eigenfunctions of the Laplacian in arbitrary domains, as well as better approximations for its eigenvalues. It must be emphasized, however, that as with the finite linear method, the inverse iteration with shift method is not capable to find all the eigenfunctions associated to a non-simple eigenvalue. It can only find an eigenfunction of the associated eigenspace. In the generic sense most domains have Laplacian spectra consisting only of simple eigenvalues (see [7,8]), although many domains of practical interest have eigenvalues with multiplicity greater than one (usually, domains which exhibit some type of symmetry, although not all of them).

Algorithm 1 below is the simplest version of the inverse iteration with shift algorithm for computing one specific eigenvalue and corresponding eigenfunction of the Laplacian.

Algorithm 1: Inverse iteration with shift for Laplacian eigenvalue and eigenfunction

1: $\phi_0 = u$
2: Set x_0 (point in Ω outside nodal surfaces, randomly chosen)
3: Set σ (shift, usually eigenvalue estimate)
4: Set m (number of iterations, depending on method used to solve Laplacian)
5: **for** $n = 0, 1, 2, \ldots, m$ **do**
6:   Solve $-\Delta_\sigma \phi_{n+1} = \phi_n$ in Ω, $\phi_{n+1} = 0$ on $\partial\Omega$
7: **end for**
8: **return** $\phi_{m+1}/\|\phi_{m+1}\|_\infty$ (L^∞-normalized eigenfunction)
9: **return** $\phi_m(x_0)/\phi_{m+1}(x_0) + \sigma$ (eigenvalue)

In principle, the function u at the start of Algorithm 1 should be chosen so that it will have components in all eigenspaces of the Laplacian and a random choice would suffice. However, in practice, due to rounding errors any simple function can be used. In our numerical tests (see Section 6), we observed that even the unit constant function could be used in order to obtain all the eigenvalues, even in a domain where it does not have an infinite number of them in its spectral decomposition.

In Line 6 of Algorithm 1 any PDE solver can be used. This allows one to choose the fastest solver available for a particular domain. In Line 9 the eigenvalue is computed according to the uniform convergence theory developed in Section 4. Since uniform convergence occurs away from nodal surfaces, a point $x_0 \in \Omega$ not in a nodal surface must be chosen; because nodal surfaces have zero N-dimensional measures, a random choice will suffice in the vast majority of cases, even taking into account that nodal surfaces change as the computed eigenfunction changes.

In finite linear algebra, the approximation to the eigenvalue is usually computed using the Rayleigh quotient. In our context, the eigenvalue can also be computed via the Rayleigh quotient of the approximated eigenfunction:

$$\mathcal{R}(\phi_{n+1}) = \frac{\langle \nabla \phi_{n+1}, \nabla \phi_{n+1} \rangle_2}{\langle \phi_{n+1}, \phi_{n+1} \rangle_2} = \frac{\|\nabla \phi_{n+1}\|_2^2}{\|\phi_{n+1}\|_2^2} = \frac{\int_\Omega |\nabla \phi_{n+1}|^2 dx}{\int_\Omega \phi_{n+1}^2 dx}. \tag{2}$$

However, due to the high oscillatory nature of high frequency eigenfunctions, in order to accurately compute the integral of the (squared) gradient of eigenfunctions associated with these eigenvalues, a much finer grid needs to be used, which affects the efficiency of the method. Therefore, the Rayleigh quotient in its original form (2) is not recommended for the computation of the eigenvalues of the Laplacian, unless one is prepared to incur the higher computational costs (see also further comments in Section 7).

Nonetheless, an integration by parts argument produces the following alternative expression for the Rayleigh quotient that avoids computations involving gradients:

$$\mathcal{R}(\phi_n) = \sigma + \frac{\int_\Omega \phi_n \phi_{n-1} dx}{\int_\Omega |\phi_n|^2 dx}. \tag{3}$$

We obtain very satisfactory results by using this sequence in Line 9 of Algorithm 1 to compute eingenvalues in our numerical tests (see Section 6).

Another alternative way to compute the eigenvalues is given by the quotient

$$\frac{\|\phi_n\|_2}{\|\phi_{n+1}\|_2} + \sigma = \frac{\int_\Omega \phi_n^2 dx}{\int_\Omega \phi_{n+1}^2 dx} + \sigma, \tag{4}$$

when the shift σ is chosen below the eigenvalue. This quotient also gives accurate approximations for the eigenvalues even using relatively coarse meshes; the computation of the integrals of the approximated eigenfunctions, instead of their gradients, does not appear to be significantly affected by the use of coarse grids (see Section 6).

We believe that, differently from what happens in finite dimensions, where much better and faster algorithms for finding the eigenvalues of linear operators (matrices), specially self-adjoint operators, are available, the inverse iteration with shift algorithm can be a very competitive method for finding the eigenvalues of the Laplacian. Typical algorithms for computing Laplacian eigenvalues involve the discretization of the Laplacian operator and the computation of the eigenvalues of the resulting discretization matrix. However, since only a small number of the eigenvalues of the discretization matrix are good approximations to the Laplacian eigenvalues (the smaller ones), huge matrices are necessary in order to obtain a sufficiently good number of eigenvalues. And some problems, particularly those arising in the study of quantum billiards, demand the computation of a very large number of eigenvalues. Needless to say, besides the requirements of memory, the size of the matrix makes it computationally costly to find its eigenvalues (see the classical [9] book, the review [3] and the more recent work [10] for details).

The inverse iteration with shift method, that requires only typical relatively modest sizes for meshes in order to solve the Poisson equation with homogeneous Dirichlet boundary condition, can be very competitive in terms of memory allocation and processing time. This is true even when one considers that in order to find accurate approximations for the highest order eigenvalues and eigenfunctions sometimes one needs to refine the mesh, due to the increase of oscillations.

Even if good estimates for the eigenvalues of a particular domain are not known in advance, a few iterations of inverse iteration with shift should be able to find good approximations to them, which can work as first estimates for the shift on a second run of the algorithm. The first choices for the shift might be concentrated around the numbers given by Weiyl's Law (see [11] or [12]).

The inverse iteration with shift method can also be used in order to find the spectral decomposition of any function $u \in L^2(\Omega)$, that is, in order to find its projections on the Laplacian eigenspaces. One has only to be careful to eliminate spurious projections, that is, projections which arise from rounding errors. This can be done through computing the Fourier coefficient associated to each eigenspace. If this coefficient becomes less than a specified very small tolerance, this projection can be safely discarded as arising from rounding errors. The two algorithms can be combined together in order to simultaneously find both the desired spectral decomposition of a given function defined on a domain and the spectrum of the Laplacian on it. The spectral decomposition algorithm is given below (Algorithm 2). Once again, Line 11 can be replaced by (3) or (4).

Algorithm 2: Spectral decomposition

1: $\phi_0 = u$
2: Set x_0 (point in Ω randomly chosen)
3: **for** $k = 0, 1, 2, \ldots$ **do**
4:     Setσ_k (shift)
5:     **for** $n = 0, 1, 2, \ldots$ **do**
6:        Solve $-\Delta_{\sigma_k} \phi_{n+1}^k = \phi_n^k$ in Ω, $\phi_{n+1}^k = 0$ on $\partial\Omega$
7:        Compute $\left\langle u, \phi_{n+1}^k / \left\| \phi_{n+1}^k \right\|_2 \right\rangle_2$ (Fourier coeficient)
8:        **if** $\left| \left\langle u, \phi_{n+1}^k / \left\| \phi_{n+1}^k \right\|_2 \right\rangle_2 \right| > $ tolerance **then**
9:           **return** $\phi_{n+1}^k / \left\| \phi_{n+1}^k \right\|_2$ (L^2 -normalized eigenfunction)
10:         **return** $\left\langle u, \phi_{n+1}^k / \left\| \phi_{n+1}^k \right\|_2 \right\rangle_2$ (Fourier coefficient)
11:         **return** $\phi_n(x_0)/\phi_{n+1}(x_0) + \sigma_k$ (eigenvalue)
              break
12:       **end if**
13:     **end for**
14: **end for**

Although for the sake of simplicity all computations here are done for the Laplacian, the same algorithm can be used for similar elliptic operators.

This paper is organized as follows. The inverse iteration with shift sequence is defined in Section 2, where most of the notation used in this paper is also established. In Section 3 some well-known results concerning the Rayleigh quotient are recalled and proven for completeness. In Sections 3 and 4 we discuss L^2 and uniform convergence of the inverse iterated sequence, respectively. In the short Section 5 we make some considerations about the normalization process on each step of (1) which is useful for computational purposes, and in Section 6 we present the results of some numerical experiments made in simple domains.

Finally, in Section 7 we discuss if the rate of convergence of the method could theoretically be improved through the use of the inverse iteration with shift given by the Rayleigh quotient, as it is standard practice in finite linear algebra.

2. Definition of the inverse iteration with shift sequence

Let Ω be a bounded domain in $\mathbb{R}^N$ and $\mathcal{H} = \{e_k\}_{k=1}^\infty \subset H_0^1(\Omega)$ be an orthogonal (not necessarily normalized) basis for $L^2(\Omega)$ consisting of eigenfunctions of the Laplacian operator with homogeneous Dirichlet boundary condition, that is,

$$\begin{cases} -\Delta e_k = \lambda_k e_k & \text{in } \Omega, \\ e_k = 0 & \text{on } \partial\Omega, \end{cases}$$

where $\{\lambda_k\}_{k=1}^\infty$ is the non-decreasing sequence of eigenvalues of the Laplacian, counting multiplicities:

$$0 < \lambda_1 < \lambda_2 \leqslant \ldots \tag{5}$$

Let $\sigma > 0$ and define the *shifted operator*

$$\Delta_\sigma := \Delta + \sigma I. \tag{6}$$

It follows that e_k is also an eigenfunction of $-\Delta_\sigma$ corresponding to the eigenvalue $\lambda_k - \sigma$.

Conversely, if λ is an eigenvalue of $-\Delta_\sigma$, then $\lambda = \lambda_k - \sigma$ for some k. Thus, the spectrum of the shifted operator equals the spectrum of the Laplacian operator shifted to the left by σ, while the corresponding eigenspaces are the same.

Given $u \in L^2(\Omega)$, let

$$u = \sum_{k=1}^\infty \alpha_k e_k$$

be the Fourier expansion of u, so that the Fourier coefficients α_k are given by

$$\alpha_k = \frac{\langle u, e_k \rangle_2}{\|e_k\|_2^2} = \frac{\int_\Omega u e_k dx}{\int_\Omega e_k^2 dx}.$$

Denote by λ_u^1 the least eigenvalue whose associated eigenspace is not orthogonal to u. That is,

$$\lambda_u^1 := \lambda_{k_1} \quad \text{where} \quad k_1 = \min\{k : \alpha_k \neq 0\}.$$

In other words, λ_u^1 is the first eigenvalue such that u has a non-zero component in the corresponding eigenspace. Note that if r_1 is the multiplicity of λ_{k_1} then

$$\lambda_u^1 = \lambda_{k_1} = \lambda_{k_1+1} = \cdots = \lambda_{k_1+r_1-1}.$$

We will denote by e_u^1 the orthogonal projection of u on the λ_u^1-eigenspace, that is

$$e_u^1 := \alpha_{k_1} e_{k_1} + \alpha_{k_1+1} e_{k_1+1} + \cdots + \alpha_{k_1+r_1-1} e_{k_1+r_1-1} = \sum_{\lambda_k = \lambda_u^1} \alpha_k e_k.$$

Thus, the Fourier expansion of u can be rewritten as

$$u = \sum_{\lambda_k \geqslant \lambda_u^1} \alpha_k e_k = e_u^1 + \sum_{\lambda_k > \lambda_u^1} \alpha_k e_k = e_u^1 + \sum_{k \geqslant k_1+r_1} \alpha_k e_k.$$

Proceeding in this way, denoting by e_u^j the orthogonal projection of u on the λ_u^j-eigenspace which is the jth-eigenspace not orthogonal to u, the eigenfunction expansion of u can be written in terms of its non-zero components in the eigenspaces of the Laplacian as

$$u = \sum_{j=1}^M e_u^j, \tag{7}$$

where either M is a positive integer or, as in most cases, $M = \infty$, and the corresponding sequence of eigenvalues $\left\{\lambda_u^j\right\}_{j=1}^\infty$ is (strictly) increasing

$$0 < \lambda_u^1 < \lambda_u^2 < \ldots$$

As is well known from the theory of compact linear operators, if σ does not belong to the spectrum of $-\Delta$ we have that $(-\Delta_\sigma)^{-1} : L^2(\Omega) \to L^2(\Omega)$ is a continuous, compact and invertible operator. Therefore, whenever σ is not an eigenvalue of the Laplacian, we can define a sequence $\{\phi_n\}_{n \in \mathbb{N}} \subset H_0^1(\Omega)$ by inverse iteration setting

$$\phi_0 = u \quad \text{and} \quad \begin{cases} -\Delta_\sigma \phi_{n+1} = \phi_n & \text{in } \Omega, \\ \phi_{n+1} = 0 & \text{on } \partial\Omega. \end{cases} \tag{8}$$

For each $u \in L^2(\Omega)$ and $\sigma > 0$ not in the Laplacian spectrum consider the sequence $\{\phi_n\}$ defined by inverse iteration in (8). Since $\phi_{n+1} = (-\Delta_\sigma)^{-1}\phi_n$, it follows from (7) that the eigenfunction expansion of ϕ_n is given by

$$\phi_n = \sum_{j=1}^{M} \frac{1}{\left(\lambda_u^j - \sigma\right)^n} e_u^j.$$

Let λ_u^σ be the Laplacian eigenvalue appearing in the spectral decomposition of u which is closest to σ, i.e.,

$$\left| \lambda_u^\sigma - \sigma \right| = \min_{j \in \mathbb{N}} \left| \lambda_u^j - \sigma \right|. \tag{9}$$

Now let e_u^σ denote the projection of u on the λ_u^σ-eigenspace. Then

$$\langle u, e_u^\sigma \rangle_2 = \langle e_u^\sigma, e_u^\sigma \rangle_2 = \| e_u^\sigma \|_2^2 \tag{10}$$

and we can write

$$\phi_n = \frac{1}{\left(\lambda_u^\sigma - \sigma\right)^n} e_u^\sigma + \sum_{\left| \lambda_u^j - \sigma \right| > \left| \lambda_u^\sigma - \sigma \right|}^{M} \frac{1}{(\lambda_u^j - \sigma)^n} e_u^j = \frac{1}{\left(\lambda_u^\sigma - \sigma\right)^n} \left(e_u^\sigma + \sum_{\left| \lambda_u^j - \sigma \right| > \left| \lambda_u^\sigma - \sigma \right|}^{M} \left(\frac{\lambda_u^\sigma - \sigma}{\lambda_j - \sigma} \right)^n e_u^j \right),$$

or

$$\phi_n = \frac{1}{\left(\lambda_u^\sigma - \sigma\right)^n} \left(e_u^\sigma + \psi_n \right), \tag{11}$$

where

$$\psi_n = \sum_{\left| \lambda_u^j - \sigma \right| > \left| \lambda_u^\sigma - \sigma \right|}^{M} \left(\frac{\lambda_u^\sigma - \sigma}{\lambda_u^j - \sigma} \right)^n e_u^j. \tag{12}$$

Throughout this paper, we will denote by λ_u^τ the Laplacian eigenvalue appearing in the spectral decomposition of u which is second closest to σ, i.e.,

$$\left| \lambda_u^\tau - \sigma \right| = \min_{\substack{j \in \mathbb{N} \\ \lambda_u^j \neq \lambda_u^\sigma}} \left| \lambda_u^j - \sigma \right|. \tag{13}$$

We will also denote by u_n the component of u in the direction of $\frac{\phi_n}{\|\phi_n\|_2}$, that is:

$$u_n := \left\langle u, \frac{\phi_n}{\|\phi_n\|_2} \right\rangle_2 \frac{\phi_n}{\|\phi_n\|_2} = \left(\int_\Omega u \frac{\phi_n}{\|\phi_n\|_2} dx \right) \frac{\phi_n}{\|\phi_n\|_2}. \tag{14}$$

3. L^2-convergence of inverse iteration with shift

In this section we expose the L^2-approach of the inverse iteration with shift. Firstly let us state some well-known results concerning the Rayleigh quotient $\mathcal{R} : H_0^1(\Omega) \setminus \{0\} \to \mathbb{R}$ defined by

$$\mathcal{R}(v) = \frac{\int_\Omega |\nabla v|^2 dx}{\int_\Omega v^2 dx}. \tag{15}$$

For ease of consultation, we give short proofs of these results.

Proposition 1. *A function $u \in H_0^1(\Omega) \setminus \{0\}$ is a critical point of $\mathcal{R}$ if and only if u is an eigenfunction of the Laplacian with homogeneous Dirichlet boundary condition and $\mathcal{R}(u)$ is the corresponding eigenvalue.*

Proof. Given $v \in H_0^1(\Omega)$, we have

$$\mathcal{R}'(u)v = \frac{2}{\|u\|_2^2} [\langle \nabla u, \nabla v \rangle_2 - \mathcal{R}(u)\langle u, v \rangle_2].$$

Therefore, $\mathcal{R}'(u) = 0$ if and only if

$$\int_{\Omega} \nabla u \cdot \nabla v = \mathcal{R}(u) \int_{\Omega} uv$$

for all $v \in W_0^{1,2}(\Omega)$, that is, u is a weak solution of

$$\begin{cases} -\Delta u = \mathcal{R}(u)u & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{cases} \qquad \square$$

Corollary 2. *The Rayleigh quotient gives a quadratically accurate estimate for the Dirichlet Laplacian eigenvalues, that is, if u is an eigenfunction of the Laplacian with homogeneous Dirichlet boundary condition with $\mathcal{R}(u)$ as the corresponding eigenvalue, then*

$$\mathcal{R}(v) - \mathcal{R}(u) = O\left(\|v - u\|^2\right)$$

as $v \to u$ in $L^2(\Omega)$.

Proof. If follows immediately from Taylor's formula, since $\mathcal{R}'(u) = 0$. $\square$

Now we give the main result of this section. Before this, we note from (11) of Section 2 that

$$\frac{\phi_n}{\|\phi_n\|_2} = \pm \frac{e_u^{\sigma} + \psi_n}{\|e_u^{\sigma} + \psi_n\|_2}, \tag{16}$$

where the sign of the right-hand side will depend on whether the shift σ is taken above or below the eigenvalue. With respect to n: if the shift is taken below the eigenvalue, the sign will always be positive, whereas if the shift is chosen above the eigenvalue the sign will be $(-1)^n$.

We note from (14) and (16) that

$$u_n = \left\langle u, \frac{e_u^{\sigma} + \psi_n}{\|e_u^{\sigma} + \psi_n\|_2} \right\rangle_2 \frac{e_u^{\sigma} + \psi_n}{\|e_u^{\sigma} + \psi_n\|_2} \tag{17}$$

and also remark that

$$\mathcal{R}(\phi_n) = \sigma + \frac{\int_{\Omega} \phi_n \phi_{n-1} dx}{\int_{\Omega} |\phi_n|^2 dx}. \tag{18}$$

This fact follows from an integration by parts after multiplying the equation $-\Delta_{\sigma}\phi_n = \phi_{n-1}$ by ϕ_n. From the computational viewpoint, (18) has the advantage of avoiding the computation of the gradient $\nabla\phi_n$ as required in (15).

Theorem 3. *Let $u \in L^2(\Omega)$.*

(i) *We have*

$$\|\psi_n\|_2 \leqslant \left|\frac{\lambda_u^{\sigma} - \sigma}{\lambda_u^{\tau} - \sigma}\right|^n \|u\|_2.$$

In particular, $\psi_n \to 0$ in $L^2(\Omega)$ with an exponential rate.

(ii) *There exists $n_0 \in \mathbb{N}$ such that*

$$\left\|\frac{e_u^{\sigma} + \psi_n}{\|e_u^{\sigma} + \psi_n\|_2} - \frac{e_u^{\sigma}}{\|e_u^{\sigma}\|_2}\right\|_2 \leqslant \frac{4}{\|e_u^{\sigma}\|_2} \|\psi_n\|_2$$

for all $n \geqslant n_0$. In particular,

$$\frac{e_u^{\sigma} + \psi_n}{\|e_u^{\sigma} + \psi_n\|_2} \to \frac{e_u^{\sigma}}{\|e_u^{\sigma}\|_2} \text{ in } L^2(\Omega),, \tag{19}$$

with an exponential rate.

(iii) *The following convergences hold:*

$$\frac{\|\phi_n\|_2}{\|\phi_{n+1}\|_2} \to |\lambda_u^{\sigma} - \sigma|, \tag{20}$$

$$u_n \to e_u^{\sigma} \text{ in } L^2(\Omega), \tag{21}$$

where u_n is defined by (14), *and*

$$\mathcal{R}(\phi_n) \to \lambda_u^\sigma, \tag{22}$$

with

$$\mathcal{R}(\phi_n) - \lambda_u^\sigma = O\left(\left|\frac{\lambda_u^\sigma - \sigma}{\lambda_u^\tau - \sigma}\right|^{2n}\right). \tag{23}$$

Proof. We have from (12) that

$$\|\psi_n\|_2^2 = \sum_{|\lambda_u^j - \sigma| > |\lambda_u^\sigma - \sigma|} \left|\frac{\lambda_u^\sigma - \sigma}{\lambda_u^j - \sigma}\right|^{2n} \|e_u^j\|_2^2 \leqslant \left|\frac{\lambda_u^\sigma - \sigma}{\lambda_u^\tau - \sigma}\right|^{2n} \sum_{|\lambda_u^j - \sigma| > |\lambda_u^\sigma - \sigma|} \|e_u^j\|_2^2 \leqslant \left|\frac{\lambda_u^\sigma - \sigma}{\lambda_u^\tau - \sigma}\right|^{2n} \|u\|_2^2.$$

Since

$$\left|\frac{\lambda_u^\sigma - \sigma}{\lambda_u^\tau - \sigma}\right| < 1,$$

it follows that $\|\psi_n\|_2 \to 0$ as $n \to \infty$, which proves *(i)*.

Let $n_0 \in \mathbb{N}$ be such that

$$\|\psi_n\|_2 \leqslant \frac{1}{2}\|e_u^\sigma\| \quad \text{for all } n \geqslant n_0.$$

Thus, if $n \geqslant n_0$ it follows that

$$\frac{1}{2}\|e_u^\sigma\|_2 = \|e_u^\sigma\|_2 - \frac{1}{2}\|e_u^\sigma\|_2 \leqslant \|e_u^\sigma + \psi_n\|_2 + \|\psi_n\|_2 - \|\psi_n\|_2 = \|e_u^\sigma + \psi_n\|_2$$

and

$$\left\|\frac{e_u^\sigma + \psi_n}{\|e_u^\sigma + \psi_n\|_2} - \frac{e_u^\sigma}{\|e_u^\sigma\|_2}\right\|_2 = \left\|\frac{\|e_u^\sigma\|_2(e_u^\sigma + \psi_n) - e_u^\sigma\|e_u^\sigma + \psi_n\|_2}{\|e_u^\sigma + \psi_n\|_2\|e_u^\sigma\|_2}\right\|_2 \leqslant \left\|\frac{e_u^\sigma\left(\|e_u^\sigma\|_2 - \|e_u^\sigma + \psi_n\|_2\right) + \|e_u^\sigma\|_2\psi_n}{(1/2)\|e_u^\sigma\|_2^2}\right\|_2$$

$$\leqslant 2\frac{\|e_u^\sigma\|_2\|\psi_n\|_2 + \|e_u^\sigma\|_2\|\psi_n\|_2}{\|e_u^\sigma\|_2^2} = \frac{4}{\|e_u^\sigma\|_2}\|\psi_n\|_2,$$

which proves (ii).

Since

$$\frac{\|\phi_n\|_2}{\|\phi_{n+1}\|_2} = |\lambda_u^\sigma - \sigma|\frac{\|e_u^\sigma + \psi_n\|_2}{\|e_u^\sigma + \psi_{n+1}\|_2},$$

(20) follows from *(i)*.

The L^2-convergence (21) follows from (17), (19) and (10).

In order to prove (22) we firstly notice that

$$\lim\left\langle\frac{\phi_{n-1}}{\|\phi_{n-1}\|_2}, \frac{\phi_n}{\|\phi_n\|_2}\right\rangle_2 = \left\langle\frac{e_u^\sigma}{\|e_u^\sigma\|_2}, \frac{e_u^\sigma}{\|e_u^\sigma\|_2}\right\rangle_2 \begin{cases} 1 & \text{if } \lambda_u^\sigma \geqslant \sigma, \\ -1 & \text{if } \lambda_u^\sigma < \sigma. \end{cases}$$

In fact, if $\lambda_u^\sigma \geqslant \sigma$ then

$$\lim\left\langle\frac{\phi_{n-1}}{\|\phi_{n-1}\|_2}, \frac{\phi_n}{\|\phi_n\|_2}\right\rangle_2 = \lim\left\langle\frac{e_u^\sigma + \psi_{n-1}}{\|e_u^\sigma + \psi_{n-1}\|_2}, \frac{e_u^\sigma + \psi_n}{\|e_u^\sigma + \psi_n\|_2}\right\rangle_2 = \left\langle\frac{e_u^\sigma}{\|e_u^\sigma\|_2}, \frac{e_u^\sigma}{\|e_u^\sigma\|_2}\right\rangle_2,$$

while if $\lambda_u^\sigma < \sigma$ then

$$\lim\left\langle\frac{\phi_{n-1}}{\|\phi_{n-1}\|_2}, \frac{\phi_n}{\|\phi_n\|_2}\right\rangle_2 = \lim\left\langle(-1)^{n-1}\frac{e_u^\sigma + \psi_{n-1}}{\|e_u^\sigma + \psi_{n-1}\|_2}, (-1)^n\frac{e_u^\sigma + \psi_n}{\|e_u^\sigma + \psi_n\|_2}\right\rangle_2 = -\left\langle\frac{e_u^\sigma}{\|e_u^\sigma\|_2}, \frac{e_u^\sigma}{\|e_u^\sigma\|_2}\right\rangle_2.$$

Thus, it follows from (18) that

$$\lim\mathcal{R}(\phi_n) = (\sigma + |\lambda_u^\sigma - \sigma|)\begin{cases} 1 & \text{if } \lambda_u^\sigma \geqslant \sigma, \\ -1 & \text{if } \lambda_u^\sigma < \sigma. \end{cases} = \lambda_u^\sigma.$$

The convergence order (23) follows from (21) and Corollary 2, since

$$\mathcal{R}(\phi_n) - \lambda_u^\sigma = \mathcal{R}(u_n) - \mathcal{R}(e_u^\sigma) = O\left(\|u_n - e_u^\sigma\|_2^2\right) = O\left(\left|\frac{\lambda_u^\sigma - \sigma}{\lambda_u^\tau - \sigma}\right|^{2n}\right). \qquad \square$$

4. Uniform convergence of inverse iteration with shift

We begin this section by stating a L^∞-estimate for an eigenfunction of the Laplacian in terms of its L^2-norm. In the following, we denote by $|\Omega|$ the Lebesgue measure of Ω.

Lemma 4. Let $e \in H_0^1(\Omega)$ be an eigenfunction of $-\Delta$ corresponding to the eigenvalue λ. Then

$$\|e\|_\infty \leqslant 4^N |\Omega|^{1/2} \lambda^{N/2} \|e\|_2. \tag{24}$$

Proof. It is shown in [13], without any smoothness assumption on $\partial\Omega$, that if e is an eigenfunction corresponding to a variational eigenvalue λ of the homogeneous Dirichlet problem for the p-Laplacian then

$$\|e\|_\infty \leqslant 4^N \lambda^{N/p} \|e\|_{L^1(\Omega)}.$$

Choosing $p = 2$, (24) follows from Hölder's inequality. $\square$

Estimates for eigenfunctions of the Laplacian with the exponent $N/2$ in the eigenvalue replaced by $N/4$ can be found in [14–17]. See also [18, Remark 5.21] for more references.

The following result refers to the nondecreasing sequence (5) of eigenvalues of the Laplacian.

Lemma 5. If $k > N/2$, then

$$\sum_{j=1}^\infty \frac{1}{\lambda_j^k} \leqslant \frac{NC^k}{2k - N} < \infty, \tag{25}$$

where C is a positive constant which depends only on N and $|\Omega|$.

Proof. It is well known (see [19,20]) that

$$\lambda_j \geqslant \frac{1}{C} j^{2/N},$$

where

$$C = \frac{N+2}{N} \frac{(\omega_N |\Omega|)^{2/N}}{4\pi^2} \tag{26}$$

and ω_N is the volume of the N-dimensional unit ball. Hence, if $j > N/2$ we have

$$\sum_{j=1}^\infty \lambda_j^{-k} \leqslant C^k \sum_{j=1}^\infty j^{-2k/N} < C^k \int_1^\infty s^{-2k/N} ds = \frac{NC^k}{2k - N}. \qquad \square$$

In the next lemma we show that the convergence of a series formed by the eigenvalues λ_u^j which appear in the spectral decomposition of a function $u \in L^2(\Omega)$ follows from the convergence of a series formed by all eigenvalues of the Laplacian.

Lemma 6. Let k be chosen so that the series $\sum_{j=1}^\infty \frac{1}{\lambda_j^k}$ is convergent. Then the series

$$\sum_{j=1}^M \frac{\left(\lambda_u^j\right)^{N/2}}{\left|\lambda_u^j - \sigma\right|^{N/2+k+1}}$$

is also convergent.

Proof. Assume that the expansion of u is not finite, i.e., $M = \infty$ (otherwise the result is trivial). Since

$$\sum_{j=1}^\infty \frac{1}{\left(\lambda_u^j\right)^k} \leqslant \sum_{j=1}^\infty \frac{1}{\lambda_j^k},$$

it suffices to show that

$$\frac{\left(\lambda_u^j\right)^{N/2}}{\left|\lambda_u^j - \sigma\right|^{N/2+k+1}} \leqslant \frac{1}{\left(\lambda_u^j\right)^k} \tag{27}$$

for all sufficiently large j.

As $\lambda_u^j \to \infty$, there exists j_0 such that $\left|\lambda_u^j - \sigma\right| = \lambda_u^j - \sigma$ for all $j \geqslant j_0$. Thus, if j is sufficiently large, we can write

$$\frac{\left(\lambda_u^j\right)^{N/2+k}}{\left|\lambda_u^j - \sigma\right|^{N/2+k}} = \frac{\left(\lambda_u^j\right)^{N/2+k}}{\left(\lambda_u^j - \sigma\right)^{N/2+k}} < \lambda_u^j - \sigma = \left|\lambda_u^j - \sigma\right|,$$

whence (27) follows.   □

In order to prove the uniform convergence of the inverse iteration sequence $\{\phi_n\}_{n\in\mathbb{N}}$, we return to (11) and write

$$\frac{\phi_n}{\|\phi_n\|_\infty} = \pm \frac{e_u^\sigma + \psi_n}{\|e_u^\sigma + \psi_n\|_\infty}. \tag{28}$$

As in (16), the sign of the right-hand side will depend on whether the shift is taken above or below the eigenvalue and on n.

Lemma 7. *The inequality*

$$\|\psi_n\|_\infty \leqslant K \left|\frac{\lambda_u^\sigma - \sigma}{\lambda_u^\tau - \sigma}\right|^{n-\theta} \tag{29}$$

holds for all sufficiently large n, for some $\theta > 0$ and a positive constant $K = K(u, \Omega, |\lambda_u^\sigma - \sigma|)$. In particular, $\psi_n \to 0$ uniformly in $\overline{\Omega}$ with an exponential rate.

Proof. From (12) and Lemma 4 we obtain

$$|\psi_n| \leqslant \sum_{\left|\lambda_u^j - \sigma\right| > \left|\lambda_u^\sigma - \sigma\right|}^M \left|\frac{\lambda_u^\sigma - \sigma}{\lambda_u^j - \sigma}\right|^n \left|e_u^j\right| \leqslant 4^N |\Omega|^{1/2} \|u\|_2 \sum_{\left|\lambda_u^j - \sigma\right| > \left|\lambda_u^\sigma - \sigma\right|}^M \left|\frac{\lambda_u^\sigma - \sigma}{\lambda_u^j - \sigma}\right|^n \left(\lambda_u^j\right)^{N/2}.$$

But, taking $\theta = N/2 + k + 1$, we have

$$\sum_{\left|\lambda_u^j - \sigma\right| > \left|\lambda_u^\sigma - \sigma\right|}^M \left|\frac{\lambda_u^\sigma - \sigma}{\lambda_u^j - \sigma}\right|^n \left(\lambda_u^j\right)^{N/2} = \left|\lambda_u^\sigma - \sigma\right|^\theta \sum_{\left|\lambda_u^j - \sigma\right| > \left|\lambda_u^\sigma - \sigma\right|}^M \left|\frac{\lambda_u^\sigma - \sigma}{\lambda_u^j - \sigma}\right|^{n-\theta} \frac{\left(\lambda_u^j\right)^{N/2}}{\left|\lambda_u^j - \sigma\right|^\theta} \leqslant \left|\lambda_u^\sigma - \sigma\right|^\theta \left|\frac{\lambda_u^\sigma - \sigma}{\lambda_u^\tau - \sigma}\right|^{n-\theta} \sum_{\left|\lambda_u^j - \sigma\right| > \left|\lambda_u^\sigma - \sigma\right|}^M \frac{\left(\lambda_u^j\right)^{N/2}}{\left|\lambda_u^j - \sigma\right|^\theta}$$

$$\leqslant \left|\frac{\lambda_u^\sigma - \sigma}{\lambda_u^\tau - \sigma}\right|^{n-\theta} \left|\lambda_u^\sigma - \sigma\right|^\theta \sum_{j=1}^M \frac{\left(\lambda_u^j\right)^{N/2}}{\left|\lambda_u^j - \sigma\right|^\theta}$$

and by Lemma 6 the last series converges. Thus, (29) follows if we take

$$K = 4^N |\Omega|^{1/2} \|u\|_2 \left|\lambda_u^\sigma - \sigma\right|^\theta \sum_{j=1}^M \frac{\left(\lambda_u^j\right)^{N/2}}{\left|\lambda_u^j - \sigma\right|^\theta}.   \quad \square$$

Theorem 8. *Let $u \in L^2(\Omega)$. Then*

(i) There exists $n_0 \in \mathbb{N}$ such that

$$\left\|\frac{e_u^\sigma + \psi_n}{\|e_u^\sigma + \psi_n\|_\infty} - \frac{e_u^\sigma}{\|e_u^\sigma\|_\infty}\right\|_\infty \leqslant \frac{4}{\|e_u^\sigma\|_\infty} \|\psi_n\|_\infty$$

for all $n \geqslant n_0$. In particular,

$$\frac{e_u^\sigma + \psi_n}{\|e_u^\sigma + \psi_n\|_\infty} \to \frac{e_u^\sigma}{\|e_u^\sigma\|_\infty} \quad \text{uniformly in } \Omega$$

with an exponential rate.

(ii) The following convergences hold

$$\frac{\|\phi_n\|_\infty}{\|\phi_{n+1}\|_\infty} \to |\lambda_u^\sigma - \sigma| \tag{30}$$

and

$$u_n \to e_u^\sigma \quad \text{uniformly in } \Omega. \tag{31}$$

(iii) If $\mathcal{K} \subset \{x : e_u^\sigma(x) \neq 0\}$ is compact, then $\frac{\phi_n}{\phi_{n+1}} \to \lambda_u^\sigma - \sigma$ uniformly and with an exponential rate.

Proof. Let n_0 be such that $\|\psi_n\|_\infty \leqslant \frac{1}{2}\|e_u^\sigma\|_\infty$ for all $n \geqslant n_0$. Then, as in the proof of *(ii)* of Theorem 3, we have for all $n \geqslant n_0$ that

$$\frac{1}{2}\|e_u^\sigma\|_\infty \leqslant \|e_u^\sigma + \psi_n\|_\infty$$

and

$$\left\|\frac{e_u^\sigma + \psi_n}{\|e_u^\sigma + \psi_n\|_\infty} - \frac{e_u^\sigma}{\|e_u^\sigma\|_\infty}\right\|_\infty \leqslant \frac{4}{\|e_u^\sigma\|_\infty}\|\psi_n\|_\infty.$$

The remaining of *(i)* follows from Lemma 7.

In order to prove *(31)*, write

$$u_n = \left(\frac{\|\phi_n\|_\infty}{\|\phi_n\|_2}\right)^2 \frac{\phi_n}{\|\phi_n\|_\infty} \int_\Omega u \frac{\phi_n}{\|\phi_n\|_\infty} dx.$$

Since

$$\lim \frac{\|\phi_n\|_\infty}{\|\phi_n\|_2} = \lim \frac{\|e_u^\sigma + \psi_n\|_\infty}{\|e_u^\sigma + \psi_n\|_2} = \frac{\|e_u^\sigma\|_\infty}{\|e_u^\sigma\|_2}$$

and, from *(i)*,

$$\frac{\phi_n}{\|\phi_n\|_\infty} \int_\Omega u \frac{\phi_n}{\|\phi_n\|_\infty} dx \to \frac{e_u^\sigma}{\|e_u^\sigma\|_\infty} \int_\Omega u \frac{e_u^\sigma}{\|e_u^\sigma\|_\infty} dx$$

uniformly in Ω, it follows from (10) that

$$u_n \to \left(\frac{\|e_u^\sigma\|_\infty}{\|e_u^\sigma\|_2}\right)^2 \frac{e_u^\sigma}{\|e_u^\sigma\|_\infty} \int_\Omega u \frac{e_u^\sigma}{\|e_u^\sigma\|_\infty} dx = \frac{e_u^\sigma}{\|e_u^\sigma\|_2^2} \int_\Omega u e_u^\sigma dx = \frac{e_u^\sigma}{\|e_u^\sigma\|_2^2} \langle u, e_u^\sigma \rangle = e_u^\sigma.$$

Since from (11) we have

$$\frac{\|\phi_n\|_\infty}{\|\phi_{n+1}\|_\infty} = |\lambda_u^\sigma - \sigma| \frac{\|e_u^\sigma + \psi_n\|_\infty}{\|e_u^\sigma + \psi_{n+1}\|_\infty}$$

and thus *(30)* also follows from Lemma 7.

Now, let $\mathcal{K} \subset\subset \operatorname{supp} e_u^\sigma$ be compact so that

$$m := \min_{\mathcal{K}}|e_u^\sigma| > 0$$

and fix $n_0 \in \mathbb{N}$ such that

$$\|\psi_n\|_\infty < \frac{m}{2} \quad \text{for all } n \geqslant n_0.$$

Thus if $n \geqslant n_0$ we have on $\mathcal{K}$

$$|e_u^\sigma + \psi_n| \geqslant |e_u^\sigma| - |\psi_n| \geqslant m - \|\psi_n\|_\infty > \frac{m}{2}.$$

Therefore, the quotient

$$\frac{\phi_n}{\phi_{n+1}} = (\lambda_u^\sigma - \sigma)\frac{e_u^\sigma + \psi_n}{e_u^\sigma + \psi_{n+1}}$$

makes sense on $\mathcal{K}$ for all sufficiently large n and again *(iii)* follows from Lemma 7 since

$$\left|\frac{\phi_n}{\phi_{n+1}} - (\lambda_u^\sigma - \sigma)\right| = |\lambda_u^\sigma - \sigma|\left|\frac{e_u^\sigma + \psi_n}{e_u^\sigma + \psi_{n+1}} - 1\right| = |\lambda_u^\sigma - \sigma|\left|\frac{\psi_n - \psi_{n+1}}{e_u^\sigma + \psi_{n+1}}\right| \leqslant \frac{2|\lambda_u^\sigma - \sigma|}{m}|\psi_n - \psi_{n+1}|. \qquad \square$$

5. Normalization at each step

In order to avoid numerical problems, such as overflow or underflow, it is usual to normalize the right-hand-side function in each inverse iteration. Although this procedure changes the sequence of iterates it maintains convergences.

In fact, let v_n be defined by

$$v_0 = \frac{u}{\|u\|} \quad \text{and} \quad \begin{cases} -\Delta_\sigma v_{n+1} = \frac{v_n}{\|v_n\|} & \text{in } \Omega, \\ v_{n+1} = 0 & \text{on } \partial\Omega. \end{cases} \tag{32}$$

where $\|\cdot\|$ may denote the L^2-norm or the L^∞-norm. Then, since σ is not an eigenvalue of $-\Delta$ it is easy to verify that

$$\phi_{n+1} = \|\phi_n\|v_{n+1}. \tag{33}$$

Hence, for example, if one uses $\|\cdot\| = \|\cdot\|_2$ then

$$\left\langle u, \frac{v_n}{\|v_n\|_2}\right\rangle_2 \frac{v_n}{\|v_n\|_2} = u_n \to e_u^\sigma, \tag{34}$$

both uniformly and in L^2. Note that this sequence is exactly the sequence $\{u_n\}$ defined by (14) and rewritten in terms of the sequence $\{v_n\}$.

Moreover, in view of (33) and (15) one also has

$$\mathcal{R}(v_n) = \mathcal{R}(\phi_n) \to \lambda_u^\sigma. \tag{35}$$

If $\|\cdot\| = \|\cdot\|_\infty$ then one has the following uniform convergence in each compact $\mathcal{K} \subset \{x : e_u^\sigma(x) \neq 0\}$:

$$\frac{v_n}{v_{n+1}} \to \frac{\lambda_u^\sigma - \sigma}{|\lambda_u^\sigma - \sigma|} = \begin{cases} 1 & \text{if } \lambda_u^\sigma > \sigma, \\ -1 & \text{if } \lambda_u^\sigma < \sigma. \end{cases}$$

6. Numerical tests

In this section we present some numerical tests on the unit interval, unit disk and unit square. The inverse iteration with shift was implemented starting from the unit constant function $u \equiv 1$ on these domains. Eigenvalue approximations were computed by running our Algorithm 1 and taking (in the line 9) the following sequences considered in this paper:

$$\mu_n := \frac{\phi_n}{\phi_{n+1}}(x_0) + \sigma, \quad \gamma_n := \frac{\|\phi_n\|_2}{\|\phi_{n+1}\|_2} + \sigma$$

and

$$\mathcal{R}(\phi_n) = \sigma + \frac{\langle\phi_n, \phi_{n-1}\rangle_2}{\|\phi_n\|_2^2}. \tag{36}$$

This last sequence is an alternative form of the Rayleigh quotient evaluated at ϕ_n according to (18). As previously remarked, the numerical advantage of writing the Rayleigh quotient in this form is that one need not compute the gradient $\nabla\phi_n$.

Taking into account (35) we also compute eigenvalue approximations using the sequence $\mathcal{R}(v_n)$ where v_n is defined by (32). Namely, we use the following alternative expression for this sequence:

$$\mathcal{R}(v_n) = \sigma + \frac{\langle v_n, v_{n-1}\rangle_2}{\|v_n\|_2^2}. \tag{37}$$

Notwithstanding the (theoretical) equality $\mathcal{R}(v_n) = \mathcal{R}(\phi_n)$, our tests indicate some remarkable numerical differences between them.

The non-normalization of the function ϕ_n on each step in Algorithm 1 tends to attribute to it smaller values at each iteration. Thus, as a numerical phenomenon, the quotient ϕ_n/ϕ_{n+1} tends to assume the value 1, what makes the sequences μ_n, γ_n and $\mathcal{R}(\phi_n)$ converge to $\sigma + 1$.

This phenomenon may restrict the use of these sequences. However, handled with care by controlling the number of iterations and points in the grid, they can provide good approximations to the eigenvalues, as our numerical tests indicate.

Table 1

Exact and approximated eigenvalues on the unit interval $[0,1]$ obtained from the inverse iteration with shift starting from the unit function. The shift $\sigma_k := \lambda_k - 0.1$ and a grid containing 101 nodes were used.

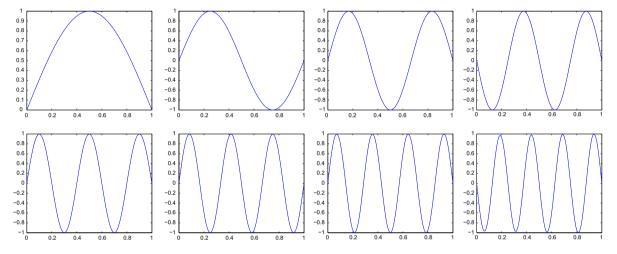| k	λ_k	μ_{10}	γ_{10}	$\mathcal{R}(\phi_{10})$	$\mathcal{R}(\nu_{10})$
1	9.8696	9.8688	9.8688	9.8688	9.8688
2	39.4784	39.4654	39.4654	39.4654	9.8691
3	88.8264	88.7607	88.7607	88.7607	88.7607
4	157.914	157.706	157.921	157.706	89.1623
5	246.740	246.233	247.047	246.233	246.233
6	355.306	354.255	356.157	356.206	252.178
7	483.611	481.665	485.356	481.665	481.665
8	631.655	628.335	634.773	632.555	514.785

Fig. 1. First eight approximated eigenfunctions of the Laplacian on $[0,1]$ obtained from the inverse iteration with shift starting from the unit function.

Table 2

Number N_λ of approximates with relative error of order ϵ for $\sigma_k := 0.99\lambda_k$, grid containing 10,001 points and 30 iterations.

ϵ	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	$\leqslant 10^{-8}$
N_λ	292	1004	156	39	6	3

On the other hand, the sequence $\mathcal{R}(\nu_n)$ seems to be more robust, since we did not observe this phenomenon when using it. Another indication of its numerical stability is its tendency to better capture the correct eigenvalues (i. e. those belonging to the spectrum of the starting function), than the other sequences.

The graphs of the eigenfunction approximations were constructed by using the sequence u_n in (34). In Algorithm 2, these approximations can be viewed as the combination of lines 9 and 10 with ϕ_{n+1}^k replaced by ν_{n+1}^k (normalizing on each step).

To show the efficiency of inverse iteration with shift we used neither the most efficient available method for solving the underlying differential equation nor a fine grid, but one of the most basic methods, finite differences, and a relatively coarse grid. Integrals were computed via the Simpson composite method.

6.1. Eigenvalues and eigenfunctions for the unit interval $[0,1]$

In this case, (8) becomes the following boundary value problem

$$\begin{cases} -\phi_{n+1}'' - \sigma\phi_{n+1} = \phi_n, \\ \phi_{n+1}(0) = \phi_{n+1}(1) = 0. \end{cases}$$

One can verify that $\lambda_k = k^2\pi^2$ and that the function $u \equiv 1$ does not have components corresponding to λ_k for k even.

We present in Table 1 exact and approximated eigenvalues of the Laplacian on the unit interval. The shift was set to the corresponding exact eigenvalue minus 0.1 (that is, $\sigma_k := \lambda_k - 0.1$), and a grid of only 101 nodes was used. As shown in the last column, the sequence $\mathcal{R}(\nu_n)$ seems to capture only the eigenvalues λ_u^σ that appear on the spectral decomposition of the

Table 3
Number N_λ of approximates with relative error of order ϵ for $\sigma_k := 0.5(\lambda_{k+1} + \lambda_k)$, grid containing 10,001 points and 30 iterations.

ϵ	10^{-4}	10^{-5}	10^{-6}	10^{-7}	$\leqslant 10^{-8}$
N_λ	1	66	25	4	4

Table 4
Numbers N_σ of shifts and N_λ of approximates with relative errors of order ϵ. Here σ was randomly chosen on the interval $(0, \lambda_{50})$. A grid containing 10,001 points and 30 iterations were used.

ϵ	$\geqslant 10^{-2}$	10^{-3}	10^{-4}	10^{-5}	10^{-6}	$\leqslant 10^{-7}$
N_σ	38	60	2	0	0	0
N_λ	0	1	2	80	16	1

function $u \equiv 1$. In fact, we note that for even values of k the shift is closer to λ_k than λ_{k-1} and even so the corresponding sequence $\mathcal{R}(v_n)$ converges to λ_{k-1} which is the correct eigenvalue.

In Fig. 1 we present the graphs of the first eight approximated eigenfunctions.

Table 1 also exemplifies the numerical convergence to $\sigma + 1$ of the non-normalized sequence $\mathcal{R}(\phi_n)$, which happened to the approximations of λ_6 and λ_8. For the first one, for example, the closest approximation achieved is $\mathcal{R}(\phi_4) = 280.278$. For $n > 4$ the quotient collapses to one and the result is spurious. In order to compute a correct approximation of this eigenvalue using this sequence, a finer grid should be used.

In Table 2 we show the result of calculating the first 1,500 eigenvalues of the unit interval using the normalized sequence $\mathcal{R}(v_n)$ with 30 iterations and a grid containing 10,001 nodes. The relative error between the computed eigenvalue $\mathcal{R}(v_n)$ and the exact eigenvalue λ is defined by

$$\epsilon(\mathcal{R}(v_n), \lambda) = \left| \frac{\mathcal{R}(v_n) - \lambda}{\lambda} \right|.$$

The shift used to make Table 2 is $\sigma_k := 0.99\lambda_k$, which has an initial relative error of 1%. Such error is huge for great eigenvalues and the interval (σ_k, λ_k) may contain many other eigenvalues. Thus, it is likely to happen that this shift makes the sequence converge to an eigenvalue λ_r different from λ_k. With this in mind, we considered that $\mathcal{R}(v_{30})$ correctly approximated an eigenvalue λ_r if $|\lambda_r - \mathcal{R}(v_{30})| = \min_s |\lambda_s - \mathcal{R}(v_{30})|$, and that $\mathcal{R}(v_{30})$ converged to λ_r if their relative error is less than 10^{-3}.

Table 2 reveals that among the 1,500 shifts used, all of them approximated an eigenvalue with a relative error of order of magnitude 10^{-3}, and that 1,208 converged with a relative error less than 10^{-3}.

Among the 1,208 converged approximations, 547 refer to eigenvalues λ_k with k even. This shows that the sequence $\mathcal{R}(v_n)$ can converge to an eigenvalue that does not belong to the spectrum of the unit function.

In order to better understand convergence of shifts with large initial relative error, we used a grid of 10,001 nodes and 30 iterations of the sequence $\mathcal{R}(v_n)$ with shifts $\sigma_k := 0.5(\lambda_{k+1} + \lambda_k)$, where k runs from 1 to 100. The result is presented in Table 3. As we can see, despite the shift being located exactly between the eigenvalues, only one did not converge to an eigenvalue.

Another numerical experiment using shifts with large initial error was done with randomly chosen shifts. We generated 100 random numbers (shifts) on the interval $(0, \lambda_{50})$ and used a grid of 10,001 nodes and 30 iterations. Table 4 shows the initial relative errors of the shifts, as well as the errors after 30 iterations of sequence $\mathcal{R}(v_n)$. As we can see, only one of these shifts did not converge to an eigenvalue, and most of them converged with a relative error of order 10^{-5}.

6.2. Radial eigenvalues and eigenfunctions for the unit disk

We computed only the radial eigenfunctions for the unit disk $\Omega = \{x \in \mathbb{R}^2 : |x| \leqslant 1\}$. In this case $\phi_n = \phi_n(r)$ where $r = |x|$, and (8) becomes the Sturm–Liouville problem type

$$\begin{cases} -\frac{(r\phi'_{n+1})'}{r} - \sigma\phi_{n+1} = \phi_n, 0 < r < 1, \\ \phi'_{n+1}(0) = 0 = \phi_{n+1}(1). \end{cases}$$

Note that the function $u \equiv 1$ has components in all radial eigenspaces. In fact, if $e = e(r)$ denotes a radial eigenfunction corresponding to an eigenvalue $\lambda > 0$ in Ω then

$$\begin{cases} \Delta_r e = \frac{(re')'}{r} = -\lambda e, 0 < r < 1, \\ e'(0) = 0 = e(1). \end{cases}$$

Therefore,

Table 5
The first eight Laplacian radial eigenvalues on the unit disk obtained from the inverse iteration with shift starting from the unit function.

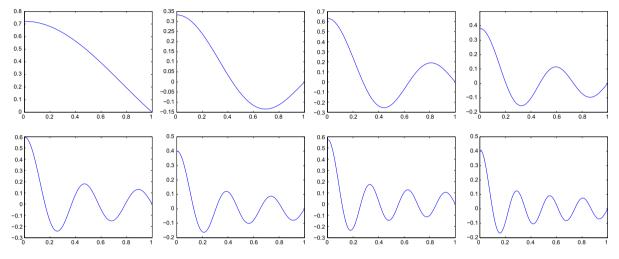| k	λ_k	μ_{10}	γ_{10}	$\mathcal{R}(\phi_{10})$	$\mathcal{R}(v_{10})$
1	5.7831	5.7834	5.7834	5.7392	5.7392
2	30.4713	30.4698	30.4698	30.4396	30.4396
3	74.887	74.865	74.865	74.847	74.847
4	139.040	138.942	138.942	138.942	138.942
5	222.932	222.646	223.018	222.674	222.674
6	326.563	325.901	327.025	325.968	326.563
7	449.934	448.611	451.057	448.729	448.729
8	593.043	590.663	595.223	590.836	590.836

Fig. 2. First eight Laplacian radial eigenfunctions on the unit disk obtained from the inverse iteration with shift.

Table 6
Exact and approximated eigenvalues of the Laplacian on the unit square.

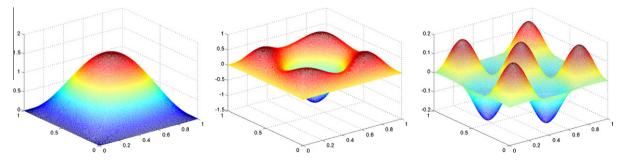| (n,m)	$\lambda_{n,m}$	μ_{10}	γ_{10}	$\mathcal{R}(\phi_{10})$	$\mathcal{R}(v_{10})$
(1,1)	19.7392	19.7388	19.7388	19.7388	19.7388
(1,2)	49.3480	49.3346	49.3446	49.3446	19.8395
(2,2)	78.9568	78.9504	78.9504	78.9504	98.6732
(1,3)	98.6960	98.6796	98.6308	98.6796	98.6796
(2,3)	128.305	128.285	128.285	128.285	98.7042
(3,3)	177.653	177.620	177.620	177.562	177.620

Fig. 3. Graphs of the approximations for the first three projections of the function $u \equiv 1$ on the unit square obtained of the inverse iteration with shift $\sigma_{n,m} := \lambda_{n,m} - 0.1$. $e_u^{\sigma_{1,1}}$ (left), $e_u^{\sigma_{1,3}}$ (center) and $e_u^{\sigma_{3,3}}$ (right).

Table 7
Approximated eigenvalues of the Laplacian on the unit square and relative errors for different grids. The exact eigenvalue is $\lambda_{3,3} = 177.6529$.

Grid	μ_{10}	$\epsilon(\mu_{10}, \lambda_{3,3})$
100×100	177.5187	7.6×10^{-4}
200×200	177.6197	1.9×10^{-4}
300×300	177.6382	8.3×10^{-5}
400×400	177.6446	4.7×10^{-5}
500×500	177.6476	3.0×10^{-5}
1000×1000	177.6516	7.4×10^{-6}
2000×2000	177.6526	1.9×10^{-6}

$$\langle u, 1 \rangle_2 = \int_{|x| \leqslant 1} e(|x|)dx = \int_0^1 \int_{|x|=r} e(r)dS_x dr = 2\pi \int_0^1 e(r)r\,dr = -\frac{2\pi}{\lambda} \int_0^1 (re'(r))'dr = -\frac{2\pi}{\lambda} e'(1) \neq 0$$

because of the uniqueness of the initial value problems for the ODE above at $r = 1$.

We present in Table 5 the exact and approximated first eight radial eigenvalues for the Laplacian on the unit disk, calculated using the shift $\sigma_k := \lambda_k - 0.1$ and a grid containing 201 nodes.

The graphs of the first eight approximated radial eigenfunctions of the Laplacian obtained by our Algorithm 2 are displayed in Fig. 2.

6.3. Unit square

The eigenvalues of the unit square $\Omega = [0, 1] \times [0, 1]$ are $\lambda_{n,m} = (n^2 + m^2)\pi^2$ and the corresponding L^∞-normalized eigenfunctions are $e_{n,m} = \sin(n\pi x)\sin(m\pi x)$. Hence it is easy to verify that the spectrum of the function $u \equiv 1$ consists precisely of those eigenvalues $\lambda_{n,m}$ for which both n and m are odd and that its first three eigenvalues are $\lambda_{1,1}, \lambda_{1,3}$ and $\lambda_{3,3}$. In Table 6 we present exact and approximated eigenvalues of the Laplacian on this domain. The shift was set $\sigma_k := \lambda_k - 0.1$ and a grid containing 201×201 nodes was used. We can see again that the sequence $\mathcal{R}(v_n)$ tends to capture only the eigenvalues λ_u^σ that appear on the spectrum of the function $u \equiv 1$, as shown in the last column. Note that the shift $\sigma_{1,2} := \lambda_{1,2} - 0.1$ is closer to $\lambda_{1,2}$ but, however, the corresponding sequence $\mathcal{R}(v_n)$ approaches the correct eigenvalue $\lambda_{1,1}$. The same behavior happens with the shifts $\sigma_{2,2} := \lambda_{2,2} - 0.1$ and $\sigma_{2,3} := \lambda_{2,3} - 0.1$ since they are closer to $\lambda_{2,2}$ and $\lambda_{2,3}$, respectively, but the corresponding sequences $\mathcal{R}(v_n)$ approach to $\lambda_{1,3}$. The graphs of the first three eigenfunctions in the spectrum of the unit function using Algorithm 2 are displayed in Fig. 3.

In Table 7 we used the sequence μ_n to show the effect of refining the grid. The shift was chosen $\sigma_{3,3} := \lambda_{3,3} - 0.1$ and 10 iterations were used. As expected, a finer grid provides a better approximation of the eigenvalue.

7. Final comments

In finite linear algebra, the iterative process itself is often used in order to generate increasingly better estimates for the eigenvalue at each iteration, meaning that the approximation obtained at any given iteration is used as the shift in the next iteration. It turns out that instead of using the estimates for the eigenvalue obtained in the process, the Rayleigh quotient of the estimates for the eigenvector obtained at each iteration give much better approximations for the eigenvalue. Indeed, if the eigenvalues of the operator or at least very good estimates of them are known in advance, inverse iteration with shift given by the Rayleigh quotient is the standard method for computing eigenvalues due to its cubic rate of convergence (see [2]). It would be only natural to extend such ideas to the Laplacian, but we were not able to do it. Instead, our (admittedly preliminary) numerical tests, not shown in this paper, did not indicate convergence to the correct eigenvalues. As previously discussed, the Rayleigh quotient may not be a good way to approximate the eigenvalue of high frequency eigenfunctions unless the grid is much further refined, due to high oscillations, and the computational cost of using too fine grids can seriously limit the efficiency of the method. Further investigation is needed. So it remains an open problem to us if inverse iteration with shift given by the Rayleigh quotient is a method that can be successfully applied to the Laplacian.

The method described in this paper uses a modification of the Rayleigh quotient that avoids the computation of gradients. Our numerical tests shown in Section 6 indicate a greater degree of convergence to the correct eigenvalues when this form is used. It seems to us that the non-necessity of calculating the gradients makes our algorithm more numerically stable.

The only reference we could find where the Rayleigh quotient was used in computing the eigenvalues of the Laplacian, and only for polygonal domains, was the work [21]; however the Rayleigh quotient was only indirectly used there, as one component of another algorithm and in a very different way from the direct approach we follow here.

Acknowledgments

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