Computer-assisted analysis of the sign-change structure for elliptic problems

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Abstract. In this paper, a method is proposed for rigorously analyzing the sign-change structure of solutions to elliptic problems with computer-assistance. Suppose that errors \( \|u - \hat{u}\|_{H^1_0} \) and \( \|u - \hat{u}\|_{L^\infty} \) are evaluated between an exact solution \( u \) and a numerically computed approximate solution \( \hat{u} \). We estimate the number of sign-changes of the solution \( u \) (the number of nodal domains) and the location of zero level-sets of \( u \) (the location of the nodal line). We present numerical examples where our method is applied to a specific semilinear elliptic problem.

Keywords: Computer-assisted proof, Elliptic problems, Numerical verification, Sign-change structure, Verified numerical computation

AMS subject classifications: 35J25, 35J61, 65N15

1 Introduction

Computer-assisted proofs for partial differential equations have been developed over the last several decades. Pioneering research on such methods began with [12, 15], and has been further developed by many researchers (see the recent survey book [13] and the references therein). At the present time, such approaches are also known as numerical verification methods, validated numerics, or verified numerical computations for partial differential equations, and have been applied to various problems, including examples where purely analytical methods have failed. One such successful application is to the semilinear elliptic equation

\[-\Delta u(x) = f(u(x)), \quad x \in \Omega, \quad (1)\]

with appropriate boundary value conditions, where \( \Omega \subset \mathbb{R}^N \) \((N = 2, 3, \cdots)\) is a given domain, \( \Delta \) is the Laplacian, and \( f: \mathbb{R} \rightarrow \mathbb{R} \) is a given nonlinear map (see, for example, the numerical results in [10, 17, 14, 9, 19, 23, 13]). Further regularity assumptions for \( \Omega \) and \( f \) will be shown later for our setting. Throughout this paper, \( H^k(\Omega) \) denotes the \( k \)-th order \( L^2 \) Sobolev space. We define \( H^1_0(\Omega) := \{u \in H^1(\Omega) : u = 0 \text{ on } \partial \Omega\} \), with the inner product \((u, v)_{H^1_0} := \langle \nabla u, \nabla v \rangle_{L^2}\) and norm \( \|u\|_{H^1_0} := \sqrt{(u, u)_{H^1_0}} \).

Computer-assisted proofs enable us to obtain an explicit ball containing exact solutions of (1). More precisely, for a “good” numerical approximation \( \hat{u} \in H^1_0(\Omega) \), they enable us to prove the existence of an exact solution \( u \in H^1_0(\Omega) \) of (1) that satisfies

\[\|u - \hat{u}\|_{H^1_0} \leq \rho, \quad (2)\]

with an explicit error bound \( \rho > 0 \). Additionally, under an appropriate condition, we can obtain an \( L^\infty \)-estimation

\[\|u - \hat{u}\|_{L^\infty} \leq \sigma, \quad (3)\]

with bound \( \sigma > 0 \). For instance, when \( u, \hat{u} \in H^2(\Omega) \), we can evaluate the \( L^\infty \)-bound \( \sigma > 0 \) by considering the embedding \( H^2(\Omega) \hookrightarrow L^\infty(\Omega) \) [16, Theorem 1 and Corollary 1]. Thus,

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this approach has the advantage that quantitative information about the solutions of a target equation is provided accurately in a strict mathematical sense. From the error estimates, we can identify the approximate shape of solutions. Despite these advantages, irrespective of how small the error bound (\(\rho\) or \(\sigma\)) is, information about the sign change of solutions is not guaranteed without additional considerations. To be more precise, we introduce the following.

**Definition 1.1.** For \(u : \Omega \rightarrow \mathbb{R}\), the connected components of the open sets

\[
\{ x \in \Omega : u(x) > 0 \} \quad \text{and} \quad \{ x \in \Omega : u(x) < 0 \}
\]

are called the **nodal domains** of \(u\) and denoted by \(\text{N.D.}(u)\). In particular, \(\{ x \in \Omega : u(x) > 0 \}\) is called the positive nodal domains of \(u\) and denoted by \(\text{P.N.D.}(u)\), and \(\{ x \in \Omega : u(x) < 0 \}\) is called the negative nodal domains of \(u\) and denoted by \(\text{N.N.D.}(u)\).

The zero level-set

\[
\{ x \in \Omega : u(x) = 0 \}
\]

is called the **nodal line** of \(u\).

Note that nodal domains and lines are usually defined for the eigenfunctions of some operators, typically elliptic operators. In this paper, we extend such definitions to general functions. According to the above definition, nodal lines do not contain the boundary of \(\Omega\); however, we interpret zero-Dirichlet boundaries as parts of nodal lines in an actual application to a specific problem (see Subsection 2.3).

An essential problem is that, in general, \#\text{N.D.}(u) (the number of \text{N.D.}(u)) does not coincide with \#\text{N.D.}(\hat{u}) (see Fig. 1). For example, when \(u\) is imposed on the homogeneous Dirichlet boundary conditions, even when \(\hat{u}\) is positive in \(\Omega\), it is possible for \(u\) to be negative near the boundary \(\partial \Omega\). In previous studies, we developed methods for verifying the positivity of solutions of \(\text{(4)}\) \([22, 24, 23]\). These methods succeeded in verifying the existence of positive solutions with precise error bounds by checking simple conditions, but determining the sign-change structure has been out of scope.

Fig. 1: Conceptual figure for the area in which \((\hat{u} - \sigma)(\hat{u} + \sigma) < 0\) between the two solid lines. Nodal lines of \(u\) lay inside the area and do not exist outside. Regardless of how small \(\sigma > 0\) is, we cannot deny the possibility that there exist (small) nodal domains in the area only from the error estimations \(\rho\) and/or \(\sigma\). If the nonexistence of nodal domains inside the area is proved, we can estimate \#\text{N.D.}(u) and determine the topology of nodal lines (i.e., how the lines intersect).

The main contribution of this paper is a proposed method for verifying the sign-change structure of solutions \(u\) of \(\text{(1)}\) subject to one of the three types of homogeneous boundary value conditions —Dirichlet type, Neumann type, and mixed type— while assuming the error estimations \(\text{(2)}\) and \(\text{(3)}\). As long as error bounds are sufficiently precise, our theorems can be
applied to the case in which \( f \) is a subcritical polynomial

\[
f(t) = \lambda t + \sum_{i=2}^{n(<p^*)} a_i t^{|i-1|}, \quad \lambda, a_i \in \mathbb{R}, a_i \neq 0 \text{ for some } i,
\]

where \( p^* = \infty \) when \( N = 2 \) and \( p^* = (N + 2)/(N - 2) \) when \( N \geq 3 \). They are also applicable for more general nonlinearities other than polynomials (see Theorems 2.4 and 3.2). In the later sections, we discuss the applicability of our method to the Dirichlet problem

\[
\begin{aligned}
-\Delta u(x) &= f(u(x)), \quad x \in \Omega, \\
u(x) &= 0, \quad x \in \partial \Omega,
\end{aligned}
\]

the Neumann problem

\[
\begin{aligned}
-\Delta u(x) &= f(u(x)), \quad x \in \Omega, \\
\frac{\partial u}{\partial n}(x) &= 0, \quad x \in \partial \Omega,
\end{aligned}
\]

and the mixed boundary value problem

\[
\begin{aligned}
-\Delta u(x) &= f(u(x)), \quad x \in \Omega, \\
u(x) &= 0, \quad x \in \Gamma_D, \\
\frac{\partial u}{\partial n}(x) &= 0, \quad x \in \Gamma_N,
\end{aligned}
\]

where \( \Gamma_D \) and \( \Gamma_N \) are subsets of \( \partial \Omega \) that satisfy \( \Gamma_D \cup \Gamma_N = \partial \Omega \). We suppose without restriction that \( \Gamma_D \) and \( \Gamma_N \) are connected sets so that, for example, when \( n = 2 \), the intersection \( \Gamma_D \cap \Gamma_N \) is composed of two points unless \( \Gamma_D = \emptyset \) or \( \Gamma_N = \emptyset \). When \( f \) is subcritical, weak solutions of (4), (5), or (6) always belong to \( L^\infty(\Omega) \) (see [2, Corollary 6.6]).

The remainder of this paper is organized as follows. In Section 2, focusing on the Dirichlet problem (4), we propose a method to estimate the number of nodal domains of solutions \( u \), and discuss the applicability of the method. This section contains numerical examples in which the method is applied to the Allen–Cahn equation (see Subsection 2.3). Subsequently, in Section 3, we extend our method to the other boundary value conditions: the Neumann type (5) and mixed type (6).

2 Verification for sign-change structure — the Dirichlet case (4)

In this section, we limit our target problem to the Dirichlet problem (4). In Section 3, our scope will be extended.

We begin by introducing required notation. We denote \( V = H_0^1(\Omega) \) and \( V^* = (\text{the topological dual of } V) \). For two Banach spaces \( X \) and \( Y \), the set of bounded linear operators from \( X \) to \( Y \) is denoted by \( \mathcal{L}(X,Y) \) with the usual supremum norm \( \|T\|_{\mathcal{L}(X,Y)} := \sup\{\|Tu\|_Y/\|u\|_X : u \in X \setminus \{0\}\} \) for \( T \in \mathcal{L}(X,Y) \). The norm bound for the embedding \( V \hookrightarrow L^{p+1}(\Omega) \) is denoted by \( C_{p+1}(\Omega) \), that is, \( C_{p+1} \) is a positive number that satisfies

\[
\|u\|_{L^{p+1}(\Omega)} \leq C_{p+1} \|u\|_V \quad \text{for all } u \in V,
\]

where \( p \in [1, \infty) \) when \( N = 2 \) and \( p \in [1, p^*] \) when \( N \geq 3 \). If no confusion arises, we use the notation \( C_{p+1} \) to represent the embedding constant on the entire domain \( \Omega \), whereas, in some parts of this paper, we need to consider an embedding constant on some subdomain \( \Omega' \subset \Omega \). This is denoted by \( C_{p+1}(\Omega') \) to avoid confusion. Moreover, \( \lambda_1(\Omega) \) denotes the first eigenvalue of \(-\Delta\)
imposed on the homogeneous Dirichlet boundary condition. More precisely, this is characterized by
\[
\lambda_1(\Omega) = \inf_{v \in V \setminus \{0\}} \frac{\|v\|_V^2}{\|v\|_{L^2}^2}. \tag{8}
\]
Throughout this paper, we assume that \( f \) is a \( C^1 \) function that satisfies
\[
|f(t)| \leq a_0|t|^p + b_0 \quad \text{for all } t \in \mathbb{R},
\]
\[
|f'(t)| \leq a_1|t|^{p-1} + b_1 \quad \text{for all } t \in \mathbb{R}
\]
for some \( a_0, a_1, b_0, b_1 \geq 0 \) and \( p < p^* \). We define the operator \( F \) by
\[
F : \left\{ \begin{array}{ll}
\ u(\cdot) & \mapsto f(u(\cdot)), \\
V & \mapsto V^*.
\end{array} \right.
\]
Moreover, we define another operator \( \mathcal{F} : V \to V^* \) by \( \mathcal{F}(u) := -\Delta u - F(u) \), which is characterized by
\[
\langle \mathcal{F}(u), v \rangle = \langle \nabla u, \nabla v \rangle_{L^2} - \langle F(u), v \rangle \quad \text{for all } u, v \in V, \tag{9}
\]
where \( \langle F(u), v \rangle = \int_{\Omega} f(u(x))v(x)dx \). The Fréchet derivatives of \( F \) and \( \mathcal{F} \) at \( \varphi \in V \), denoted by \( F' \) and \( \mathcal{F}' \), respectively, are given by
\[
\langle F'\varphi u, v \rangle = \int_{\Omega} f'(\varphi(x))u(x)v(x)dx \quad \text{for all } u, v \in V, \tag{10}
\]
\[
\langle \mathcal{F}'\varphi u, v \rangle = \langle \nabla u, \nabla v \rangle_{L^2} - \langle F'\varphi u, v \rangle \quad \text{for all } u, v \in V. \tag{11}
\]
Under the notation and assumptions, we look for solutions \( u \in V \) of
\[
\mathcal{F}(u) = 0, \tag{12}
\]
which corresponds to the weak form of (4). We call this the D-problem to prevent confusion with the other boundary value problems to be discussed in Section 3. Recall that the weak solution \( u \in V \) of the D-problem is in \( L^\infty(\Omega) \); see [2, Corollary 6.6]. We assume that some computer-assisted method succeeds in proving the existence of a solution \( u \in V \cap L^\infty(\Omega) \) of (12) in
\[
\overline{B}(\hat{u}, \rho, \| \cdot \|_V) := \{ v \in V : \| v - \hat{u} \|_V \leq \rho \}, \tag{13}
\]
\[
\overline{B}(\hat{u}, \sigma, \| \cdot \|_{L^\infty}) := \{ v \in L^\infty(\Omega) : \| v - \hat{u} \|_{L^\infty} \leq \sigma \} \tag{14}
\]
given \( \hat{u} \in V \cap L^\infty(\Omega) \) and \( \rho, \sigma > 0 \). Although the regularity assumption for \( \hat{u} \) (to be in \( V \cap L^\infty(\Omega) \)) is sufficient to obtain the error bounds [13] and [14] in theory, we further assume that \( \hat{u} \) is continuous or piecewise continuous. This assumption impairs little of the flexibility of actual numerical computation methods. Indeed, past computer-assisted results were implemented with such approximate solutions \( \hat{u} \); again, see [10, 17, 14, 9, 19, 23, 13]. Then, we use the following notation:

- \( \Omega_+ := \{ x \in \Omega : \hat{u} - \sigma > 0 \} \) where \( u > 0 \) therein;
- \( \Omega_- := \{ x \in \Omega : \hat{u} + \sigma < 0 \} \) where \( u < 0 \) therein;
- \( \Omega_0 := \Omega \setminus (\Omega_+ \cup \Omega_-) \).

The subset \( \Omega_0 \) approximates the nodal line of \( u \), and therefore the location of \( \Omega_0 \) is essential for determining the topological information of the nodal line. In practice, \( \Omega_+ \) and \( \Omega_- \) are set to a subset of \( \{ x \in \Omega : \hat{u} - \sigma > 0 \} \) and \( \{ x \in \Omega : \hat{u} + \sigma < 0 \} \), respectively, then \( \Omega_0 \) is defined as above. This generalization can be applied directly to our theory. Throughout this paper, we assume that \( \sigma \) is small so that \( \Omega_0 \neq \Omega \), and \( \Omega_0 \) can be decomposed into a finite number of connected components \( \Omega^j_0 \) \( (j = 1, 2, \cdots) \).
2.1 Main theorem

The following lemma plays an essential role for our main result.

**Lemma 2.1.** Let \( f \) satisfy

\[
    tf(t) \leq \lambda t^2 + \sum_{i=1}^{n} a_i |t|^{p_i+1} \quad \text{for all } t \in \mathbb{R}
\]

for some \( \lambda < \lambda_1(\Omega) \), nonnegative coefficients \( a_1, a_2, \ldots, a_n \), and subcritical exponents \( p_1, p_2, \ldots, p_n \in (1, p^*) \). If a solution \( u \in V \) of the D-problem (12) satisfies the inequality

\[
    \sum_{i=1}^{n} a_i C_{p_i+1}^2 \|u\|_{L^{p_i+1}}^{p_i-1} < 1 - \frac{\lambda}{\lambda_1(\Omega)},
\]

then \( u \) is the trivial solution \( u \equiv 0 \), where \( C_{p_i+1} = C_{p_i+1}(\Omega) \).

**Remark 2.2.** The left-hand side of (16) converges to zero as \( \|u\|_{L^{p_i+1}} \downarrow 0 \). Therefore, if the solution \( u \) of (12) is sufficiently small to satisfy (16), then \( u \) must vanish.

**Remark 2.3.** The inequality (15) can be reduced to a combination of the following inequalities:

\[
    f(t) \leq \lambda t + \sum_{i=1}^{n} a_i t^{p_i} \quad \text{for all } t \geq 0;
\]

\[
    -f(-t) \leq \lambda t + \sum_{i=1}^{n} a_i t^{p_i} \quad \text{for all } t \geq 0.
\]

Therefore, the polynomial \( f(t) = \lambda t + \sum_{i=1}^{n} a_i t^{p_i} \) with \( \lambda < \lambda_1(\Omega) \) and \( a_i \in \mathbb{R} \) obviously satisfies the required inequality (15). Indeed, for the set of subscripts \( \Lambda_+ \) for which \( a_i \geq 0 \) \( (i \in \Lambda_+) \) and \( a_i < 0 \) \( (\text{otherwise}) \), we have

\[
    f(t) \leq \lambda t + \sum_{i \in \Lambda_+} a_i t^i \quad \text{and} \quad -f(-t) \leq \lambda t + \sum_{i \in \Lambda_+} a_i t^i \quad \text{for all } t \geq 0.
\]

**Proof of Lemma 2.1**

We prove that \( \|u\|_V = 0 \). Because \( u \) satisfies

\[
    (\nabla u, \nabla v)_{L^2} = \langle F(u), v \rangle \quad \text{for all } v \in V,
\]

by fixing \( v = u \), we have

\[
    \|u\|_V^2 \leq \int_{\Omega} \left\{ \lambda (u(x))^2 + \sum_{i=1}^{n} a_i |u(x)|^{p_i+1} \right\} \, dx
\]

\[
    = \lambda \|u\|_{L^2}^2 + \sum_{i=1}^{n} a_i \|u\|_{L^{p_i+1}}^{p_i+1}
\]

\[
    \leq \left\{ \frac{\lambda}{\lambda_1(\Omega)} + \sum_{i=1}^{n} a_i C_{p_i+1}^2 \|u\|_{L^{p_i+1}}^{p_i-1} \right\} \|u\|_V^2.
\]

Therefore, (16) ensures that \( \|u\|_V = 0 \). \( \square \)

On the basis of Lemma 2.1, the following theorem evaluates the number of nodal domains of \( u \) from the inclusions (13) and (14) for \( \hat{u} \).
Theorem 2.4. Let $f$ satisfy (15) for some $\lambda < \lambda_1(\Omega_0)$. We denote $C_{p+1} = C_{p+1}(\Omega)$. If

$$
\sum_{i=1}^{n} a_i C_{p+1}(\Omega_0) \left( \|u\|_{L_{p+1}(\Omega_0)} + C_{p+1}\rho \right)^{p_i - 1} < 1 - \frac{\lambda}{\lambda_1(\Omega_0)},
$$

then the verified solution $u \in V \cap L^\infty(\Omega)$ of the D-problem (12) in the balls (13) and (14) satisfies

$$
\text{#C.C.}(\Omega_+ \cup \Omega_0) \leq \text{#P.N.D.}(u) \leq \text{#C.C.}(\Omega_+),
$$

(19)

$$
\text{#C.C.}(\Omega_- \cup \Omega_0) \leq \text{#N.N.D.}(u) \leq \text{#C.C.}(\Omega_-),
$$

(20)

where #C.C.($\Omega$) is the number of connected components of $\Omega$. Note that if $\Omega_0$ is disconnected, (18) is understood as the set of inequalities for all connected components $\Omega_0^j$ ($j = 1, 2, \cdots$) of $\Omega_0$. If $\Omega_0$ is empty, $\lambda_1(\Omega_0)$ is understood as $\infty$ so that $\lambda/\lambda_1(\Omega_0) = 0$.

Remark 2.5. The formula inside the parentheses in (18) converges to 0 as $\rho \downarrow 0$ and $|\Omega_0| \downarrow 0$ which is equivalent to $\sigma \downarrow 0$ when $\dot{u}$ is continuous. Therefore, as long as verification succeeds for a continuous approximation $\dot{u}$ with sufficient accuracy, the number of nodal domains of $u$ can be evaluated using Theorem 2.4.

Remark 2.6. The connected components on either side of the inequalities (19) and (20) can be determined only from the information of the approximation $\dot{u}$ and the $L^\infty$-error $\sigma$ as in (14); see the definitions of $\Omega_+$, $\Omega_-$, and $\Omega_0$ located just before Lemma 2.1.

Remark 2.7. Explicitly estimating a lower bound for $\lambda_1(\Omega_0)$ and upper bounds for $C_{p+1}(\Omega_0)$ and $C_{p+1}(\Omega_0)$ is essential for Theorem 2.4. This topic is discussed in Appendix A.

Proof of Theorem 2.4

The goal is to prove that there is no nodal domain of $u$ inside $\Omega_0$. To achieve this, we prove that, for some subdomain $\Omega' \subset \Omega_0$, if $u|_{\Omega'}$ (the restriction of $u$ over $\Omega'$) can be regarded as a solution of the D-problem (12) with the notational replacement $\Omega \to \Omega'$, then $u|_{\Omega'}$ should be a trivial solution that satisfies $u|_{\Omega'} \equiv 0$.

Suppose that there exists such a subdomain $\Omega'$ so that $u|_{\Omega'} \in H^1_0(\Omega') (\subset V)$ is a solution of the D-problem (12) with the replacement $\Omega \to \Omega'$. We express $u \in V$ as $u = \dot{u} + \rho \omega$, where $\omega \in V$ satisfies $\|\omega\|_V \leq 1$. This ensures that, for $p \in (1, p^*)$,

$$
\|u\|_{L^{p+1}(\Omega')} \leq \|\dot{u}\|_{L^{p+1}(\Omega')} + C_{p+1}\rho
$$

(21)

because $\|\omega\|_{L^{p+1}(\Omega')} \leq \|\omega\|_{L^{p+1}(\Omega)} \leq C_{p+1} \|\omega\|_V \leq C_{p+1}$. Therefore, it readily follows from $\|\dot{u}\|_{L^{p+1}(\Omega')} \leq \|\dot{u}\|_{L^{p+1}(\Omega_0)}$ that

$$
\|u\|_{L^{p+1}(\Omega')} \leq \|\dot{u}\|_{L^{p+1}(\Omega_0)} + C_{p+1}\rho.
$$

(22)

Therefore, (18) and (22) ensure that

$$
\sum_{i=1}^{n} a_i C_{p+1}(\Omega')^2 \|u|_{\Omega'}\|_{L^{p_i+1}(\Omega')}^{p_i - 1} \leq \sum_{i=1}^{n} a_i C_{p+1}(\Omega_0)^2 \|u|_{\Omega'}\|_{L^{p_i+1}(\Omega')}^{p_i - 1} < 1 - \frac{\lambda}{\lambda_1(\Omega_0)} \leq 1 - \frac{\lambda}{\lambda_1(\Omega')} ,
$$

where $\lambda_1(\Omega') \geq \lambda_1(\Omega_0)$, $C_{p+1}(\Omega') \leq C_{p+1}(\Omega_0)$, and $\|u\|_{L^{p+1}(\Omega')} = \|u|_{\Omega'}\|_{L^{p+1}(\Omega')}$. Hence, it follows from Lemma 2.1 that $u|_{\Omega'} \equiv 0$.

Thus, there is no nodal domain in $\Omega_0$. This implies the evaluations (19) and (20) for the number of positive (negative) nodal domains. □
2.2 Further discussion on the main theorem

In this subsection, we provide some remarks about Theorem 2.4.

2.2.1 Inequality (15) can be weakened

Assuming the $L^\infty$-error estimation (3) (or (14)), we ensure that the range of $u$ is taken over $[\min\{\hat{u}\} - \sigma, \max\{\hat{u}\} + \sigma]$. Therefore, the condition (15) imposed on $f$ is replaceable with

$$tf(t) \leq \lambda t^2 + \sum_{i=1}^{n} a_i|t|^{p_i+1} \text{ for all } t \in [\min\{\hat{u}\} - \sigma, \max\{\hat{u}\} + \sigma]$$

(23)

because (17) is confirmed in the same manner when the $L^\infty$-error $\sigma$ is explicitly estimated.

2.2.2 When assuming only $L^\infty$-error

Given $\sigma$ satisfying (3), $u$ can be written as $u = \hat{u} + \sigma \omega$ with $\omega \in L^\infty(\Omega)$ that satisfies $\|\omega\|_{L^\infty(\Omega)} \leq 1$.

Therefore, applying the inequality

$$\|u\|_{L^{p+1}(\Omega')} \leq \|\hat{u}\|_{L^{p+1}(\Omega_0)} + \sigma|\Omega_0|^{\frac{1}{p+1}}$$

(24)

instead of (22), we have the following similar theorem without assuming an $H^1_0$-error $\rho$ but only an $L^\infty$-error $\sigma$.

**Theorem 2.8.** Let $f$ satisfy (15) for some $\lambda < \lambda_1(\Omega_0)$. If

$$\sum_{i=1}^{n} a_i C_{p_i+1}(\Omega')^2 \left(\|\hat{u}\|_{L^{p_i+1}(\Omega_0)} + \sigma|\Omega_0|^{\frac{1}{p_i+1}}\right)^{p_i-1} < 1 - \frac{\lambda}{\lambda_1(\Omega_0)}.$$  (25)

then the verified solution $u \in V \cap L^\infty(\Omega)$ of the $D$-problem (12) in the ball (14) satisfies (19) and (20).

Note that almost all existing verification methods for the partial differential equation (1) estimate an $L^\infty$-error $\sigma$ after deriving an $H^1_0$-error $\rho$, as described in Subsection 2.3 (see, e.g., [13]). However, if $\sigma$ is obtained directly without computing $\rho$, Theorem 2.8 becomes useful.

2.2.3 Sufficient conditions for (18)

Because $C_{p_i+1}(\Omega_0) \leq C_{p_i+1}(\Omega)$, the following simplified inequality is sufficient for (18) when $C_{p_i+1}(\Omega_0)$ is replaced by $C_{p_i+1}(\Omega)$:

$$\sum_{i=1}^{n} a_i C_{p_i+1}^2 \left(\|\hat{u}\|_{L^{p_i+1}(\Omega_0)} + C_{p_i+1}\rho\right)^{p_i-1} < 1 - \frac{\lambda}{\lambda_1(\Omega)}.$$  (26)

As long as we have $\lambda < \lambda_1(\Omega)$, this is further reduced to

$$\sum_{i=1}^{n} a_i C_{p_i+1}^2 \left(\|\hat{u}\|_{L^{p_i+1}(\Omega_0)} + C_{p_i+1}\rho\right)^{p_i-1} < 1 - \frac{\lambda}{\lambda_1(\Omega)}$$

because $\lambda_1(\Omega_0) \geq \lambda_1(\Omega)$; this is confirmed by considering an extension outside $\Omega_0$. Generally, the shape of $\Omega_0$ tends to be more complicated than $\Omega$, which makes the evaluation of $C_{p_i+1}(\Omega_0)$ and/or $\lambda_1(\Omega_0)$ difficult. The above sufficient inequalities can be useful in such cases.
2.2.4 Application to specific nonlinearities

We apply Theorem 2.4 to two specific problems in which we are interested. The first problem is \((4)\) with the nonlinearity \(f(t) = \lambda t + t|t|^{p-1}, p \in (1,p^*)\). Adapting Theorem 2.4 to this case, we have the following.

**Corollary 2.9.** Let \(f(t) = \lambda t + t|t|^{p-1}, p \in (1,p^*)\). If

\[
C_{p+1}(\Omega_0)^2 \left( \|\hat{u}\|_{L^{p+1}(\Omega_0)} + C_{p+1} \rho \right)^{p-1} < 1 - \frac{\lambda}{\lambda_1(\Omega_0)},
\]

then the verified solution \(u \in V\) of the D-problem \((12)\) in the balls \((13)\) and \((14)\) satisfies \((19)\) and \((20)\).

The second problem is the case in which \(f(t) = \varepsilon^{-2}(t - t^3) (\varepsilon > 0)\). Because \(tf(t) \leq \varepsilon^{-2}t^2\) for all \(t \in \mathbb{R}\), applying Theorem 2.4 to this nonlinearity, we have the following.

**Corollary 2.10.** Let \(f(t) = \varepsilon^{-2}(t - t^3), \varepsilon^{-2} \geq \lambda_1(\Omega)\). If

\[
\varepsilon^{-2} < \lambda(\Omega_0),
\]

then the verified solution \(u \in V\) of the D-problem \((12)\) in the balls \((13)\) and \((14)\) satisfies \((19)\) and \((20)\).

In the next subsection, Corollary 2.10 is applied to an important problem.

2.3 Numerical example

In this subsection, we consider the stationary problem of the Allen–Cahn equation:

\[
\begin{dcases}
-\Delta u(x) = \varepsilon^{-2}(u(x) - u(x)^3), & x \in \Omega, \\
u(x) = 0, & x \in \partial\Omega
\end{dcases}
\]

for which Corollary 2.10 can be used. We demonstrated the applicability of our theory to the problem on square \(\Omega = (0,1)^2\). All computations were implemented on a computer with 2.20 GHz Intel Xeon E7-4830 CPUs \(\times 4\), 2 TB RAM, and CentOS 7 using MATLAB 2019b with GCC version 6.3.0. All rounding errors were strictly estimated using the toolboxes INTLAB version 11 [18] and kv library version 0.4.48 [4]. Therefore, the accuracy of all results was guaranteed mathematically. We constructed approximate solutions of \((12)\) for the domain via a Legendre polynomial basis. Specifically, we define a finite-dimensional subspace \(V_{M_u} \subset V\) as the tensor product \(V_{M_u} = \text{span}\{\phi_1, \phi_2, \cdots, \phi_{M_u}\} \otimes \text{span}\{\phi_1, \phi_2, \cdots, \phi_{M_u}\}\), where each \(\phi_n (n = 1,2,3,\cdots)\) is defined as

\[
\phi_n(x) = \frac{1}{n(n+1)} x(1-x) Q_n(x)
\]

with \(Q_n = \frac{(-1)^n}{n!} \left( \frac{d}{dx} \right)^n x^n(1-x)^n, \ n = 1,2,3,\cdots\).

For a fixed integer \(M_u \geq 1\), we constructed \(\hat{u}\) in \(V_{M_u}\) as

\[
\hat{u}(x,y) = \sum_{i=1}^{M_u} \sum_{j=1}^{M_u} u_{i,j} \phi_i(x) \phi_j(y), \ u_{i,j} \in \mathbb{R}.
\]
Note that our method does not limit the basis functions that constitute approximate solutions, but can be applied to many types of bases other than the Legendre polynomial basis, such as the finite element basis and Fourier basis.

In actual computations to obtain $H^1_0$-errors $\rho$ using the methods proposed in [17, 25], verification was implemented on the solution space $V$ with the generalized inner product and norm

$$(u,v)_\tau = (\nabla u, \nabla v)_{L^2} + \tau (u,v)_{L^2}, \quad \|u\|_\tau = \sqrt{(u,u)_\tau},$$

where $\tau$ is a nonnegative number chosen as

$$\tau > -f'(\hat{u}(x)) = \varepsilon^{-2}(-1 + 3\hat{a}^2) \text{ for all } x \in \Omega.$$  

However, because the norm $\|\cdot\|_\tau$ monotonically increases with $\tau$, the usual norm $\|\cdot\|_V = \|\nabla \cdot\|_{L^2}$ is bounded by $\|\cdot\|_\tau$ for any $\tau \geq 0$. Therefore, we can use the error bound $\|u - \hat{u}\|_\tau$ as the error bound $\rho$ in the sense of the usual norm that is desired in Subsection 2.1 whereas we should allow some overestimation for $\rho$ (see, Table I for estimation results).

We used [5, Theorem 2.3] to obtain an explicit interpolation error constant $C(M)$ ($M \geq 1$) satisfying

$$\|v - P_M v\|_V \leq C(M) \|\Delta v\|_{L^2} \text{ for all } v \in V \cap H^2(\Omega),$$

where the orthogonal projection $P_M$ from $V$ to $V_M$ is defined as

$$(v - P_M v, v_M)_V = 0 \text{ for all } v \in V \text{ and } v_M \in V_M.$$  

The interpolation error constant $C^\tau(M)$ ($M \geq 1$) corresponding to the generalized norm [32] is defined as

$$\|v - P_M^\tau v\|_\tau \leq C^\tau(M) \|\Delta v + \tau v\|_{L^2} \text{ for all } v \in V \cap H^2(\Omega),$$

where $P_M^\tau$ is the orthogonal projection from $V$ to $V_M$ corresponding to [32] that satisfies

$$(v - P_M^\tau v, v_M)_\tau = 0 \text{ for all } v \in V \text{ and } v_M \in V_M.$$  

This generalized constant $C^\tau(M)$ can be estimated from $C(M)$ as follows:

$$C^\tau(M) \leq C(M) \sqrt{1 + \tau C(M)^2};$$

see [21, Remark A.4]. This constant $C^\tau(M)$ was used for obtaining $K$, a key constant for error estimation introduced below. Lower bounds for $\lambda(\Omega_0)$ were estimated using Corollary A.2.

We proved the existence of solutions $u$ of the D-problem [12] (i.e., weak solutions of [29]) in $B(\hat{u}, \rho, \|\cdot\|_V)$ and $B(\hat{u}, \sigma, \|\cdot\|_{L^\infty})$ given approximate solutions $\hat{u}$ constructed as [31]. The proof was achieved by combining the methods described in [17] and [25] using computer assistance. On the basis of [17, Theorem 1], we obtained $H^1_0$-error estimates $\rho$. The required constants $\delta$ and $K$, and function $g$ in the theorem were computed as follows:

- $\delta$ was evaluated as $\delta \leq C_2 \|\Delta \hat{u} + \varepsilon^{-2}(\hat{u} - \hat{u}^3)\|_{L^2}$ with $C_2 = (2\pi^2 + \tau)^{-\frac{1}{2}}$. This $L^2$-norm was computed using a numerical integration method with strict estimation of rounding errors using [4].
- $K$, the norm of the inverse operator, was computed using the method described in [25], with $C^\tau(M_K)$ defined above given $M_K \geq 1$.  

• $g$ was taken as $g(t) = 6\varepsilon^{-2}C_4^3 t \left( \|\hat{u}\|_{L^4(\Omega)} + C_4 t \right)$; see [17, Subsection 4.4] for the construction of $g$. An upper bound for $C_4$ was evaluated using the smaller estimation from [23, Corollary A.2] and [17, Lemma 2] (see, Corollary A.4 and Theorem A.5). Although [23, Corollary A.2] estimates $C_4$ in the sense of the usual norm $\|\cdot\|_V$, it becomes an upper bound for the embedding constant with the generalized norm (32) because $\|\cdot\|_V \leq \|\cdot\|_\tau$ for any nonnegative $\tau$.

By applying the bound for the embedding $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ [16, Corollary 1] to the residual $u - \hat{u} \in H^2(\Omega)$, we also obtained the $L^\infty$-error $\sigma$. Note that the verified solution has the regularity to be in $H^2(\Omega)$. Indeed, for each $h \in L^2(\Omega)$, the problem

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

has a unique solution $u \in H^2(\Omega)$, such as when $\Omega$ is a bounded convex polygonal domain (see [3, Section 3.3]).

Table 1 shows the verification results for (29). The values in rows $\tau$, $C(M_K)$, $\delta$, $K$, $\rho$, $\sigma$, $|\Omega_0|$, and $\varepsilon^{-2}$ represent strict upper bounds in decimal form; for instance, $6.0e\!-\!03$ means $6.0 \times 10^{-3}$. The values in row $\lambda_1(\Omega_0)$ are lower bounds, which were estimated using Corollary A.2. Integers $M_u$, $M_K$, and $2^m$ are displayed as strict integers. Volumes $|\Omega_0|$ were estimated by dividing $\Omega$ into $2^m$ smaller congruent squares and implementing interval arithmetic on them to confirm $(\hat{u} + \sigma)(\hat{u} - \sigma) \leq 0$. Approximate solutions $\hat{u}$ and the corresponding defect bounds $\delta$ were computed in double-double precision using type “dd” or “interval<dd>” equipped in the kv library [4]. Although the values in row $\rho$ represent the error bounds in the sense of the norm (32) for corresponding $\tau$s, these can be regarded as upper bounds for them in the sense of the usual norm $\|\cdot\|_V$ required in Subsection 2.1.

In all cases, the numbers of nodal domains were estimated on the basis of Corollary 2.10 under the condition (28). The number of N.N.D.($u$) for type (A) was evaluated to be 1 or 2, and not determined exactly. This is because it is difficult to determine whether N.N.D.($u$) that appear to be divided in two parts are connected through the boundary (see Fig. 3 (A)). As we can see in column (B) of Table 1, both #P.N.D.($u$) and #N.N.D.($u$) were not determined for solutions type (B). In fact, the evaluations for #N.D.($u$) for this type can be refined to 3 or 4 by considering the topology of nodal lines, that is, “how the lines intersect.” As shown in Fig. 3 (B), the topology depends on the sign of $u$ at the center of $\Omega$. If $u(x) = 0$ at the center exactly, the number of nodal domains is 4, otherwise, that is, when $u(x) > 0$ or $u(x) < 0$, the number of nodal domains is 3. In theory, confirming the exact sign of $u$ at the center, where $\hat{u}(x) = 0$, is impossible unless $\sigma = 0$. Therefore, another or an additional approach is required to strictly determine #N.D.($u$) for type (B). However, without Corollary 2.10 no rigorous information can be obtained about the sign-change structure of such verified solutions from the error bounds (13) or/and (14) only. The corollary provides rough but rigorous estimates for nodal domains and lines. By contrast, for solution type (C), both #P.N.D.($u$) and #N.N.D.($u$) were strictly determined. This solution is special in the sense that the inner nodal line does not touch the original boundary $\partial\Omega$ (see Fig. 3 (C)). In this sense, the inner nodal line can be regarded as a “new” nontrivial Dirichlet boundary. To the best of our knowledge, the existence of such solutions of problem (29) has not been proved. Our method confirmed the existence on the basis of the computer-assisted approaches [17, 16, 25] and Corollary 2.10.
Table 1: Verification results for (29) on $\Omega = (0, 1)^2$.

| ID | (A) | | (B) | | (C) | |
|----|-----|---|-----|---|-----|---|
| $\varepsilon$ | 0.1 | 0.08 | 0.06 | 0.1 | 0.08 | 0.06 | 0.1 | 0.08 | 0.06 |
| $M_u$ | 100 | 100 | 100 | 80 | 80 | 80 | 100 | 100 | 100 |
| $M_K$ | 80 | 80 | 80 | 80 | 80 | 80 | 50 | 100 | 100 |
| $\tau$ | 0 | 102.3 | 436.3 | 0 | 126.1 | 481.7 | 0 | 217.5 | 545.6 |
| $C^\tau(M_K)$ | 6.0e-03 | 6.0e-03 | 6.1e-03 | 6.0e-03 | 6.1e-03 | 6.1e-03 | 9.4e-03 | 4.9e-03 | 4.9e-03 |
| $\delta$ | 1.6e-16 | 5.4e-13 | 2.8e-08 | 1.5e-16 | 1.1e-12 | 1.5e-08 | 1.5e-16 | 3.7e-15 | 7.2e-13 |
| $K$ | 1113 | 10.4 | 53.4 | 263 | 12.9 | 13.4 | 261 | 14.8 | 12.3 |
| $\rho$ | 4.0e-14 | 5.1e-13 | 6.9e-08 | 8.8e-15 | 1.2e-12 | 8.6e-09 | 8.8e-15 | 4.1e-15 | 3.8e-13 |
| $\sigma$ | 1.5e-13 | 1.1e-11 | 3.2e-06 | 3.2e-14 | 1.9e-11 | 3.3e-07 | 3.2e-14 | 5.5e-14 | 1.4e-11 |
| $2^m$ | $2^{20}$ | $2^{20}$ | $2^{20}$ | $2^{20}$ | $2^{22}$ | $2^{24}$ | $2^{20}$ | $2^{20}$ | $2^{20}$ |
| $|\Omega_0|$ | 9.5e-02 | 1.1e-02 | 1.1e-02 | 4.6e-02 | 2.9e-02 | 1.6e-02 | 9.0e-03 | 1.1e-02 | 1.4e-02 |
| $\lambda_1(\Omega_0) \geq$ | 664.6 | 625.7 | 597.6 | 137.5 | 222.8 | 396.3 | 704.7 | 574.1 | 459.0 |
| $\varepsilon^{-2}$ | 100.0 | 156.3 | 277.8 | 100.0 | 156.3 | 277.8 | 100.0 | 156.3 | 277.8 |
| #P.N.D.$(u)$ | 1 | 1–2 | | 1 | 1–2 | |
| #N.N.D.$(u)$ | 1–2 | 1–2 | | 1 | |
| #N.D.$(u)$ | 2–3 | 2–4 | | 2 | |

$\varepsilon$: the positive parameter in (29).
$M_u$: the number of basis functions for constructing approximate solution $\hat{u}$; see (31).
$M_K$: the number of basis functions for calculating $K$.
$\tau$: the nonnegative number satisfying (33).
$C^\tau(M_K)$: the interpolation constant calculated by (36).
$\delta$: the defect bound required in [17, Theorem 1].
$K$: the norm of the inverse operator required in [17, Theorem 1].
$\rho$: $H^{1}_0$-error bound.
$\sigma$: $L^{\infty}$-error bound.
$|\Omega_0|$: the volume of $\Omega_0$; $\Omega_0$ is defined just before Subsection 2.1.
$\lambda_1(\Omega_0)$: the first eigenvalue of $-\Delta$ on $\Omega_0$ defined by (8).
$\varepsilon^{-2}$: the number of positive (negative) nodal domains of $u$; see Definition 1.1.
#N.D.$(u)$: the number of nodal domains that satisfies #N.D.$(u) = \#P.N.D.$(u) + \#N.N.D.$(u)$.

3 Extension to other boundary value conditions

In this section, we extend the results from Section 2 to Neumann type (5) and mixed type (6) boundary value conditions. Because (6) coincides with (5) when $\Gamma_D = \emptyset$ and $\Gamma_N = \partial \Omega$, we discuss the application to (6). The Dirichlet problem (4) is regarded as (5) with the specialization $\Gamma_N = \emptyset$ and $\Gamma_D = \partial \Omega$. Therefore, the generalization to (6) is considered as an extension of the method provided in Section 2.

We introduce (or replace) some required notation. We extend the solution space $V$ to $V := \{u \in H^1(\Omega) : u = 0 \text{ on } \partial \Gamma_D\}$, adapting to the corresponding boundary value condition. The inner product endowed with $V$ should be changed according to the boundary value conditions. When $\Gamma_D = \emptyset$ (i.e., Neumann type), we endow $V$ with the inner product $(u, v)_V = (\nabla u, \nabla v)_{L^2} + (u, v)_{L^2}$; otherwise (i.e., Dirichlet type or mixed type), we endow it with $(u, v)_V = (\nabla u, \nabla v)_{L^2}$. The norm endowed with $V$ is always $\|u\|_V = \sqrt{(u, u)_V}$ regardless of the boundary value conditions. Additionally, the topological dual of $V$ is denoted by $V^\ast$. In this function space setting, the weak form of (6) is characterized by the form (12) with
Figure 2: Sign-changing solutions to (29) on $\Omega = (0, 1)^2$.

Figure 3: Verified nodal lines of the solutions (A), (B), and (C) for $\varepsilon = 0.08$. We confirmed that $(\hat{u} + \sigma)(\hat{u} - \sigma) \leq 0$ on red squares. For ease of viewing, these were drawn with a rough accuracy by dividing the domain $\Omega$ into $2^{12}$ smaller congruent squares and implementing interval arithmetic on each of them (see Fig. 4 for a more accurate nodal line). For each solution, our method proved that there exists no nodal domain of $u$ in the union of the red squares. Simultaneously, the sign of $u$ is strictly determined in the blanks.
the same assumptions for nonlinearity $f$ introduced in Section 2. To avoid confusion, we call (12) corresponding to (5) (assuming $\Gamma_D = \emptyset$ and $\Gamma_N = \partial \Omega$) the N-problem, and call (12) corresponding to (6) (assuming $\Gamma_D \neq \emptyset$ and $\Gamma_N \neq \emptyset$) the M-problem.

We extend the definition of embedding constants. The norm bound $C_{p+1} (= C_{p+1}(\Omega, \Gamma_D))$ for the embedding $V(\Omega, \Gamma_D) \hookrightarrow L^{p+1}(\Omega)$ is defined as
\[
\|u\|_{L^{p+1}(\Omega)} \leq C_{p+1} \|u\|_{V(\Omega, \Gamma_D)} \quad \text{for all } u \in V,
\] where $p \in [1, \infty)$ when $N = 2$ and $p \in [1, p^*)$ when $N \geq 3$. In the following definition (38), we assume $\Gamma_D \neq \emptyset$; considering this case is sufficient for completing the later discussion. The first eigenvalue of $-\Delta$ on $V(\Omega, \Gamma_D)$ is denoted by $\lambda_1(\Omega, \Gamma_D)$, the definition of which is
\[
\lambda_1(\Omega, \Gamma_D) := \inf_{\{v \neq 0\} \subset V \{0\}} \frac{\|v\|^2_{V(\Omega, \Gamma_D)}}{\|v\|^2_{L^2(\Omega)}}.
\] (38)

**Lemma 3.1.** The same argument in Lemma 2.1 is true for the M-problem (12) with a nonempty $\Gamma_D$, where the old notation of eigenvalue $\lambda_1(\Omega)$ and embedding constants $C_{p+1}(\Omega)$ is replaced with new notation: $\lambda_1(\Omega, \Gamma_D)$ and $C_{p+1}(\Omega, \Gamma_D)$, respectively.

**Proof.** Inequality (17) holds for the notational replacements. \hfill \square

We also continue to assume $\Omega_0 \neq \Omega$, as in Section 2. Recall that the connected components of $\Omega_0$ are denoted by $\Omega_0^j (j = 1, 2, \cdots)$, the number of which is assumed to be finite. Note that $\partial \Omega_0^j \setminus \Gamma_N$ should not be empty because $\partial \Omega_0^j \setminus \partial \Omega \neq \emptyset$ is ensured from $\Omega_0 \neq \Omega$ as long as $\Omega_0 \neq \emptyset$.

Moreover, we recall our assumption: some computer-assisted method succeeds in proving the existence of a solution $u \in V \cap L^\infty(\Omega)$ of the D-, N-, or M-problem of (12) in both balls (13) and (14) in this “extended” setting.

**Theorem 3.2.** Let $f$ satisfy (15) for some $\lambda < \min_j \{\lambda_1(\Omega_0^j, \partial \Omega_0^j \setminus \Gamma_N)\}$. Let $C_{p+1} = C_{p+1}(\Omega, \partial \Gamma_D)$, $C_{p+1}^j = C_{p+1}(\Omega_0^j, \partial \Omega_0^j \setminus \Gamma_N)$, and $\lambda_1^j = \lambda_1(\Omega_0^j, \partial \Omega_0^j \setminus \Gamma_N)$. If we have
\[
\sum_{i=1}^n a_i(C_{p+1}^j)^2 \left(\|\hat{u}\|_{L^{p+1}(\Omega_0^j)} + C_{p+1}^j \rho\right)^{p_i-1} < 1 - \frac{\lambda}{\lambda_1^j},
\] (39)
for each $j$, then the verified solution $u \in V \cap L^\infty(\Omega)$ of the D-, N-, or M-problem of (12) in balls (13) and (14) satisfies (19) and (20), where $\lambda_1^j$ is understood as $\infty$ so that $\lambda/\lambda_1^j = 0$ when $\Omega_0^j$ is empty.

**Remark 3.3.** Explicit estimation for a lower bound of $\lambda_1^j$ and upper bounds of $C_{p+1}$ and $C_{p+1}^j$ are discussed in Section A.
Proof of Theorem 3.2

We prove the nonexistence of nodal domains inside \( \Omega_0^j \) for every \( j \), as well as in the proof of Theorem 2.4. To achieve this, we consider the following two cases with respect to the intersection \( \partial \Omega_0^j \cap \Gamma_N \). Hereafter, we denote the \((n - 1)\)-dimensional measure of \( \partial \Omega_0^j \cap \Gamma_N \) by \( |\partial \Omega_0^j \cap \Gamma_N| \).

Case 1 — when \(|\partial \Omega_0^j \cap \Gamma_N| = 0\)

In this case, almost the same discussion in the proof of Theorem 2.4 can be applied (see \( \Omega_0^1 \) or \( \Omega_0^3 \) in Fig. 5).

Suppose that there exists a subdomain \( \Omega' \subset \Omega_0^j \) such that \( u|_{\Omega'} \in H_0^1(\Omega') \subset H_0^1(\Omega_0^j) \) is a solution of the D-problem (12) with the replacement \( \Omega \to \Omega' \). We express \( u \in V (= V(\Omega, \Gamma_D)) \) as \( u = \hat{u} + \rho \omega \), where \( \omega \in V \) satisfies \( \|\omega\|_V \leq 1 \). This ensures that, for \( p \in (1, p^*) \),

\[
\|u\|_{L^{p+1}(\Omega')} \leq \|\hat{u}\|_{L^{p+1}(\Omega')} + C_{p+1} \rho
\]

because \( \|\omega\|_{L^{p+1}(\Omega')} \leq \|\omega\|_{L^{p+1}(\Omega)} \leq C_{p+1} \|\omega\|_V \leq C_{p+1} \), where \( C_{p+1} = C_{p+1}(\Omega, \Gamma_D) \). It readily follows from \( \|\hat{u}\|_{L^{p+1}(\Omega_0^j)} \leq \|u\|_{L^{p+1}(\Omega_0^j)} \) that

\[
\|u\|_{L^{p+1}(\Omega')} \leq \|\hat{u}\|_{L^{p+1}(\Omega_0^j)} + C_{p+1} \rho.
\]

Therefore, (39) and (40) ensure that

\[
\sum_{i=1}^{n} a_i(C'_{p+1})^2 \|u|_{\Omega'}|_{L^{p+1}(\Omega')} \leq \sum_{i=1}^{n} a_i(C_{p+1})^2 \left( \|\hat{u}\|_{L^{p+1}(\Omega_0^j)} + C_{p+1} \rho \right)^{p_i-1}
\]

\[
< 1 - \frac{\lambda}{\lambda_1} \leq 1 - \frac{\lambda}{\lambda_1(\Omega')},
\]

where \( C'_{p+1}(\Omega', \partial \Omega') \leq C_{p+1} \rho \) and \( \lambda(\Omega') \geq \lambda_1 \). Hence, it follows from Lemma 2.1 that \( u|_{\Omega'} \equiv 0 \).

Case 2 — when \(|\partial \Omega_0^j \cap \Gamma_N| \neq 0\)

The main difference from Theorem 2.4 is the possibility of this case (see, \( \Omega_0^2 \) in Fig. 5). Let \( \Omega' \) be an arbitrary subdomain of \( \Omega_0^j \). To reach the desired fact (there exists no nodal domain of \( u \) inside \( \Omega_0^j \)), it is necessary to prove that \( u|_{\Omega'} \) vanishes if it can be considered as a solution of the D- or M-problem of (12) with the notational replacements \( \Omega \to \Omega', \Gamma_D \to \Gamma'_D \), and \( \Gamma_N \to \Gamma'_N \), where \( \Gamma'_N = \partial \Omega' \cap \Gamma_N \) (allowed to be empty) and \( \Gamma'_D = \partial \Omega' \setminus \Gamma'_N \). When \(|\partial \Omega' \cap \Gamma_N| = 0 \), \( u \) can be considered as a solution of the D-problem on \( \Omega' \); therefore, the same argument as that in Case 1 is true.

We are left to consider the case in which \( u|_{\Omega'} \) is a solution of the M-problem where \(|\partial \Omega' \cap \Gamma_N| \neq 0 \). Considering the zero extension outside \( \Omega' \) to \( \Omega_0^j \), the restriction \( u|_{\Omega'} \) can be regarded as a function in \( V(\Omega_0^j, \partial \Omega_0^j \setminus \Gamma_N) \); note that \( u|_{\partial \Omega'} \) can be nonzero only on a subset of \( \Gamma_N \) (again, see \( \partial \Omega_0^j \) in Fig. 5). Therefore, we have \( \lambda(\Omega', \Gamma'_D) \geq \lambda(\Omega_0^j, \partial \Omega_0^j \setminus \Gamma_N) \) and \( C_{p+1}(\Omega', \Gamma'_D) \leq C_{p+1}(\Omega_0^j, \partial \Omega_0^j \setminus \Gamma_N) \), thereby making the same argument as that in Case 1 combined with Lemma 3.1.

4 Conclusion

We proposed a rigorous numerical method for analyzing the sign-change structure of solutions to the elliptic problem (1) with computer-assistance. Given two types of error estimates \( \|u - \hat{u}\|_{H^1_0} \)
Figure 5: Conceptual image of domains \( \Omega, \Omega_+, \Omega_-, \) and \( \Omega_0 \). The upper side (black line) is imposed on the Neumann boundary condition. The lower side (green line) is imposed on the Dirichlet boundary condition. Green lines satisfy \( \Omega_0 = \Omega_0^1 \cup \Omega_0^2 \cup \Omega_0^3 \), which includes the part of \( \overline{\Omega} \) where \( |\hat{u}| \leq \sigma \). These green lines are expected to topologically approximate the nodal lines of \( u \) in the sense that no nodal domain exists inside them. Note that \( \partial \Omega_0^1 \) and \( \partial \Omega_0^3 \) are Dirichlet boundaries in their entirety, whereas some parts of \( \partial \Omega_0^2 \) are Neumann boundaries located on its “sides”.

and \( \|u - \hat{u}\|_{L^\infty} \) between an exact solution \( u \) and a numerically computed approximate solution \( \hat{u} \), we provided a method for estimating the number of nodal domains (see Theorems 2.4 and 3.2). The location of the nodal line of \( u \) can be determined via the information of \( \hat{u} \) and a verified \( L^\infty \)-error \( \sigma \). Our method was applied to the analysis of the sign-change structure of the Allen–Cahn equation (29) subject to the homogeneous Dirichlet boundary condition. In Section 3, our method was extended to Neumann type and mixed type of boundary value conditions (see Theorem 3.2).

A Required constants — eigenvalues and embedding constants

In this section, we discuss evaluating the minimal eigenvalue \( \lambda_1(\Omega_0) \) and embedding constants \( C_{p+1} \) required in Theorems 2.4 and 3.2.

The following theorem can be used to obtain an explicit lower bound for the \( k \)-th eigenvalue \( \lambda_k(\Omega) \) of the Laplacian imposed on the homogeneous Dirichlet boundary condition for a bounded domain \( \Omega \).

**Theorem A.1** ([6]). *Let \( \Omega \) be a bounded domain in \( \Omega \subset \mathbb{R}^N \) \( (N = 1, 2, 3, \cdots) \). We have*

\[
\lambda_k(\Omega) \geq \frac{4\pi^2N}{N + 2} \left( \frac{k}{B_N |\Omega|} \right)^2
\]

*(41)*

*where \( |\Omega| \) and \( B_N \) denote the volume of \( \Omega \) and the unit \( N \)-ball, respectively.*

Adapting Theorem A.1 to the case in which \( N = 2, 3 \), we have the following estimations for the first eigenvalue.
Corollary A.2. Under the same assumption of Theorem [A.1] we have
\[
\lambda_1(\Omega) \geq 2\pi|\Omega|^{-1}, \\
\lambda_1(\Omega) \geq \frac{3 \times 6^\frac{3}{5}}{5} \pi^\frac{2}{5} |\Omega|^{-\frac{2}{5}},
\]
for \( N = 2,3 \).

Theorem [A.1] (or Corollary [A.2]) is reasonable for obtaining rough lower bounds for \( \lambda_1(\Omega_0) \) (= \( \lambda_1(\Omega_0, \partial \Omega_0) \)). If more accuracy is required to satisfy the inequalities assumed in Theorems 2.4 and 3.2 we can use Liu’s method in [3, 7] based on the finite element method. Liu’s method can be further applied to estimate the eigenvalues \( \lambda_1(\Omega_0^j, \partial \Omega_0^j \setminus \Gamma_N) \) (subject to a mixed boundary value condition) required in Theorem 3.2.

Upper bounds for \( C_p(\Omega) (= C_p(\Omega, \partial \Omega)) \) can be estimated via [23, Corollary A.2] or [17, Lemma 2], which are used in the numerical examples in Subsection 2.3. Before introducing them, we quote the following famous result about the best constant in the classical Sobolev inequality. Hereafter, the range of \( p \) is shifted by 1 (in place of \( p + 1 \)) to fit the original notation.

**Theorem A.3** ([1] and [20]). Let \( u \) be any function in \( W^{1,q}(\mathbb{R}^N) \) \((N = 2,3,\ldots)\). Moreover, let \( q \) be any real number such that \( 1 < q < N \), and let \( p = Nq/(N - q) \). Then,
\[
\left( \int_{\mathbb{R}^N} |u(x)|^p \, dx \right)^{\frac{1}{p}} \leq T_p \left( \int_{\mathbb{R}^N} |\nabla u(x)|_2^q \, dx \right)^{\frac{1}{q}}
\]
holds for
\[
T_p = \pi^{-\frac{1}{q}} N^{-\frac{1}{q}} \left( \frac{q - 1}{N - q} \right)^{1 - \frac{1}{q}} \left\{ \frac{\Gamma \left( 1 + \frac{N}{q} \right) \Gamma (N)}{\Gamma \left( \frac{N}{q} \right) \Gamma \left( 1 + N - \frac{N}{q} \right)} \right\}^{\frac{1}{N}}, \tag{42}
\]

where \( |\nabla u|_2 = \left( (\partial u/\partial x_1)^2 + (\partial u/\partial x_2)^2 + \cdots + (\partial u/\partial x_N)^2 \right)^{1/2} \), and \( \Gamma \) denotes the gamma function.

The following corollary obtained from Theorem [A.3] provides a simple bound for the embedding constant from \( H_0^1(\Omega) \) to \( L^p(\Omega) \) for a bounded domain \( \Omega \), where \( H_0^1(\Omega) \) is endowed with the usual norm \( \|\nabla \cdot \|_{L^2} \). Recall that this can be used as an upper bound for the embedding constant with the generalized norm [32].

**Corollary A.4** ([23, Corollary A.2]). Let \( \Omega \subset \mathbb{R}^N \) \((N = 2,3,\ldots)\) be a bounded domain. Let \( p \) be a real number such that \( p \in (N/(N - 1), 2N/(N - 2)] \) if \( N \geq 3 \) and \( p \in (2,\infty) \) if \( N = 2 \). Additionally, set \( q = Np/(N + p) \). Then, (7) holds for
\[
C_p(\Omega) = |\Omega|^{\frac{2q - p}{2q}} T_p,
\]
where \( T_p \) is the constant in (42).

The following theorem estimates the embedding constants where \( H_0^1(\Omega) \) is endowed with the generalized norm [32].

**Theorem A.5** ([17, Lemma 2]). Let \( \lambda_1 \in [0,\infty) \) denote the minimal point of the spectrum of \( -\Delta \) on \( H_0^1(\Omega) \) endowed with the inner product (32), where \( \tau \) is selected so that \( \tau > 0 \) when \( \lambda_1 = 0 \).

a) Let \( n = 2 \) and \( p \in [2,\infty) \). With the largest integer \( \nu \) satisfying \( \nu \leq p/2 \), (7) holds for
\[
C_p(\Omega) = \left( \frac{1}{2} \right)^{\frac{1}{2} + \frac{2q - 3}{p}} \left[ \frac{p}{2} \left( \frac{p}{2} - 1 \right) \cdots \left( \frac{p}{2} - \nu + 2 \right) \right]^{\frac{1}{2}} \left( \lambda_1 + \frac{p}{2} \tau \right)^{-\frac{1}{2}},
\]

b) Let \( n \geq 3 \) and \( p \in [2,\infty) \). With the largest integer \( \nu \) satisfying \( \nu \leq p/2 \), (7) holds for
\[
C_p(\Omega) = \left( \frac{1}{2} \right)^{\frac{1}{2} + \frac{2q - 3}{p}} \left[ \frac{p}{2} \left( \frac{p}{2} - 1 \right) \cdots \left( \frac{p}{2} - \nu + 2 \right) \right]^{\frac{1}{2}} \left( \lambda_1 + \frac{p}{2} \tau \right)^{-\frac{1}{2}},
\]
where \( \frac{p}{2} \left( \frac{p}{2} - 1 \right) \cdots \left( \frac{p}{2} - \nu + 2 \right) = 1 \) if \( \nu = 1 \).

b) Let \( n \geq 3 \) and \( p \in [2, 2n/(n-2)] \). With \( s := n(p-1 - 2^{-1} + n^{-1}) \in [0, 1] \), (7) holds for
\[
C_p(\Omega) = \left( \frac{n - 1}{\sqrt{n}(n-2)} \right)^{1-s} \left( \frac{s}{s\lambda_1 + \tau} \right)^{\frac{\nu}{2}}.
\]

Although Corollary A.4 and Theorem A.5 are reasonable for evaluating embedding constants under the homogeneous Dirichlet boundary conditions, Theorem 3.2 requires upper bounds for more general constants \( C_{p+1}(\Omega, \partial \Omega \cap \Gamma_N) \) and \( C_{p+1}(\Omega_{\theta}, \partial \Omega_{\theta} \cap \Gamma_N) \). Generally, directly evaluating the best values of these embedding constants is not easy. Instead of a direct estimation, we can use the bound for embedding \( H^1(\Omega) \rightarrow L^{p+1}(\Omega) \) as an upper bound. Such an upper bound is provided, for example, in [21, 11] although estimations derived using these methods are rather larger than those in the homogeneous Dirichlet case. Therefore, when \( |\partial \Omega_{\theta} \cap \Gamma_N| \neq 0 \) (corresponding to Case 2 in the proof of Theorem 3.2), inequality (39) is less likely to hold than in Case 1. In the following, we introduce [11, Theorems 2.1 and 3.3], which provide reasonable estimates for the embedding constant. These can be applied to a domain \( \Omega \) that can be divided into a finite number of bounded convex domains \( \Omega_i \) \( (i = 1, 2, 3, \cdots, n) \) such that
\[
\Omega = \bigcup_{1 \leq i \leq n} \Omega_i \quad \text{and} \quad \Omega_i \cap \Omega_j = \emptyset \quad (i \neq j). \tag{43}
\]

**Theorem A.6.** Let \( \Omega \subset \mathbb{R}^N \) be a bounded convex domain. Moreover, let \( d_\Omega := \sup_{x,y \in \Omega} |x-y| \), \( \Omega_x := \{x-y : y \in \Omega\} \) for \( x \in \Omega \), and \( U := \cup_{x \in \Omega \Omega_x} \). Suppose that \( 1 \leq q \leq p < qN/(N-q) \) if \( N > q \), and \( 1 \leq q \leq p < \infty \) if \( N = q \). Then, we have
\[
\|u - u_\Omega\|_{L^p(\Omega)} \leq D_p(\Omega)\|\nabla u\|_{L^q(\Omega)} \quad \text{for all} \quad u \in W^{1,q}(\Omega) \tag{44}
\]
with
\[
D_p(\Omega) = \frac{d_\Omega^N}{N|\Omega|} (A_p A_q A_{p'})^N \|x|^{1-N}\|_{L^r(U)},
\]
where \( r = qp/(q-1)p + q \) and
\[
A_m = \begin{cases} \sqrt{m^{-1}(m-1)^{1-\frac{1}{m}}} & (1 < m < \infty), \\ 1 & (m = 1, \infty). \end{cases}
\]

**Theorem A.7.** Let \( \Omega \subset \mathbb{R}^N \) be a bounded domain, and let \( p \) and \( q \) satisfy \( 1 \leq q \leq p \leq \infty \). Suppose that there exists a finite number of bounded domains \( \Omega_i \) \( (i = 1, 2, 3, \cdots, n) \) satisfying (43). Moreover, suppose that for every \( \Omega_i \) \( (i = 1, 2, 3, \cdots, n) \) there exist constants \( D_p(\Omega_i) \) such that
\[
\|u - u_{\Omega_i}\|_{L^p(\Omega_i)} \leq D_p(\Omega_i)\|\nabla u\|_{L^q(\Omega_i)} \quad \text{for all} \quad u \in W^{1,q}(\Omega_i). \tag{45}
\]
Then,
\[
\left( \int_\Omega |u(x)|^p \, dx \right)^{\frac{1}{p}} \leq C_p'(\Omega) \left( \int_\Omega |u(x)|^q \, dx + \int_\Omega |\nabla u(x)|^q \, dx \right)^{\frac{1}{q}} \tag{46}
\]
holds for
\[
C_p'(\Omega) = \begin{cases} \max \left( 1, \max_{1 \leq i \leq n} D_{\infty}(\Omega_i) \right) & (p = q = \infty), \\ 2^{1-\frac{1}{q}} \max \left( \max_{1 \leq i \leq n} |\Omega_i|^{\frac{1}{p} - \frac{1}{q}}, \max_{1 \leq i \leq n} D_p(\Omega_i) \right) & (\text{otherwise}), \end{cases} \tag{47}
\]
where this formula is understood with \( 1/\infty = 0 \) when \( p = \infty \) and/or \( q = \infty \).
Using Theorems A.6 and A.7 with $q = 2$, we can estimate required bounds for embedding constants. Indeed, $C'_p(\Omega)$ in (46) with $q = 2$ becomes an upper bound for $C_p(\Omega, \Gamma_D)$ for any choices of $\Gamma_D$.

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