Convergence analysis of Galerkin finite element approximations to shape gradients in eigenvalue optimization

Shengfeng Zhu\(^1\) · Xianliang Hu\(^2\) · Qifeng Liao\(^3\)

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Abstract
This paper concerns the accuracy of Galerkin finite element approximations to two types of shape gradients for eigenvalue optimization. Under certain regularity assumptions on domains, a priori error estimates are obtained for the two approximate shape gradients. Our convergence analysis shows that the volume integral formula converges faster and offers higher accuracy than the boundary integral formula. Numerical experiments validate the theoretical results for the problem with a pure Dirichlet boundary condition. For the problem with a pure Neumann boundary condition, the boundary formulation numerically converges as fast as the distributed type.

Keywords Shape optimization · Shape gradient · Eigenvalue problem · Finite element · Error estimate · Multiple eigenvalue

Mathematics Subject Classification 49Q10 · 65N25 · 65N30

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Shengfeng Zhu
sfzhu@math.ecnu.edu.cn

Xianliang Hu
xlhu@zju.edu.cn

Qifeng Liao
liaoqf@shanghaitech.edu.cn

\(^1\) Department of Data Mathematics and Shanghai Key Laboratory of Pure Mathematics and Mathematical Practice, School of Mathematical Sciences, East China Normal University, Shanghai 200241, China

\(^2\) School of Mathematical Sciences, Zhejiang University, Hangzhou 310027, Zhejiang, China

\(^3\) School of Information Science and Technology, ShanghaiTech University, Shanghai 201210, China

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1 Introduction

Shape optimization has become important and promising in many fields of engineering [12,32,35], e.g., structural mechanics [6], acoustics [29], and computational fluid dynamics [32]. For shape design of practical complex systems, numerical methods such as gradient-type algorithms are usually employed. These include the optimize-then-discretize approach [35] and the discretize-then-optimize approach [6]. They are not equivalent in certain circumstances. For optimize-then-discretize, the so-called Eulerian derivative and the corresponding shape gradient of a shape functional are usually derived by shape sensitivity analysis with respect to domain variations [12,35]. In 1907, Hadamard computed the Eulerian derivative of the first eigenvalue of a clamped plate with $C^\infty$ smooth boundary [16]. Later, a structure theorem was developed by Zolésio for general shape functionals on $C^{\zeta+1}$-domains ($\zeta \geq 0$). By the structure theorem, the Eulerian derivative can be expressed as a boundary integral. This type of Eulerian derivative has attracted much attention in both shape optimization theory [12,35] and existing numerical shape gradient algorithms [32]. However, this Eulerian derivative formula actually fails to hold when the boundary is not smooth enough. In this situation, another general type of Eulerian derivatives expressed as a domain integral can be considered [12]. These two types of Eulerian derivatives are shown to be equivalent through integration by parts if the boundary is regular enough.

For shape gradient computations, numerical approaches such as finite elements, finite differences [39] and boundary element methods [3] are used to solve the state and possible adjoint constraints. The Galerkin finite element method [9] is popular to discretize PDEs in shape optimization [27,37,40,42]. This method based on domain triangulation is a flexible approach for shape representation and shape changes in shape optimization. The accuracy of finite element approximations of shape gradients is essential for implementation of numerical optimization algorithms. Delfour and Zolésio (Remark 2.3 on p. 531 [12]) pointed out that “the boundary integral expression is not suitable since the finite element solution does not have the appropriate smoothness under which the boundary integral formula is obtained”. Pironneau et al. (p. 210 [28]) presented convergence analysis for consistent approximations of boundary shape gradients in linear elliptic problems. Berggren [7] remarked that “the sensitivity information-directional derivatives of objective functions and constraints needs to be very accurately computed in order for the optimization algorithms to fully converge”. Using domain expressions of Eulerian derivatives is promising. Recently, Hiptmair et al. [21] first showed that the Galerkin finite element approximation of shape gradients in the distributed type converges faster and is more accurate than that in the boundary integral for linear elliptic problems. In shape optimization of Stokes flow [43], a priori error estimates were given for mixed finite element approximations to distributed and surface shape gradients. The discretizations of distributed formulations were shown to have higher convergence rates than surface formulations. They were used numerically for shape reconstruction problems [26]. The distributed shape gradients were derived and used for numerical shape optimization algorithms in magnetic induction tomography [20] and parabolic diffusion problems [34], respectively. Boundary shape gradients are popular when combined with level set methods for shape optimization [11,27,29]. Recently, the volume type Eulerian derivative was
also incorporated numerically into the level set method for shape and topology optimization [25]. In [23], an eigenvalue optimization problem was transformed to be an optimal control problem and a priori error estimates were obtained after finite element discretizations.

In this paper, we prove the convergence of Galerkin finite element approximations for shape gradients in eigenvalue optimization. Our motivation arises from the following aspects. First, eigenvalue problems in optimal shape design have fundamental importance for science and engineering, especially in structural mechanics [2,6,12,19,33,35,39]. Second, finite element approximations to shape gradients of eigenvalues in boundary formulations are widely used for numerical algorithms in eigenvalue optimization [2,3,12,19,29,30,35]. Moreover, numerical results in [41] show the potential advantages for using the new volume type of shape gradients in algorithms for shape optimization of simple and multiple Laplace eigenvalue problems. In this paper, we provide a theoretical analysis for numerical algorithms of [41]. For both Dirichlet and Neumann Laplace eigenvalue problems [3,10,19,22,30], we prove the convergence of the finite element approximations to shape gradients in both boundary and volume formulations. Novel a priori error estimates are developed in an infinite-dimensional operator norm. Numerical results are presented to verify the convergence of shape gradient approximations.

The rest of the paper is organized as follows. In the next section, a priori error estimates for finite element approximations of Laplace eigenvalue problems with Dirichlet and Neumann boundary conditions are developed, and shape calculus is introduced to give the Eulerian derivatives of eigenvalues in the forms of boundary and volume integrals. Our novel a priori convergence analysis of the finite element approximations to shape gradients in boundary and volume formulations is presented in Sect. 3. Numerical results are discussed in Sect. 4.

2 Problem formulation

Let $\Omega$ be a bounded domain in $\mathbb{R}^d$ ($d = 2, 3$) with a Lipschitz continuous boundary $\partial \Omega$. We consider the Laplace eigenvalue problem:

\[
\begin{cases}
-\Delta u = \lambda u & \text{in } \Omega \\
u = 0 \quad \text{or} \quad \frac{\partial u}{\partial n} = 0 & \text{on } \partial \Omega,
\end{cases}
\]

where $\Delta = \sum_{i=1}^{d} \partial^2 / \partial x_i^2$ is the Laplacian operator. In $\mathbb{R}^2$, the homogeneous Dirichlet boundary condition and the homogeneous Neumann boundary condition physically correspond to vibrating planar membranes being fixed and free, respectively.

We start with introducing notations on Sobolev spaces following [1]. For $1 \leq p \leq \infty$, the Banach space $L^p(\Omega)$ consists of measurable functions $v$ such that the associated norm $\|v\|_{L^p(\Omega)} < \infty$. For each integer $m \geq 0$, the Banach space is equipped with the norm $\|\cdot\|_{W^{m,p}(\Omega)}$. In particular, when $p = 2$, we write $H^m(\Omega)$ instead of $W^{m,2}(\Omega)$ and $\|\cdot\|_{H^m(\Omega)}$ instead of $\|\cdot\|_{W^{m,2}(\Omega)}$. Note that $H^m(\Omega)$ is indeed a Hilbert space with respect to the inner product $(w, v)_{H^m(\Omega)} := \sum_{|\alpha| \leq m} (D^\alpha w, D^\alpha v)$ with
\((\cdot, \cdot)\) being the usual \(L^2\) inner product. Let \(W_0^{m,p}(\Omega)\) denote the closure of \(C_0^\infty(\Omega)\) with respect to the norm \(\|\cdot\|_{W^{m,p}(\Omega)}\). We write \(H_0^m(\Omega)\) instead of \(W_0^{m,2}(\Omega)\) when \(p = 2\). For simplicity, we use the same notations for Sobolev norms of vector-valued and scalar functions.

The variational formulation of (1) is to find \(\lambda \in \mathbb{R}, 0 \neq u \in V\) such that [5]
\[
(\nabla u, \nabla v) = \lambda (u, v) \quad \forall v \in V,
\]
where \(V\) refers to \(H^1_0(\Omega)\) when considering the pure homogeneous Dirichlet boundary condition and it refers to \(\{v \in H^1(\Omega) | \int_{\Omega} v dx = 0\}\) when considering the pure homogeneous Neumann boundary condition. Due to the positiveness, self-adjointness and the compactness of the inverse of negative Laplacian operator, there exists a sequence of eigenpairs \(\{\lambda_i, u_i\}_{i=0}^\infty\) for (2) with eigenvalues
\[
0 < \lambda_1 \leq \lambda_2 \leq \cdots \nearrow +\infty
\]
and corresponding normalized eigenfunctions \(u_1, u_2, \ldots\) satisfying
\[
(u_i, u_j) = \delta_{ij},
\]
where \(\delta_{ij}\) is the Kronecker delta. Note that when the pure homogeneous Neumann boundary condition is applied, \(\lambda_1 \geq 0\).

### 2.1 A priori error estimates for Laplace eigenvalue problems

We consider the standard Ritz-Galerkin finite element method [9] to discretize the variational formulation (2). For the shape gradient deformation algorithm discussed in this paper, the domain \(\Omega\) at each iteration step is assumed to be a polygon/polyhedron, such that there is no geometric error introduced for the domain triangulation.

**Remark 1** For Dirichlet Laplace eigenvalue problems posed on planar polygonals (see Remark 4.2 [5]), we have the following regularity result similar to the results for linear elliptic problems in [15]. Let \(\omega\pi (0 < \omega \leq 2)\) be the maximal interior angle of the vertices of \(\Omega\). Then, any eigenfunction satisfies
\[
u \in H^r(\Omega) \cap H^1_0(\Omega) \quad \text{with} \quad 1 < r < 1 + \frac{1}{\omega},
\]
i.e., \(r\) can be \(1 + \frac{1}{\omega} - \epsilon\) for any small \(\epsilon > 0\). If \(\Omega\) is a convex polygon, then \(\nu \in H^2(\Omega)\).

Consider a family of triangulations \(\{\mathcal{T}_h\}_{h>0}\) satisfying that \(\mathcal{B} = \bigcup_{K \in \mathcal{T}_h} K\), where the mesh size is denoted by \(h := \max_{K \in \mathcal{T}_h} h_K\) with \(h_K := \text{diam}\{K\}\) for any \(K \in \mathcal{T}_h\). Let \(\{V_h\}_{h>0}\) be a family of finite-dimensional subspaces of \(H^1_0(\Omega)\). For the linear Lagrange elements, letting \(\mathbb{P}_1(K)\) denote the set of piecewise linear polynomials on \(K\), we define \(V_h := \{v_h \in C^0(\Omega) \cap H^1_0(\Omega) : v_h|_K \in \mathbb{P}_1(K) \forall K \in \mathcal{T}_h\}\) for the pure Dirichlet problem, and \(V_h = \{v_h \in C^0(\mathcal{B}) : v_h|_K \in \mathbb{P}_1(K) \forall K \in \mathcal{T}_h, \int_{\Omega} v_h dx = 0\}\).
Convergence analysis of Galerkin finite element... for the pure Neumann problem. For $0 < s \leq 1$, we define $r := 1 + s$. Throughout this paper, we denote by $C$ a general constant, which may differ at different occurrences and may depend on the mesh aspect ratio and the shape of $\Omega$, but it is always independent of the eigenfunctions and the mesh size $h$. We assume that the mesh family $\{T_h\}_{h>0}$ is regular so that the following approximation property holds [9]:

$$\inf_{v_h \in V_h} (\|u - v_h\|_{L^2(\Omega)} + h\|\nabla u - \nabla v_h\|_{L^2(\Omega)}) \leq Chr |u|_{H^{r}(\Omega)} \forall u \in H^{r}(\Omega). \quad (5)$$

Suppose that the mesh is quasi-uniform so that the inverse inequality holds (see e.g. Theorem 4.5.11 [9]). The weak formulation for conforming finite element approximation of the problem (2) reads: find $\lambda_h \in \mathbb{R}$ and $0 \neq u_h \in V_h$ such that

$$(\nabla u_h, \nabla v_h) = \lambda_h (u_h, v_h) \quad \forall v_h \in V_h. \quad (6)$$

For (6), there exist a finite sequence of eigenvalues

$$0 < \lambda_{1,h} \leq \lambda_{2,h} \leq \cdots \leq \lambda_{N,h}, \quad N = \dim V_h,$$

and corresponding normalized eigenvectors

$$u_{1,h}, u_{2,h} \cdots u_{N,h},$$

with

$$(u_{i,h}, u_{j,h}) = \delta_{ij}. \quad (7)$$

For $i = 1, 2, \ldots$, we suppose that $k_i$ is the lowest index of the $i$th distinct eigenvalue of (2) with $l_i$ being its multiplicity, i.e.,

$$\lambda_{k_i-1+l_i-1-1} = \lambda_{k_i-1} < \lambda_{k_i} = \lambda_{k_i+1} = \cdots = \lambda_{k_i+l_i-1} < \lambda_{k_i+l_i} = \lambda_{k_i+1}.$$

We have the following a priori error estimates on approximate eigenvalues and eigenfunctions.

**Lemma 1** Assume that $\Omega$ is a polygon/polyhedron and $\{T_h\}_{h>0}$ are quasi-uniform. Let $(\lambda_{k_i+j-1,h}, u_{k_i+j-1})$ and $(\lambda_{k_i+j-1-1,h}, u_{k_i+j-1,h})$ be eigenpairs of (2) and (6) respectively with $u_{k_i+j-1} \in H^{1+s}(\Omega) \ (0 < s \leq 1)$. Then,

$$\lambda_{k_i+j-1} \leq \lambda_{k_i+j-1,h} \leq \lambda_{k_i+j-1} + Ch^{2s}|u_{k_i+j-1}|_{H^{1+s}(\Omega)},$$

and $u_1, u_2, \ldots$ can be chosen so that (7) holds and

$$\|u_{k_i+j-1} - u_{k_i+j-1,h}\|_{L^2(\Omega)} + h\|\nabla u_{k_i+j-1} - \nabla u_{k_i+j-1,h}\|_{L^2(\Omega)} \leq Ch^{1+s}|u_{k_i+j-1}|_{H^{1+s}(\Omega)},$$

$$\|\nabla u_{k_i+j-1} - \nabla u_{k_i+j-1,h}\|_{H^{-s}(\Omega)} \leq Ch^{2s}|u_{k_i+j-1}|_{H^{1+s}(\Omega)},$$

where $j = 1, 2, \ldots, q_i$ with $i = 1, 2, \ldots$. 

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Proof By combining (3.25) [24] and Theorem 5.1 [4], we obtain the first two a priori error estimates above. To prove the last inequality, we first have

\[
\| \nabla u - \nabla u_h \|_{H^{-1}(\Omega)} = \sup_{0 \neq v \in H^1_0(\Omega)^d} \frac{\langle \nabla u - \nabla u_h, v \rangle}{\|v\|_{H^1(\Omega)}} \\
= \sup_{0 \neq v \in H^1_0(\Omega)^d} \frac{(u - u_h, \text{div} v)}{\|v\|_{H^1(\Omega)}} \\
\leq \|u - u_h\|_{L^2(\Omega)} \sup_{0 \neq v \in H^1_0(\Omega)^d} \frac{\|\text{div} v\|_{L^2(\Omega)}}{\|v\|_{H^1(\Omega)}} \\
\leq C \|u - u_h\|_{L^2(\Omega)} \\
\leq C h^2 |u|_{H^2(\Omega)} \quad \text{for} \quad u \in H^2(\Omega),
\]

where we have omitted the subscript \(k_i + j - 1\) for notational simplicity. On the other hand,

\[
\| \nabla u - \nabla u_h \|_{L^2(\Omega)} \leq C |u|_{H^1(\Omega)} \quad \text{for} \quad u \in H^1(\Omega).
\]

Using the operator interpolation theorem (Lemma 22.3 [36]) to (8) and (9), we have

\[
\| \nabla u - \nabla u_h \|_{H^{-s}(\Omega)} \leq C h^2 |u|_{H^{1+s}(\Omega)} \quad \text{for} \quad u \in H^{1+s}(\Omega), \quad 0 \leq s \leq 1.
\]

Note that this Lemma includes results for the special case of simple eigenvalues, i.e., \(l_i = 1\). In the following, we omit the index number for a specific eigenvalue and eigenfunction for simplicity. Let \((\lambda, u)\) and \((\lambda_h, u_h)\) be eigenpairs of (2) and (6), respectively.

**Lemma 2** Assume that \(\Omega\) is a convex polygon/polyhedron. Then,

\[
\| \nabla (P_h u - u_h) \|_{L^2(\Omega)} \leq C h^2 |u|_{H^2(\Omega)}.
\]

**Proof** Let us first define the Ritz projection \(P_h : H^1_0(\Omega) \to V_h\) such that for \(w \in H^1_0(\Omega)\),

\[
(\nabla P_h w, \nabla v_h) = (\nabla w, \nabla v_h) \quad \forall v_h \in V_h.
\]

We take \(v_h = P_h u - u_h\) in (2), (6) and (10). Then, we have

\[
(\nabla (P_h u - u_h), \nabla (P_h u - u_h)) = (\lambda u - \lambda_h u_h, P_h u - u_h) \\
= (\lambda(u - u_h) + (\lambda - \lambda_h)u_h, P_h u - u_h).
\]
Then, by the Cauchy-Schwarz inequality and triangle inequality,
\[
\|\nabla (P_h u - u_h)\|_{L^2(\Omega)}^2 \leq (\lambda \|u - u_h\|_{L^2(\Omega)} + |\lambda - \lambda_h| \|u_h\|_{L^2(\Omega)}) \|P_h u - u_h\|_{L^2(\Omega)}
= (\lambda \|u - u_h\|_{L^2(\Omega)} + |\lambda - \lambda_h|) \|P_h u - u_h\|_{L^2(\Omega)}
\leq C (\lambda \|u - u_h\|_{L^2(\Omega)} + |\lambda - \lambda_h|) \|\nabla (P_h u - u_h)\|_{L^2(\Omega)},
\]
where the Poincaré inequality is used in the last inequality. Therefore,
\[
\|\nabla (P_h u - u_h)\|_{L^2(\Omega)} \leq C (\lambda \|u - u_h\|_{L^2(\Omega)} + |\lambda - \lambda_h|) \leq C \lambda \|u - u_h\|_{L^2(\Omega)} + |\lambda - \lambda h| \|u_h\|_{L^2(\Omega)}.
\]
Using Lemma 1 and the fact on regularity that \(u \in H^2(\Omega)\) [8] due to convexity of \(\Omega\).

Lemma 3 Assume that \(u \in W^{2,4}(\Omega)\). Then,
\[
\|\nabla u - \nabla u_h\|_{L^4(\Omega)} \leq Ch |u|_{W^{2,4}(\Omega)}.
\]

Proof By the triangle inequality, we have
\[
\|\nabla u - \nabla u_h\|_{L^4(\Omega)} \leq \|\nabla u - \nabla P_h u\|_{L^4(\Omega)} + \|\nabla P_h u - \nabla u_h\|_{L^4(\Omega)}.
\]
By (8.5.4) on p. 230 [9] and the approximation property (4.4.28) on p. 110 [9],
\[
\|\nabla u - \nabla P_h u\|_{L^4(\Omega)} \leq C \inf_{v \in V_h} \|\nabla u - \nabla v\|_{L^4(\Omega)} \leq Ch |u|_{W^{2,4}(\Omega)},
\]
By the inverse inequality (4.5.12) on p. 112 [9] and Lemma 2, we have
\[
\|\nabla P_h u - \nabla u_h\|_{L^4(\Omega)} \leq C h^{-\frac{d}{4}} \|\nabla P_h u - \nabla u_h\|_{L^2(\Omega)} \leq Ch^{2-\frac{d}{4}} |u|_{H^2(\Omega)}.
\]
Combining (13), (14) and (15) gives (12).

2.2 Shape sensitivity analysis

As a tool in shape optimization, shape calculus/shape sensitivity analysis can be performed by the velocity (speed) method [12,35] and the perturbation of identity method [32]. These two approaches are equivalent in the sense of the first-order expansion with respect to domain perturbations. We review basic shape calculus using the speed method (Sec. 2.9, pp. 54 and 98 of [35]).

For a variable \(t \in [0, \tau)\) with \(\tau > 0\), we introduce a velocity field \(\mathcal{V}(t, x) \in C([0, \tau]; \mathcal{G}^1(\mathbb{R}^d, \mathbb{R}^d))\) with \(\mathcal{G}^1(\mathbb{R}^d, \mathbb{R}^d)\) denoting the space of continuously differentiable transformations of \(\mathbb{R}^d\). Then, we define a family of transformations \(T_t : \Omega \rightarrow \Omega_t\)
with $\Omega_t = T_t(\mathcal{V})(\Omega)$. For $x = x(t, X) \in \Omega_t$ with $X \in \Omega$, it satisfies the following flow system

$$\frac{dx}{dt}(t, X) = \mathcal{V}(t, x(t, X)), \ x(0, X) = X.$$  \hspace{1cm} (16)

For some domain $\Omega$, a shape functional depending on the shape is denoted by $J(\Omega)$ with $J(\cdot) : \Omega \mapsto \mathbb{R}$. We denote $\mathcal{V} = \mathcal{V}(0, X)$ in the following for simplicity.

**Definition 1** The Eulerian derivative of $J(\Omega)$ at $\Omega$ in the direction $\mathcal{V}$ is defined by

$$dJ(\Omega; \mathcal{V}) := \lim_{t \searrow 0} \frac{J(\Omega_t) - J(\Omega)}{t}$$  \hspace{1cm} (17)

if the limit exists [12].

**Definition 2** The shape functional $J(\Omega)$ is called shape differentiable at $\Omega$ if (i) there exist Eulerian derivatives for all directions $\mathcal{V}$; (ii) the map $\mathcal{V} \rightarrow dJ(\Omega; \mathcal{V})$ is linear and continuous from $C([0, \tau]; \mathcal{D}^1(\mathbb{R}^d, \mathbb{R}^d))$ to $\mathbb{R}$.

**Definition 3** The material derivative in some Sobolev space $W(\Omega)$ of a state variable $u = u(\Omega) \in W(\Omega)$ in a direction $\mathcal{V}$ is denoted as

$$\dot{u}(\Omega; \mathcal{V}) := \lim_{t \searrow 0} \frac{u(\Omega_t) \circ T_t(\mathcal{V})(\Omega) - u(\Omega)}{t}$$  \hspace{1cm} (18)

if the limit exists.

When considering the strong convergence in $W(\Omega)$ for the limit, the material derivative is specified by the strong derivative; when considering the weak convergence, it is specified by the weak derivative. In addition, material derivatives on the boundary $\partial \Omega$ can be defined analogously.

We remark that there may exist non-differentiable cases, e.g., when the Eulerian derivative exists but the mapping $\mathcal{V} \mapsto dJ(\Omega; \mathcal{V})$ is nonlinear. Such cases occur for the shape functionals of multiple eigenvalues.

The structure theorem [11, Corollary 1, p. 480] states that the boundary Eulerian derivative of shape functional only depends on the normal part of the velocity on the boundary when certain smoothness of the boundary is satisfied. The volume formulation of Eulerian derivatives actually holds with less smoothness requirement on boundary [25] and offers more accuracy [21], compared with the boundary formulation.

In shape optimization associated with eigenvalue problems, the usual objective is to minimize/maximize certain eigenvalue subject to a volume constraint [3,10,19,22,30]. By the speed method, we can obtain the Eulerian derivatives of simple and multiple eigenvalues for both Dirichlet and Neumann boundary conditions. We denote $\mathcal{V}_n =$
\(\nabla (0) \cdot n\). The Eulerian derivative of an eigenvalue \(\lambda = \lambda(\Omega)\) (depending on \(\Omega\)) in the direction \(\Psi\) is defined to be

\[
d\lambda(\Omega; \Psi) := \lim_{t \rightarrow 0} \frac{\lambda(\Omega_t) - \lambda(\Omega)}{t}. \tag{19}
\]

**Proposition 1** Let \((\lambda, u)\) be an eigenpair of the problem (2). Assume that \(\lambda\) is simple. Then, \(\lambda(\Omega)\) is shape differentiable and can be written as

\[
d\lambda(\Omega; \Psi) = \int_{\Omega} \left[-2 \nabla u \cdot D\Psi \nabla u + \text{div} \Psi (|\nabla u|^2 - \lambda u^2)\right] dx, \tag{20}
\]

where \(D\Psi\) denotes the Jacobian of \(\Psi\). If, furthermore, \(\Omega\) is convex or if it is of class \(C^2\), then the boundary Eulerian derivative of Dirichlet eigenvalue is

\[
d\lambda(\Omega; \Psi) = -\int_{\partial\Omega} \left(\frac{\partial u}{\partial n}\right)^2 \Psi_n ds. \tag{21}
\]

If \(\Omega\) is of class \(C^3\) for the Neumann case, then the boundary Eulerian derivative is

\[
d\lambda(\Omega; \Psi) = \int_{\partial\Omega} \left(|\nabla \Gamma u|^2 - \lambda u^2\right) \Psi_n ds, \tag{22}
\]

where the tangential gradient \(\nabla \Gamma u\) is defined as

\[
\nabla \Gamma u := \nabla u - \frac{\partial u}{\partial n} n.
\]

**Proof** Closely following [19] and Section 4.2 of Chapter 10 [12] on the first Dirichlet eigenvalue, we give a heuristic and formal derivation for self-containedness of the paper. We only consider the Dirichlet case for simplicity. The results for the Neumann case can be derived similarly. The variational formulation on \(\Omega_t\) is to find \(\lambda(\Omega_t) \in \mathbb{R}\), \(0 \neq u(\Omega_t) \in H^1_0(\Omega_t)\) such that

\[
\int_{\Omega_t} \nabla u(\Omega_t) \cdot \nabla v dx = \lambda(\Omega_t) \int_{\Omega_t} u(\Omega_t) v dx \quad \forall v \in C_0^\infty(\Omega_t). \tag{23}
\]

From (23) and (2), for all \(\psi = v \circ T_t \in C_0^\infty(\Omega)\), we have

\[
\int_{\Omega_t} \lim_{t \rightarrow 0} (B(t) \nabla (u(\Omega_t) \circ T_t) - \nabla u) \cdot \nabla \psi dx = \int_{\Omega_t} \lim_{t \rightarrow 0} \left(\lambda(\Omega_t) \omega(t) u(\Omega_t) - \lambda(\Omega) u(\Omega)\right) \psi dx,
\]

where

\[
B(t) = \omega(t) D T_t^{-1} D T_t^{-T}.
\]
with \( \omega(t) := \det(\mathbf{D}T_t) \). The product rule for differentiation yields
\[
\int_\Omega (B'(0) \nabla u + \nabla \dot{u}) \cdot \nabla \psi \, dx = \int_\Omega \left( d\lambda(\Omega; \mathbf{v}')u + \lambda \dot{u} + \lambda u \text{div} \mathbf{v}' \right) \psi \, dx, \tag{24}
\]
where
\[
B'(0) = \text{div} \mathbf{v}' I - D \mathbf{v}' - (D \mathbf{v}')^T
\]
with \( I \in \mathbb{R}^{d \times d} \) being the identity operator. Choosing \( \psi = u \) in (24), we have
\[
\int_\Omega (B'(0) \nabla u \cdot \nabla u + \nabla \dot{u} \cdot \nabla u) \, dx = \int_\Omega \left( d\lambda(\Omega; \mathbf{v}')u^2 + \lambda u \dot{u} + \lambda u^2 \text{div} \mathbf{v}' \right) \, dx. \tag{25}
\]
Then,
\[
\int_\Omega u^2(\Omega_t) \, dx = 1 \tag{26}
\]
corresponding to (4). Taking the derivative with respect to \( t \) at 0, we get
\[
\int_\Omega 2u\dot{u} \, dx + \int_\Omega u^2 \text{div} \, dx = 0. \tag{27}
\]
Based on (4) and (27), (25) implies that
\[
d\lambda(\Omega; \mathbf{v}') = \int_\Omega (B'(0) \nabla u \cdot \nabla u + \nabla u \cdot \nabla \dot{u} + \lambda u \dot{u}) \, dx. \tag{28}
\]
On the other hand, \( \dot{u} = 0 \) on \( \partial \Omega \) since \( u(\Omega_t) \) vanishes \( \partial \Omega_t \). Thus, \( \dot{u} \in H^1_0(\Omega) \) if \( u \in H^1_0(\Omega) \). Taking \( v = \dot{u} \) in (2), we obtain
\[
\int_\Omega \nabla u \cdot \nabla \dot{u} \, dx = \lambda \int_\Omega u \dot{u} \, dx. \tag{29}
\]
A combination of (27), (28) and (29) yields the result (20).

If, furthermore, \( \Omega \) is convex or if it is of class \( C^2 \), then \( u \in H^2(\Omega) \cap H^1_0(\Omega) \) [5]. We can simplify the volume integral expression (20) as a boundary integral expression (21). Taking \( v = u \) in the identity from vector calculus, we have
\[
\mathbf{v}' \cdot \nabla (\nabla u \cdot \nabla v) + \nabla u \cdot (D \mathbf{v}' + (D \mathbf{v}')^T) \nabla v = \nabla (\mathbf{v}' \cdot \nabla u) \cdot \nabla v + \nabla u \cdot \nabla (\mathbf{v}' \cdot \nabla v),
\]
and Eq. (20) then implies

\[
\mathrm{d} \lambda(\Omega; \mathcal{V}) = \int_{\Omega} \left( \nabla \cdot \nabla (|\nabla u|^2) - 2 \nabla (\nabla \cdot \nabla u) \cdot \nabla u + \text{div} \mathcal{V} (|\nabla u|^2 - \lambda u^2) \right) \, dx \\
= \int_{\Omega} \left( \text{div}(|\nabla u|^2 \mathcal{V}) - 2 \nabla (\nabla \cdot \nabla u) \cdot \nabla u - \lambda \text{div} \mathcal{V} u^2 \right) \, dx. \tag{30}
\]

By Green’s theorem, we have

\[
\mathrm{d} \lambda(\Omega; \mathcal{V}) = \int_{\partial \Omega} \left( \left| \nabla u \right|^2 \mathcal{V}_n \, ds - 2 \nabla \cdot \nabla \mathcal{V} \frac{\partial u}{\partial n} \right) \, ds + \int_{\Omega} \left( 2 \nabla \cdot \nabla u \Delta u - \lambda \text{div} \mathcal{V} u^2 \right) \, dx \\
= -\int_{\partial \Omega} \left( \left| \nabla u \right|^2 \mathcal{V}_n \, ds - \lambda \int_{\partial \Omega} \text{div}(u^2 \mathcal{V}) \, ds \right) \\
= -\int_{\partial \Omega} \left( \left| \nabla u \right|^2 \mathcal{V}_n \, ds - \lambda \int_{\partial \Omega} u^2 \mathcal{V}_n \, ds \right),
\]

which gives (21) since \( u \) vanishes on \( \partial \Omega \). \( \square \)

When \( u \) is sufficiently regular, the expression (20) is consistent with the results in [19] (Theorem 2.5.1 and Theorem 2.5.7 in [19]):

\[
\mathrm{d} \lambda(\Omega; \mathcal{V}) = \begin{cases} 
-\int_{\Omega} \text{div}(|\nabla u|^2 \mathcal{V}) \, dx & \text{for the Dirichlet problem,} \\
\int_{\Omega} \text{div}(|\nabla u|^2 - \lambda u^2) \mathcal{V} \, dx & \text{for the Neumann problem.} 
\end{cases} \tag{31}
\]

We note that (31) cannot be used for discretization in general—the usual \( C^0 \) Lagrange finite element discretization of (31) fails to hold, since \( \nabla u_h \) is not continuously differentiable. We thus consider (20) for discretization.

For the multiple eigenvalue case, we simplify \( \lambda_{ki} \) as \( \lambda \) and let \( u_i (i = 1, 2, \ldots, l) \) be its eigenfunctions satisfying (4). In this situation, while \( \lambda \) is no longer shape differentiable, two alternative strategies can be considered: the sub-differential and directional derivatives [19,33,35]. We adopt the latter one following the derivations of directional derivatives for the Dirichlet problem as in Theorem 2.5.8 of [19]. Then we can have the following results for both boundary conditions:

**Proposition 2** Assume that \( \lambda = \lambda(\Omega) \) is a multiple eigenvalue of order \( l \geq 2 \) for (1) with the homogeneous Dirichlet boundary condition. Letting \( u_1, u_2, \ldots, u_l \) be an \( L^2 \)-orthonormal basis of the eigenspace associated with \( \lambda \), the Eulerian derivative is one of the eigenvalues of the matrix \( \mathcal{M} \in \mathbb{R}^{l \times l} \) with each entry defined as

\[
m_{i,j} = \int_{\Omega} \left[ - (D^2 \mathcal{V} + D \nabla \mathcal{V}) \nabla u_i \cdot \nabla u_j + \text{div} \mathcal{V} (\nabla u_i \cdot \nabla u_j - \lambda u_i u_j) \right] \, dx. \tag{32}
\]
If, furthermore, \( \Omega \) is convex or if it is of class \( C^2 \), then we have

\[
m_{i,j} = -\int_{\partial \Omega} \frac{\partial u_i}{\partial n} \frac{\partial u_j}{\partial n} \mathcal{V}_n ds. \tag{33}
\]

For the Neumann problem,

\[
m_{i,j} = \int_{\Omega} \left[ - (D\mathcal{V} + D\mathcal{V}^T) \nabla u_i \cdot \nabla u_j + \text{div} \mathcal{V} (\nabla u_i \cdot \nabla u_j - \lambda u_i u_j) \right] dx. \tag{34}
\]

If \( \Omega \) is of class \( C^3 \), then

\[
m_{i,j} = \int_{\partial \Omega} (\nabla \Gamma u_i \cdot \nabla \Gamma u_j - \lambda u_i u_j) \mathcal{V}_n ds. \tag{35}
\]

with \( i, j = 1, \ldots, l \).

**Proof** The results for the case of Neumann boundary condition can follow similar clue as the those for the Dirichlet case. We can obtain (33) from (32) by Gauss’s formula. What left is to prove (32). We first refer [17] for details to prove differentiability of eigenvalues (Theorem 2 [17]), whose proof is rather technical and involves the use of the resolvent in the complex plane and the Dunford integral representation of the spectral projector. Then, explicit computation for sensitivity analysis is needed (Corollary 2 [17]). \( \square \)

### 3 A priori error estimates of approximate shape gradients in Eulerian derivatives

With the Galerkin finite element method to discretize the Laplace eigenvalue problem, we compute the approximate Eulerian derivatives and resulting shape gradients. We analyze the convergence rates with a priori error estimates in an infinite-dimensional operator norm. For simplicity, we only discuss the Dirichlet problem. The results below however can be similarly extended to the Neumann problem. The simple eigenvalue case is discussed in Sect. 3.1, while the multiple eigenvalue case is discussed in Sect. 3.2. In order to distinguish notations for the boundary and volume type Eulerian derivatives, we denote (20) and (21) by \( d\lambda(\Omega; \mathcal{V})_\Omega \) and \( d\lambda(\Omega; \mathcal{V})_{\partial \Omega} \), respectively. The finite element approximations of (20) and (21) then read respectively:

\[
d\lambda(\Omega; \mathcal{V})_{\Omega,h} := \int_{\Omega} \left[ - 2\nabla u_h \cdot D\mathcal{V} \nabla u_h + \text{div} \mathcal{V} (|\nabla u_h|^2 - \lambda_h u_h^2) \right] dx \tag{36}
\]

and

\[
d\lambda(\Omega; \mathcal{V})_{\partial \Omega,h} := -\int_{\partial \Omega} \left( \frac{\partial u_h}{\partial n} \right)^2 \mathcal{V}_n ds. \tag{37}
\]
In the continuous setting, \( d\lambda(\Omega; \mathcal{V}) = d\lambda(\Omega; \mathcal{V})_{\partial\Omega} \) if \( \partial\Omega \) is \( C^2 \). With \((\lambda, u)\) discretized by finite elements, we have \( d\lambda(\Omega; \mathcal{V})_{\Omega, h} \neq d\lambda(\Omega; \mathcal{V})_{\partial\Omega, h} \).

For the case of multiple eigenvalues, the matrices associated with (32) and (33) are denoted by \( \mathcal{M}_\Omega \) and \( \mathcal{M}_{\partial\Omega} \) respectively, and the eigenvalues of \( \mathcal{M}_\Omega \) and \( \mathcal{M}_{\partial\Omega} \) are denoted by \( \{\sigma_{\Omega, i}\}_{i=1}^{l} \) and \( \{\sigma_{\partial\Omega, i}\}_{i=1}^{l} \) respectively. The approximations of (32) and (33) are

\[
m_{i,j}^h(\Omega; \mathcal{V}) := \int_\Omega \left[ - (D\mathcal{V} + D\mathcal{V}^T) \nabla u_{i,h} \cdot \nabla u_{j,h} + \text{div}\mathcal{V}(\nabla u_{i,h} \cdot \nabla u_{j,h} - \lambda u_{i,h} u_{j,h}) \right] dx \tag{38}
\]

and

\[
m_{i,j}^h(\Omega; \mathcal{V})_{\partial\Omega} := - \int_{\partial\Omega} \frac{\partial u_{i,h}}{\partial n} \frac{\partial u_{j,h}}{\partial n} \mathcal{V}_n ds \tag{39}
\]

with \( i, j = 1, 2, \ldots, l \). The corresponding matrices associated with (38) and (39) are denoted by \( \mathcal{M}_h^\Omega \) and \( \mathcal{M}_h^{\partial\Omega} \) respectively, and the eigenvalues of \( \mathcal{M}_h^\Omega \) and \( \mathcal{M}_h^{\partial\Omega} \) are denoted by \( \{\sigma_{\Omega, i}^h\}_{i=1}^{l} \) and \( \{\sigma_{\partial\Omega, i}^h\}_{i=1}^{l} \) respectively.

For each simple/multiple eigenvalue case, a priori error estimates are presented for two kinds (volume and boundary) of finite element approximations of Eulerian derivatives and corresponding shape gradients. We first consider the case of simple eigenvalues and next consider the case of multiple eigenvalues.

**Remark 2** The domain \( \Omega \) is usually assumed to be polyhedral in standard shape gradient algorithms, so that no geometric error is introduced during triangulations. In our convergence analysis of approximate Eulerian derivatives, the geometric approximation error is not considered. When the domain is smooth (e.g., \( C^2 \)), we assume that the geometric errors can be negligible by using isoparametric finite elements or sufficiently fine meshes on boundaries, so that boundary formulas of Eulerian derivatives hold.

### 3.1 Simple eigenvalue case

For the continuous formulas (20) and (21), we present convergence analysis of the approximate Eulerian derivatives with the volume integral (36) and the boundary integral (37), respectively. For the volume type, we have

**Theorem 1** Let assumptions in Lemma 1 hold. Let \((\lambda, u)\) be a single eigenpair of (2) and \((\lambda_h, u_h)\) be its Galerkin Lagrange finite element approximation in (6). If \( \mathcal{V} \in W^{1+s, \infty}(\Omega) \), then

\[
|d\lambda(\Omega; \mathcal{V})_{\Omega} - d\lambda(\Omega; \mathcal{V})_{\Omega, h}| \leq C h^2 s |u|_{H^{1+s}(\Omega)} |\mathcal{V}|_{W^{1+s, \infty}(\Omega)} , \quad 0 < s \leq 1. \tag{40}
\]
If \( \mathcal{V} \in H^2(\Omega)^d \) and \( u \in W^{2,4}(\Omega) \), we have
\[
|d\lambda(\Omega; \mathcal{V}) - d\lambda(\Omega; \mathcal{V})| \leq Ch^2|u|_{W^{2,4}(\Omega)}|\mathcal{V}|_{H^2(\Omega)}.
\] (41)

If \( \mathcal{V} \in W^{2,4}(\Omega)^d \) and \( u \in H^2(\Omega) \), we have
\[
|d\lambda(\Omega; \mathcal{V}) - d\lambda(\Omega; \mathcal{V})| \leq Ch^2|u|_{H^2(\Omega)}|\mathcal{V}|_{W^{2,4}(\Omega)}.
\] (42)

**Proof** First, by (20), (36) and the triangle inequality, we have
\[
|d\lambda(\Omega; \mathcal{V}) - d\lambda(\Omega; \mathcal{V})| \leq \left| \int_{\Omega} (2\nabla u \cdot D\mathcal{V} \nabla u - 2\nabla u_h \cdot D\mathcal{V} \nabla u_h) \, dx \right| + \left| \int_{\Omega} \text{div} \mathcal{V} (|\nabla u|^2 - |\nabla u_h|^2) \, dx \right| + \left| \int_{\Omega} \text{div} \mathcal{V} (\lambda u^2 - \lambda h u_h^2) \, dx \right|.
\] (43)

For the first term in R.H.S. of (43),
\[
\left| \int_{\Omega} (2\nabla u \cdot D\mathcal{V} \nabla u - 2\nabla u_h \cdot D\mathcal{V} \nabla u_h) \, dx \right|
\leq 2\|u - u_h\|_{H^{1-\epsilon}(\Omega)} \|\text{div}(D\mathcal{V} + D\mathcal{V}^T)\nabla u\|_{H^{1-\epsilon}(\Omega)} + 2\|\text{div}\mathcal{V}\|_{L^\infty(\Omega)} \|\nabla u - \nabla u_h\|_{L^2(\Omega)}^2
\leq Ch^2|u|_{H^{1+\epsilon}(\Omega)}^2 |\mathcal{V}|_{W^{1,\infty}(\Omega)} + Ch^2|u|_{H^{1+\epsilon}(\Omega)}^2 |\mathcal{V}|_{W^{1,\infty}(\Omega)}.
\] (44)

where the Green’s formula and Lemma 1 are used. For the second term in R.H.S. of (43), we have analogously
\[
\left| \int_{\Omega} \text{div} \mathcal{V} (|\nabla u|^2 - |\nabla u_h|^2) \, dx \right|
\leq 2\|\text{div}(\nabla u)\|_{H^{1-\epsilon}(\Omega)} \|\nabla u - \nabla u_h\|_{H^{1-\epsilon}(\Omega)} + \|\text{div}\mathcal{V}\|_{L^\infty(\Omega)} \|\nabla u - \nabla u_h\|_{L^2(\Omega)}^2
\leq Ch^2|u|_{H^{1+\epsilon}(\Omega)}^2 |\mathcal{V}|_{W^{1,\infty}(\Omega)} + Ch^2|u|_{H^{1+\epsilon}(\Omega)}^2 |\mathcal{V}|_{W^{1,\infty}(\Omega)}.
\] (45)
For the third term in R.H.S. of (43), simple estimations yield

\[
\left| \int_{\Omega} \text{div} \mathcal{V}(\lambda u^2 - \lambda_h u_h^2) dx \right| = \left| \int_{\Omega} \text{div} \mathcal{V}[2\lambda u(u - u_h) - \lambda(u - u_h)^2 + (\lambda - \lambda_h)u_h^2] dx \right|
\leq \|\mathcal{V}\|_{L^\infty(\Omega)} \left( \int_{\Omega} |2\lambda u(u - u_h)| dx + \int_{\Omega} |\lambda(u - u_h)|^2 dx \right) + |\lambda - \lambda_h| \int_{\Omega} u_h^2 dx
\leq C\|\mathcal{V}\|_{W^{1,\infty}(\Omega)} \left(2\lambda u \| L^2(\Omega) \| u - u_h \| L^2(\Omega) + \lambda \| u - u_h \| L^2(\Omega)^2 \right)
+ |\lambda - \lambda_h| \| u_h \| L^2(\Omega)^2
\leq C\|\mathcal{V}\|_{W^{1,\infty}(\Omega)} (C\lambda \| H^{1+s} \| u \| H^{1+s}(\Omega) + C\lambda h^{2+2s} \| u \| _{H^{1+s}(\Omega)}^2
+ Ch^{2s} \| u \| _{H^{1+s}(\Omega)}),
\]

where \( \|u\|_{L^2(\Omega)} = 1 \), \( \|u_h\|_{L^2(\Omega)} = 1 \) and Lemma 1 are used. Therefore,

\[
\left| \int_{\Omega} \text{div} \mathcal{V}(\lambda u^2 - \lambda_h u_h^2) dx \right| \leq Ch^{2s} \|\mathcal{V}\|_{W^{1,\infty}(\Omega)} \| u \| _{H^{1+s}(\Omega)}. \tag{46}
\]

Substituting (44), (45) and (46) into (43) allows (40) to hold.

The result (42) can be obtained analogous to (41). We next prove (41) when \( \mathcal{V} \in H^2(\Omega)^d \) and \( u \in W^{2,4}(\Omega) \). Each term on R.H.S. of (43) is estimated differently from above due to different regularities on \( u \) and \( \mathcal{V} \). By Hölder’s inequality, Lemma 1, Lemma 3, and the Sobolev embedding theorem, we have

\[
\left| \int_{\Omega} (2\nabla u \cdot \mathcal{V} \nabla u - 2\nabla u_h \cdot \mathcal{V} \nabla u_h) dx \right|
\leq 2\|u - u_h\|_{L^2(\Omega)} \| \text{div}(\mathcal{V} \nabla u) \|_{L^2(\Omega)} + 2\|\mathcal{V}\|_{L^4(\Omega)} \| \nabla u - \nabla u_h \|_{L^4(\Omega)} \| \nabla u
- \nabla u_h \|_{L^2(\Omega)}
\leq Ch^2 \| u \| _{H^2(\Omega)} \| \mathcal{V} \| _{W^{1,\infty}(\Omega)} + \| \mathcal{V} \| _{W^{1,4}(\Omega)} \| u \| _{W^{2,4}(\Omega)}
+ Ch^2 \| u \| _{H^2(\Omega)} \| \mathcal{V} \| _{W^{1,4}(\Omega)} \| u \| _{W^{2,4}(\Omega)}
\leq Ch^2 \| u \| _{H^2(\Omega)} \| \mathcal{V} \| _{H^2(\Omega)} \| u \| _{W^{2,4}(\Omega)} + Ch^2 \| u \| _{H^2(\Omega)} \| \mathcal{V} \| _{W^{1,4}(\Omega)} \| u \| _{H^1(\Omega)}
\]

and

\[
\left| \int_{\Omega} \text{div} \mathcal{V} (|\nabla u|^2 - |\nabla u_h|^2) dx \right|
\leq 2 \int_{\Omega} \text{div}(\text{div} \mathcal{V} \nabla u)(u - u_h) dx + \int_{\Omega} \text{div} \mathcal{V} (|\nabla u - \nabla u_h|^2) dx
\leq 2\|\text{div}(\mathcal{V} \nabla u)\|_{L^2(\Omega)} \| u - u_h\|_{L^2(\Omega)} + \|\text{div} \mathcal{V}\|_{L^4(\Omega)} \| \nabla u
- \nabla u_h \|_{L^4(\Omega)} \| \nabla u - \nabla u_h \|_{L^2(\Omega)}
\leq Ch^2 \| u \| _{H^2(\Omega)} \| \text{div} \mathcal{V} \| _{H^1(\Omega)} + Ch^2 \| u \| _{H^2(\Omega)} \| u \| _{W^{2,4}(\Omega)} \| \mathcal{V} \| _{W^{1,4}(\Omega)}
\]
Theorem 2

Let the assumptions in Theorem 1 be satisfied. For the case of $V^2$ and its derivative (37). First we have to assume that the result (41) is obtained under more regularity assumptions: $\lambda$ is convex and $\lambda \in W^{1,\infty}(\Omega)$.

\[
\leq C^2 |\lambda| W^{1,\infty}(\Omega) + |\lambda'| W^{1,\infty}(\Omega)
\]

\[
\leq C^2 |\lambda| W^{1,\infty}(\Omega) + |\lambda'| W^{1,\infty}(\Omega),
\]

respectively.

For the third term in R.H.S. of (43), simple estimations by the Hölder’s inequality, the Sobolev embedding theorem (p. 85 [1]), and Lemma 1 with $s=1$ yield

\[
\left| \int_{\Omega} \text{div} \varphi(\lambda u^2 - \lambda h u_h^2) \, dx \right|
\leq \left| \int_{\Omega} \text{div} \varphi(2\lambda u(u - u_h) - \lambda (u - u_h)^2 + (\lambda - \lambda h) u_h^2) \, dx \right|
\leq \| \text{div} \varphi \|_{L^4(\Omega)} \| \lambda \|_{L^4(\Omega)} \| u - u_h \|_{L^2(\Omega)}
+ \lambda \| u - u_h \|_{L^2(\Omega)} \| u - u_h \|_{L^2(\Omega)} + |\lambda - \lambda h| \| u_h \|_{L^4(\Omega)} \| u_h \|_{L^2(\Omega)}
\leq C |\varphi|_{H^2(\Omega)} \left( \| \lambda \|_{H^1(\Omega)} \| u - u_h \|_{H^1(\Omega)} + \lambda \| u - u_h \|_{H^1(\Omega)} \| u - u_h \|_{H^1(\Omega)}
+ |\lambda - \lambda h| \| u_h \|_{H^1(\Omega)} \| u_h \|_{L^2(\Omega)} \right)
\leq C |\varphi|_{H^2(\Omega)} \left( C \lambda h^2 \| u \|_{H^1(\Omega)} \| u_h \|_{H^1(\Omega)} + C \lambda h^3 \| u \|_{H^2(\Omega)} \| u_h \|_{H^1(\Omega)} \| u_h \|_{H^1(\Omega)} \right),
\]

in which

\[
\| u \|_{H^1(\Omega)} = \sqrt{\| u \|_{L^2(\Omega)}^2 + |u|_{H^1(\Omega)}^2} = \sqrt{1 + \lambda}
\]

and

\[
\| u_h \|_{H^1(\Omega)} = \sqrt{\| u_h \|_{L^2(\Omega)}^2 + |u_h|_{H^1(\Omega)}^2} = \sqrt{1 + \lambda h} \leq \sqrt{1 + \lambda + C^2 |\lambda|_{W^{1,\infty}(\Omega)}},
\]

Thus, the conclusion follows by combining the above results.

**Remark 3** In [21], $H^2$ regularity is assumed for the convergence analysis of approximate shape gradients in linear elliptic problems. In Theorem 1, the more general regularity $H^{1+s}$ ($0 < s \leq 1$) assumption is made for (40). Moreover, another new result (41) is obtained under more regularity assumptions: $u$ is assumed to be in $W^{2,4}$ and $\varphi$ is assumed to be in $H^2$ rather than $W^{1,\infty}$.

Now, we perform the convergence analysis for the approximate boundary Eulerian derivative (37). First we have to assume that $\Omega$ is convex ($d = 2$) or $C^2$, such that $u \in H^2(\Omega)$ and the continuous boundary formula (33) holds.

**Theorem 2** Let the assumptions in Theorem 1 hold with $s = 1$. Assume further that

\[
\| u \|_{W^{2,p}(\Omega)} \leq C p \lambda \| u \|_{L^p(\Omega)}
\]

for $1 < p < \mu$ with some $\mu > d$. Then,

\[
|d\lambda(\Omega; \varphi)_{a\Omega} - \delta\lambda(\Omega; \varphi)_{a\Omega,h}| \leq C |\log h|^{1-\frac{d}{2}} h |u|_{W^{2,\infty}(\Omega)} \| \varphi \|_{L^\infty(\partial\Omega)}.
\]
Proof By (21) and (37), we first have

\[
|d\lambda(\Omega; \mathcal{V}) - d\lambda(\Omega; \mathcal{V})|_{\partial\Omega, h} = \left| \int_{\partial\Omega} - \left( \frac{\partial u}{\partial n} \right)^2 - \left( \frac{\partial u_h}{\partial n} \right)^2 \right| \mathcal{K}_n ds \leq \|\mathcal{K}_n\|_{L^\infty(\partial\Omega)} \int_{\partial\Omega} \left| \left( \frac{\partial u}{\partial n} \right)^2 - \left( \frac{\partial u_h}{\partial n} \right)^2 \right| ds \leq \|\mathcal{K}_n\|_{L^\infty(\partial\Omega)} \left( 2 \left\| \frac{\partial u}{\partial n} \right\|_{L^1(\partial\Omega)} \left\| \frac{\partial (u - u_h)}{\partial n} \right\|_{L^\infty(\partial\Omega)} + |\partial\Omega| \left\| \frac{\partial (u - u_h)}{\partial n} \right\|_{L^\infty(\partial\Omega)}^2 \right),
\]

(50)

where we have used the Hölder inequality in the last inequality. By the trace theorem [1], (50) implies that

\[
|d\lambda(\Omega; \mathcal{V}) - d\lambda(\Omega; \mathcal{V})|_{\partial\Omega, h} \leq C \|\mathcal{K}_n\|_{L^\infty(\partial\Omega)} \left( 2 \left\| \frac{\partial u}{\partial n} \right\|_{L^1(\partial\Omega)} \left\| \frac{\partial (u - u_h)}{\partial n} \right\|_{L^\infty(\partial\Omega)} + |\partial\Omega| \left\| \frac{\partial (u - u_h)}{\partial n} \right\|_{L^\infty(\partial\Omega)}^2 \right).
\]

(51)

Then, the conclusion follows using the a priori error estimates in the norm $W^{1,\infty}(\Omega)$ [9]:

\[
\|u - u_h\|_{W^{1,\infty}(\Omega)} = C \log h^{1 - \frac{1}{d}} \|u\|_{W^{2,\infty}(\Omega)}.
\]

(52)

What left now is to prove (52). First, we split the error and use the triangle inequality to obtain

\[
\|u - u_h\|_{W^{1,\infty}(\Omega)} \leq \|u - P_h u\|_{W^{1,\infty}(\Omega)} + \|P_h u - u_h\|_{W^{1,\infty}(\Omega)},
\]

(53)

where $P_h : H^1_0(\Omega) \to V_h$ is defined in (10). In (53), the error estimate for the first term on the R.H.S. is standard (Corollary 8.1.12 [9]):

\[
\|u - P_h u\|_{W^{1,\infty}(\Omega)} \leq C h \|u\|_{W^{2,\infty}(\Omega)}.
\]

(54)

To estimate $\|P_h u - u_h\|_{W^{1,\infty}(\Omega)}$, the methods we use are different for $d = 2$ and $d = 3$. We discuss them separately. For $d = 2$, by the inverse inequality (see e.g., [9]), the discrete Sobolev inequality (Lemma 4.9.2 of [9]) and Lemma 2, we obtain

\[
\|P_h u - u_h\|_{W^{1,\infty}(\Omega)} \leq C h^{-1} \|P_h u - u_h\|_{L^\infty(\Omega)} \leq C h^{-1} \log h^{1/2} \|\nabla (P_h u - u_h)\|_{L^2(\Omega)} \leq C \log h^{1/2} \|u\|_{H^2(\Omega)}, \quad d = 2.
\]

(55)
For \( d = 3 \), we have to use different arguments since no result as Lemma 4.9.2 of [9] is available. Let \( p < 3 \). By the inverse inequality [9], Theorem 7.10 and its remark in [14]
\[
\| P_h u - u_h \|_{W^{1,\infty}(\Omega)} \leq C h^{-1 - \frac{3-p}{p}} \| P_h u - u_h \|_{L^{3p/(3-p)}(\Omega)}
\]
\[
\leq C C_{p} h^{-1 - \frac{3-p}{p}} \| \nabla (P_h u - u_h) \|_{L^{p}(\Omega)},
\]
where
\[
C_p = \frac{1}{3 \sqrt{\pi}} \left( \frac{3! \Gamma(3/2)}{2 \Gamma(3/p) \Gamma(4 - 3/p)} \right)^{1/3} \left[ \frac{3(p-1)}{3-p} \right]^{1-1/p}
\]
with \( \Gamma(\cdot) \) denotes the gamma function. Using the Hölder’s inequality
\[
\| v \|_{L^{p}(\Omega)} \leq |\Omega|^{\frac{3-p}{3p}} \| v \|_{L^{3}(\Omega)} \quad \forall v \in L^{3}(\Omega)
\]
in (56) and choosing \( p \) such that \((3-p)|\log h| = p\), we get
\[
\| P_h u - u_h \|_{W^{1,\infty}(\Omega)} \leq C h^{-1 - \frac{3-p}{p}} |\Omega|^{\frac{3-p}{3p}} \| \nabla (P_h u - u_h) \|_{L^{3}(\Omega)}
\]
\[
\leq C h^{-1} |\log h|^{2/3} \| \nabla (P_h u - u_h) \|_{L^{3}(\Omega)}.
\]
Since
\[
\| \nabla (P_h u - u_h) \|_{L^{3}(\Omega)} \leq C \sup_{0 \neq v_h \in V_h} \frac{\| \nabla (P_h u - u_h), \nabla v_h \|}{|v_h|_{W^{1,3/2}(\Omega)}} \quad \text{(Proposition 8.6.2 [9])}
\]
\[
= C \sup_{0 \neq v_h \in V_h} \frac{\lambda (u - u_h) + (\lambda - \lambda_h) u_h, v_h}{|v_h|_{W^{1,3/2}(\Omega)}}
\]
\[
\leq C \sup_{0 \neq v_h \in V_h} \frac{(\lambda \| u - u_h \|_{L^{2}(\Omega)} + |\lambda - \lambda_h|) \| v_h \|_{L^{2}(\Omega)}}{|v_h|_{W^{1,3/2}(\Omega)}} \quad \text{(Lemma 1)}
\]
\[
\leq C h^2 |u|_{H^{2}(\Omega)} \sup_{0 \neq v_h \in V_h} \frac{\| v_h \|_{L^{2}(\Omega)}}{|v_h|_{W^{1,3/2}(\Omega)}}
\]
\[
\leq C h^2 |u|_{H^{2}(\Omega)} \sup_{0 \neq v_h \in V_h} \frac{\| v_h \|_{L^{2}(\Omega)}}{|v_h|_{L^{3}(\Omega)}}
\]
\[
\leq C h^2 |u|_{H^{2}(\Omega)} |\Omega|^{1/6}
\]
using the Sobolev embedding Theorem (p. 85 [1]) and (57) in the last two inequalities, (58) implies that
\[
\| P_h u - u_h \|_{W^{1,\infty}(\Omega)} = C |\Omega|^{1/6} |\log h|^{2/3} h |u|_{H^{2}(\Omega)}, \quad d = 3.
\]
Finally, a combination of (54), (55) and (59) gives (52). \(\square\)
Remark 4  Compared with Theorem 1, a stronger regularity assumption on $u$ is required in Theorem 2. However, the converge rate (interpreted as $O(h^{1-\epsilon})$ for any small $\epsilon > 0$) obtained in Theorem 2 is lower than that in Theorem 1 (which is $O(h^2)$).

3.2 Multiple eigenvalue case

We now consider the multiple eigenvalue case, and show the a priori error estimates for the approximate volume and boundary Eulerian derivatives. The directional derivatives for this case are stated in Proposition 2. We first review the Weyl’s inequality to estimate perturbations of the spectrum in matrix theory [38].

Lemma 4  Let matrices $A = [a_{ij}]$ and $A^h = [a^h_{ij}] \in \mathbb{R}^{l \times l}$ be symmetric. If the entries satisfy that $|a_{ij} - a^h_{ij}| = O(h^\theta)$ with some $\theta > 0$ for $i, j = 1, 2, \ldots, l$. We denote the eigenvalues of $A$ and $A^h$ by $\{\theta_i\}_{i=1}^l$ and $\{\theta^h_i\}_{i=1}^l$ respectively. Then,

$$\max_{1 \leq i \leq l} |\theta_i - \theta^h_i| = O(l^{3/2} h^{\theta}).$$  (60)

Proof  We first obtain the symmetry of $A - A^h$ since both $A$ and $A^h$ are symmetric. Then, the spectral norm and eigenvalues satisfy that $\|A - A^h\|_2 = \max_{1 \leq i \leq l} |\theta_i - \theta^h_i|$. For matrix norms, we easily have [13]

$$\|A - A^h\|_2 \leq \sqrt{l} \|A - A^h\|_\infty.$$

Thus,

$$\max_{1 \leq i \leq l} |\theta_i - \theta^h_i| \leq \sqrt{l} \|A - A^h\|_\infty = \sqrt{l} \max_{1 \leq i \leq l} \sum_{j=1}^l |a_{ij} - a^h_{ij}|.$$

The result follows from the known condition on perturbation bounds of entries. \qed

Then, we obtain approximations (38) and (39) for the multiple eigenvalue case as follows.

Theorem 3  Let the assumptions in Lemma 1 and Proposition 2 hold. Denote by $\{u_i, h\}_{i=1}^l$ the Lagrange finite element approximations of eigenfunctions $\{u_i\}_{i=1}^l$. Then,

$$\max_{1 \leq i \leq l} |\sigma_{\Omega, i} \sigma^h_{\Omega, i}| \leq C l^{3/2} h^{2s} \max_{1 \leq i \leq l} |u_i|_{H^{1+s}(\Omega)} |\mathcal{V}|_{W^{1+s, \infty}(\Omega)}, \quad 0 < s \leq 1.$$

If $\mathcal{V} \in H^2(\Omega)^d$ and moreover $u \in W^{2,4}(\Omega)$, then

$$\max_{1 \leq i \leq l} |\sigma_{\Omega, i} \sigma^h_{\Omega, i}| \leq C l^{3/2} h^2 \max_{1 \leq i \leq l} |u_i|_{W^{2,4}(\Omega)} |\mathcal{V}|_{H^2(\Omega)}.$$

Assume that $u_i \in W^{2, \infty}(\Omega)$ for the boundary formula ($i = 1, 2, \ldots, l$). We have

$$\max_{1 \leq i \leq l} |\sigma_{\partial \Omega, i} \sigma^h_{\partial \Omega, i}| \leq C l^{3/2} h^{1-\epsilon} \max_{1 \leq i \leq l} |u_i|_{W^{2, \infty}(\Omega)} |\mathcal{V}_n|_{L^\infty(\partial \Omega)}, \quad 0 < \epsilon \ll 1.$$
Proof We can modify the arguments in Theorem 1 and Theorem 2 for the simple eigenvalue case to obtain

\[ |m_{i,j}(\Omega; \mathcal{Y})\Omega - m_{i,j}^h(\Omega; \mathcal{Y})\Omega| \leq C h^{2\epsilon} \max_{1 \leq i \leq l} |u_i|_{H^{1+\epsilon}(\Omega)} |\mathcal{Y}'|_{W^{1+\epsilon,\infty}(\Omega)}, \]

\[ |m_{i,j}(\Omega; \mathcal{Y})\Omega - m_{i,j}^h(\Omega; \mathcal{Y})\Omega| \leq C h^2 \max_{1 \leq i \leq l} |u_i|_{W^{2,4}(\Omega)} |\mathcal{Y}'|_{H^2(\Omega)} \]

and

\[ |m_{i,j}(\Omega; \mathcal{Y})\partial\Omega - m_{i,j}^h(\Omega; \mathcal{Y})\partial\Omega| \leq C h^{1-\epsilon} \max_{1 \leq i \leq l} |u_i|_{W^{2,\infty}(\Omega)} |\mathcal{Y}'_n|_{L^\infty(\partial\Omega)} \]

for \(i, j = 1, \ldots, l\) and \(\epsilon > 0\). By Lemma 4, the conclusions hold.

Remark 5 The results for Laplacian above can be generalized for a self-adjoint and uniform elliptic second-order differential operator \(L\) such that

\[ Lu := -\sum_{i,j=1}^d \frac{\partial}{\partial x_i} \left( a_{ij}(x) \frac{\partial u}{\partial x_j} \right) + a_0(x) u \]

with coefficients \(a_0(x)\) and \(a_{ij}(x) \in C^1(\overline{\Omega})\) for \(i, j = 1, \ldots, d\).

4 Numerical results

We perform numerical experiments with FreeFem++ [18]. Here we consider only the cases of simple eigenvalues. For the multiple eigenvalue case in shape optimization, we refer to [41] for using distributed shape gradients. Examples corresponding to both Dirichlet and Neumann boundary conditions are presented. We consider three cases of computational domains in \(\mathbb{R}^2\): a unit square, a unit disk and a L-shaped domain \((-1, 1)^2\) missing the upper right quarter. In Fig. 1, one level of triangulation is illustrated. To study \(h\)-convergence, the uniform refinement is employed. The eigenfunctions in the first two cases have enough smoothness and even can be extended to entire functions, whereas the eigenfunction on the L-shaped domain has singularities at the reentrant corner. The Lagrange linear element is employed in all three cases. We approximate the first eigenvalue and the first non-zero eigenvalue for the Dirichlet boundary condition and the Neumann boundary condition, respectively.

We first numerically verify the theoretical results in Sect. 3. The shape gradient for the simple eigenvalue is a linear continuous operator on \(W^{1,\infty}(\mathbb{R}^d; \mathbb{R}^d)\) and belongs to its dual space in either the volume or the boundary type Eulerian derivative. As noted in [21], it is challenging to compute numerically in the continuous infinite-dimensional operator norm for the approximate shape gradients. This norm can be approximately replaced by a tractable one on a finite-dimensional subspace of \(W^{1,\infty}(\mathbb{R}^d; \mathbb{R}^d)\). More precisely, given a positive integer \(\gamma\) as in [21], we consider an approximate operator norm on a finite-dimensional space consisting of vector fields in \(\mathcal{D}_{\gamma,\gamma}(\mathbb{R}^d; \mathbb{R}^d)(\subset W^{1,\infty}(\mathbb{R}^d; \mathbb{R}^d))\), whose components are multivariate polynomials of degree up to
Based on the equivalence of norms over finite-dimensional spaces, we replace the $W^{1,\infty}$-norm with the $H^1$-norm (which is easier to compute compared with the $W^{1,\infty}$-norm). Finally, we compute the approximate dual norms

$$
\mathcal{E}_\Omega := \left( \max_{0 \neq \varphi \in \mathcal{H}_{Y,\gamma}^\Omega} \frac{|d\lambda(\Omega; \varphi)_\Omega - d\lambda(\Omega; \varphi)_\Omega; h|^2}{\|\varphi\|^2_{H^1(\Omega)}} \right)^{1/2},
$$

$$
\mathcal{E}_{\partial\Omega} := \left( \max_{0 \neq \varphi \in \mathcal{H}_{Y,\gamma}^{\partial\Omega}} \frac{|d\lambda(\Omega; \varphi)_{\partial\Omega} - d\lambda(\Omega; \varphi)_{\partial\Omega}; h|^2}{\|\varphi\|^2_{H^1(\Omega)}} \right)^{1/2}.
$$

(61)

We take a basis \( \{ \varphi_i \}_{i=1}^q \) of vector fields in \( \mathcal{H}_{Y,\gamma}(\mathbb{R}^d;\mathbb{R}^d) \) with \( q = dC^d_{\gamma+d} \) denoting the combination coefficient and

\[
\{ \varphi_i \}_{i=1}^q = \left\{ [\Pi_{i=1}^d x_i^{\beta_i}, 0, \ldots, 0, \ldots, 0, \Pi_{i=1}^d x_i^{\beta_i}] \right\}_{i=1}^q
\]

where \( \beta_i (i = 1, \ldots, d) \) are non-negative integers. We denote the Gramian matrix associated with the $H^1(\Omega)$ inner product by \( \mathbb{K} = [(\varphi_i, \varphi_j)_{H^1(\Omega)}]_{i,j=1}^q \in \mathbb{R}^{q \times q} \). For the simple eigenvalue case, the errors (61) can be obtained by

$$
\mathcal{E} := \left( w^T \mathbb{K}^{-1} w \right)^{1/2},
$$

(62)

where \( \mathcal{E} = \mathcal{E}_\Omega \) or \( \mathcal{E}_{\partial\Omega} \) corresponds to \( w = w_\Omega \) or \( w_{\partial\Omega} \) with the vectors

\[
w_\Omega := [d\lambda(\Omega; \varphi_i)_\Omega - d\lambda(\Omega; \varphi_i)_\Omega; h]_{i=1}^q \quad \text{and} \quad w_{\partial\Omega} := [d\lambda(\Omega; \varphi_i)_{\partial\Omega} - d\lambda(\Omega; \varphi_i)_{\partial\Omega}; h]_{i=1}^q.
\]

### 4.1 The Dirichlet problem

For square, a uniform triangulation is used, and the exact first eigenpair is \( (2\pi^2, 2\sin(\pi x_1) \sin(\pi x_2)) \).

In Fig. 2, a linear finite element approximation of the first eigenfunction with \( h = \sqrt{2}/256 \) is illustrated, where the quadratic and linear convergence rates of approximate
shape gradients in approximate operator norms agree well with the predicted results of Theorems 1 and 2. For the disk domain, the exact first eigenpair is

\[ (j_{0,1}^2, \frac{1}{\sqrt{\pi}} \frac{1}{|J'_0(j_{0,1})|} J_0(j_{0,1}R)) \]

where \( j_{0,1} \) is the first zero of the Bessel function \( J_0 \) and \( R \) is the radial variable. The quasi-uniform triangulations based on the uniform refinement are used. Figure 3 shows the eigenfunction computed using the finest mesh. The convergence rates of approximate shape gradients are consistent with theoretical results.

In order to compute errors for the L-shape domain case, we use quasi-uniform meshes and compute the finite element solution on a fine mesh with 850523 degrees of freedom as the reference solution shown in Fig. 4. The eigenfunction for the L-shaped domain belongs to \( H^{\frac{5}{3}-\epsilon}(\Omega) \) and thus the \( H^2 \)-regularity for this eigenvalue.
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Fig. 4 Finite element approximation of the eigenfunction on the L-shaped domain (left) and the convergence history of approximate shape gradients (right)

Fig. 5 Convergence history of approximate shape gradients for the Neumann boundary condition
4.2 The Neumann problem

The first non-zero eigenvalue for the square domain is multiple and we consider the second one. The exact eigenpair is \((2\pi^2, 2\cos\pi x_1 \cos\pi x_2)\). For the disk domain, we consider the approximation for the first exact non-zero eigenpair

\[
\left( j_{0,1}', \frac{1}{\sqrt{\pi}} \frac{1}{|J_0'(j_{0,1}')|} J_0(j_{0,1}'R) \right).
\]

In Fig. 6b, d, the quadratic convergence rates of the boundary integral formula are unexpected, as observed in [31] for the elliptic problem with the Neumann boundary condition. For the L-shaped domain which does not guarantee the \(H^2\)-regularity of the eigenfunction, Fig. 5 shows that the volume integral expression is superior to the boundary integral expression in terms of both accuracy and convergence rates. Finally, Fig. 6 shows the measured errors for the two boundary conditions for both square and...
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disk conditions where the degree of multivariate polynomials is set to $\gamma = 2$. The accuracy and the converge rates agree well with those above when $\gamma = 3$, which shows the norm of the operator computed though the finite-dimensional subspace of multivariate polynomials vector fields is independent of $\gamma$.

5 Conclusions

In this work, the convergence analysis for Galerkin finite element approximations of the shape gradients arising from optimizing Dirichlet/Neumann type elliptic eigenvalue problems is preformed. The a priori error estimates are presented for the two types of approximate shape gradients in Eulerian derivatives. For the Dirichlet problem, our theoretical analysis and numerical results show that the volume type formula converges faster and usually offers better accuracy than the boundary type formula. For the Neumann problem, however, the boundary formulation is surprisingly competitive with the volume type formulation.

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