偏微分方程式に対する精度保証付き数値計算と符号変化構造解析への応用

Verified numerical computation for partial differential equations and application to sign-change structure analysis

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About me

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Institute for Mathematical Science / 数理科学研究所

- Starts from April 2018
- 13 members belong
- One of the seven priority research areas of Waseda Research Institute for Science and Engineering / 理工学術院総合研究所
- Consists of three groups:
  - Nonlinear Analysis Research Group (Nonlinear Partial Differential Equations, Fluid Mathematics, Fluid Engineering, Nonlinear Dynamical Systems)
  - Computational Mathematics Research Group (Development of innovative numerical methods, simulation techniques, and algorithms for elucidating complex phenomena)
  - Statistical Mathematics Research Group (Mathematical Theory of Data Science, Mathematics of Large Data, Mathematics of Modeling, Financial and Social Mathematics, Mathematics of Network Data, Arithmetic Statistics)

Keywords

- Verified numerical computation / 精度保証付き数値計算
- Numerical verification method / 数値的検証法
- Computer-assisted proofs (analysis) / 計算機援用証明（解析）
- Reliable computing
- Rigorous numerics
- Validated numerics
- Self-validating numerical methods
- Self-validated numerical methods

Verified numerical computation

- Numerical methods strictly estimating errors therein, e.g., rounding errors, truncation errors, and discretization errors.
- Mathematical reliability is added to computation results.
- It can be applied to computer-assisted proofs.
- Interval arithmetic plays an important role for implementing verified numerical computations.

Interval arithmetic

History:

- The origin of interval arithmetic is the seminal master thesis by Teruo Sunaga (須永照夫), handwritten in Japanese, submitted on February 29, 1956.
- R. E. Moore wrote a book concerning interval arithmetic in 1966.
- S. M. Rump and S. Oishi extended it to fast arithmetics for vectors and matrices around 2000.

Example of implementation:

- Let $\mathbb{F}$ be the set of floating point numbers.
- For $\mathbf{a} = [\underline{a}, \overline{a}]$ and $\mathbf{b} = [\underline{b}, \overline{b}]$ $(\underline{a}, \overline{a}, \underline{b}, \overline{b} \in \mathbb{F})$, we calculate

$$\mathbf{a} + \mathbf{b} = [\triangledown(\underline{a} + \underline{b}), \vartriangle(\overline{a} + \overline{b})],$$

where $\triangledown$($\vartriangle$) stands for round down (up).

Do computational errors cause fatal result?

W. M. Kahan,1989

Significant discrepancies (between the computed and the true result) are very rare, too rare to worry about all the time, yet not rare enough to ignore.
ちょっと意訳：数値計算結果と正しい結果の間に著しい食い違いがあることは極めて稀である。極めて稀であるため、常に心配する必要はない。ただ、無視できるほどに稀というわけでもない。

(from Wikipedia)

Rump's example

- Rump [1] found the following example:

$$f(x,y) = (333.75 - a^2)b^6 + a^2(11a^2b^2 - 121b^4 - 2) + 5.5b^8 + \frac{a}{2b}.$$

- For example, when $a = 77617$ and $b = 33096$ (what's happen with computers?).

Spurious solution of Emden's equation

- Breuer-Plum-McKenna observed a spurious solution of Emden's equation $-\Delta u = u^2$ due to discretization errors [2].
- The existence of asymmetric solutions has been denied by Gidas-Ni-Nirenberg's theory.

76 B. Breuer et al.

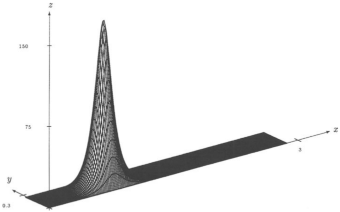


Figure 6.3. "Spurious" approximate solution of (22) for $\zeta = 2.9$

$$\Delta u + u^2 = 0$$

[2] B. Breuer, M. Plum, and P. McKenna, "Inclusions and existence proofs for solutions of a nonlinear boundary value problem by spectral numerical methods," in *Topics in Numerical Analysis*, pp. 61–77, Springer, 2001

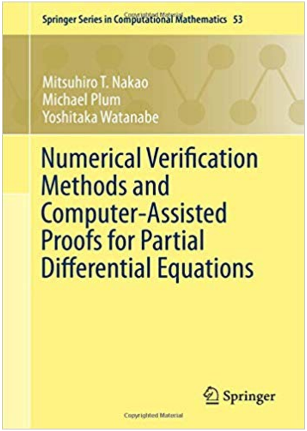
Patriot Missile Failure

- An American Patriot Missile failed to track and intercept an incoming Iraqi Scud missile.
  - Date: February 25, 1991, during the Gulf War
  - Location: Dhahran, Saudi Arabia
  - Number of deaths: 28
  - Number of injuries: 100

Quoted from:

http://www.sydrose.com/case100/298/
http://www-users.math.umn.edu/~arnold//disasters/patriot.html

Books



[3] S. Oishi and etc, *Foundation of Verified Numerical Computations (in Japanese)*. Corona Publishing Co., Ltd., 2018
[4] M. T. Nakao, M. Plum, and Y. Watanabe, *Numerical Verification Methods and Computer-Assisted Proofs for Partial Differential Equations*. Springer Series in Computational Mathematics, 2019

Libraries

- Intlab: a MATLAB/Octave toolbox for verified numerical computation by S.M. Rump.
  `http://www.ti3.tu-harburg.de/rump/intlab/`
- kv library: a library written in C++ developed by M. Kashiwagi.
  `http://verifiedby.me/kv/`
- VCP library: a library for “Verified Computation for PDEs” by K. Sekine. This has been developed on the basis of kv library.
  `https://verified.computation.jp/`

Interest: Computer-assisted proofs

- Four color theorem, 1976
- Double bubble conjecture, 1995
- Kepler conjecture, 1998
- Lorenz attractor, 2002
  *14th of Smale's problems proved by Warwick Tucker

Computer-assisted proofs for PDEs with verified numerical computation

- The breakthrough is goes back to the works around 1990 [5, 6].
- Recent methods are mainly based on
  - Newton-Kantorovich's theorem or its improvement
  - Direct application of several fixed point theorems (e.g., Banach's or Schauder's)
  - Semigroup theories for parabolic equations
  - Sub- and super-solution methods
- Recent developments are found in, e.g., [3, 4].

[3] S. Oishi and etc, *Foundation of Verified Numerical Computations (in Japanese)*. Corona Publishing Co., Ltd., 2018

[4] M. T. Nakao, M. Plum, and Y. Watanabe, *Numerical Verification Methods and Computer-Assisted Proofs for Partial Differential Equations*. Springer Series in Computational Mathematics, 2019

[5] M. T. Nakao, "A numerical approach to the proof of existence of solutions for elliptic problems," *Japan Journal of Applied Mathematics*, vol. 5, no. 2, pp. 313–332, 1988

[6] M. Plum, "Computer-assisted existence proofs for two-point boundary value problems," *Computing*, vol. 46, no. 1, pp. 19–34, 1991

What is proved?

- If a certain "good" approximate solution $\hat{u}$ is obtained, the existence of an exact solution u is proved as in the form of the inequality:

$$\|u - \hat{u}\| \leq r$$

Exact
Unknown

Approx.
with computers

Error bound
Unknown

- That is, we prove the existence of solutions with quantitative information; moreover, under suitable conditions, multiplicity, local uniqueness, and nondegeneracy are proved together.
- But, only from the inequality, we cannot obtain *qualitative* information other than them, such that sign (positivity and negativity), the number of sign-changes, convexity, etc.

Scope: Nodal domain (sign change)

Definition 1

For a function $u : \Omega \to \mathbb{R}$, the connected components of the open sets

$$\{x \in \Omega \ : \ u(x) > 0\} \ \textit{and} \ \{x \in \Omega \ : \ u(x) < 0\}$$

are called **the nodal domains** *of u. The zero level-set $\{x \in \Omega \ : \ u(x) = 0\}$ is called* **the nodal line** *of u.*

#N.D.(u): the nodal number of the nodal domains of u

Question: $\#\text{N.D.}(u) = \#\text{N.D.}(\hat{u})$?

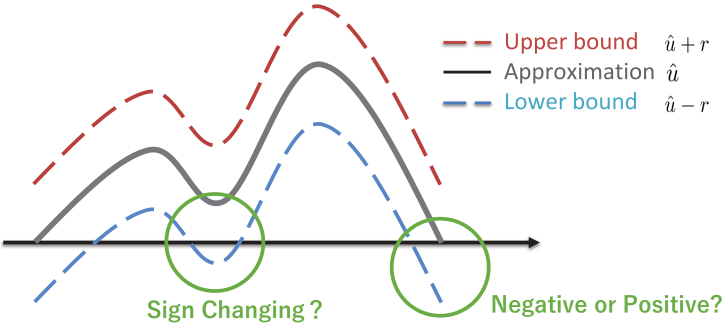
Answer: No! (generally)

$$\|u - \hat{u}\| \leq r$$

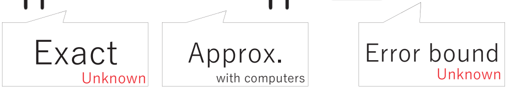
Exact
Unknown

Approx.
with computers

Error bound
Unknown



$$\|u - \hat{u}\| \le r$$


Exact
Unknown
Approx.
with computers
Error bound
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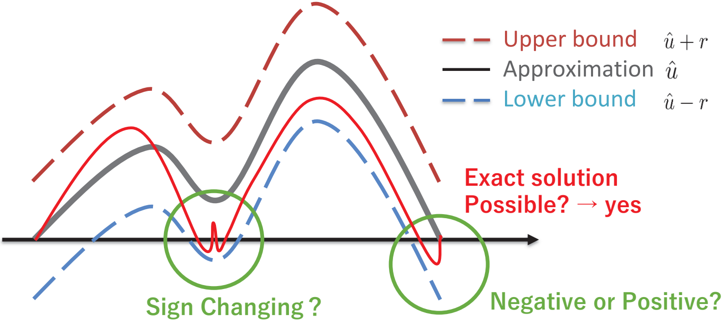
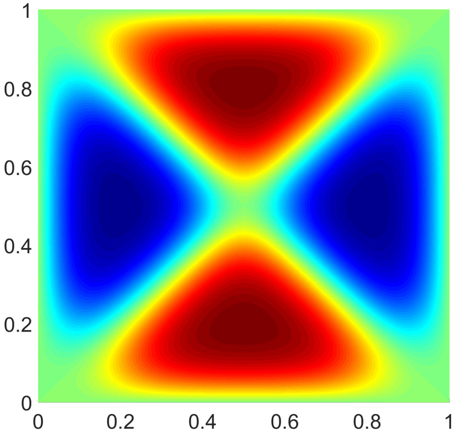
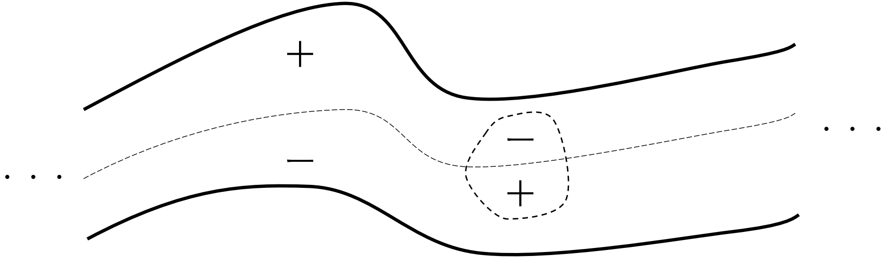

Upper bound $\hat{u} + r$
Approximation $\hat{u}$
Lower bound $\hat{u} - r$
Exact solution
Possible? → yes
Sign Changing ?
Negative or Positive?



It seems and I hope that #N.D.$(u) = 4$...



Conceptional figure for the area where $(\hat{u} - \sigma)(\hat{u} + \sigma) < 0$ between the two solid lines.

Purpose

- Let $\Omega \subset \mathbb{R}^n$ $(n = 1, 2, 3)$ be a bounded domain.
- Our objective is the semilinear elliptic problem

$$\begin{cases} -\Delta u(x) = f(u(x)) & x \in \Omega, \\ \text{B.C.} \end{cases}$$

- The purpose is to

Rigorously estimate $\#\text{N.D.}(u)$

as well as to reveal the topological information of the nodal lines, the zero level sets of u, (how they intersect).

Contents

Contents

Dirichlet problem

In this section, we discuss verification method for the homogeneous Dirichlet problem:

$$\begin{cases} -\Delta u(x) = f(u(x)), & x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega, \end{cases} \tag{D}$$

where f is a C^1 function satisfying

$$|f(t)| \leq a_0|t|^p + b_0 \quad \text{for all} \quad t \in \mathbb{R},$$
$$|f'(t)| \leq a_1|t|^{p-1} + b_1 \quad \text{for all} \quad t \in \mathbb{R}$$

for some $a_0, a_1, b_0, b_1 \geq 0$ and $p < p^*$.

Notation

- $L^p(\Omega)$ $(1 \le p < \infty)$: the functional space of p-th power Lebesgue integrable functions over Ω.
- $L^\infty(\Omega)$: the functional space of Lebesgue measurable functions over Ω, with the norm $\|u\|_{L^\infty(\Omega)} := \operatorname{ess\,sup}\{|u(x)| \mid x \in \Omega\}$ for $u \in L^\infty(\Omega)$.
- $H^k(\Omega)$: the kth order L^2 Sobolev space on Ω.
- $H_0^1(\Omega) := \left\{u \in H^1(\Omega) : u = 0 \text{ on } \partial\Omega \text{ in the trace sense}\right\}$, i.e., the closure of $C_0^\infty(\Omega)$ in $H^1(\Omega)$.
- We denote $V = H_0^1(\Omega)$ and $V^* =$(the dual space of V).
- The norm bound for the embedding $V \hookrightarrow L^{p+1}(\Omega)$ is denoted by $C_{p+1} (= C_{p+1}(\Omega))$, that is, C_{p+1} is a positive number that satisfies

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

where $p \in [1, \infty)$ when $N = 1, 2$ and $p \in [1, p^*]$ when $N \ge 3$.

Weak form

We define the operator F by

$$F : \begin{cases} u(\cdot) & \mapsto & f(u(\cdot)), \\ V & \to & V^*. \end{cases}$$

Moreover, we define another operator $\mathcal{F} : V \to V^*$ by $\mathcal{F}(u) := -\Delta u - F(u)$, which is characterized by

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

where $\langle F(u), v \rangle = \int_\Omega f(u(x))v(x)dx$. Under these notation and assumptions, we look for solutions $u \in V$ of

$$\mathcal{F}(u) = 0, \tag{P}$$

which corresponds to the weak form of (D). We call this *D-problem* preventing confusion with the other boundary value problems.

Theorem 1 (Newton-Kantorovitch's theorem)

Suppose that there exists some $\alpha > 0$ satisfying

$$\|\mathcal{F}_{\hat{u}}'^{-1}\mathcal{F}(\hat{u})\|_V \leq \alpha. \tag{1}$$

Moreover, suppose that there exists some $\beta > 0$ satisfying

$$\|\mathcal{F}_{\hat{u}}'^{-1}(\mathcal{F}_v' - \mathcal{F}_w')\|_{\mathcal{L}(V,V)} \leq \beta\|v - w\|_V \text{ for all } v, w \in D, \tag{2}$$

where $D = B(\hat{u}, 2\alpha + \delta)$ is an open ball depending on $\alpha > 0$ and small $\delta > 0$. If $\alpha\beta \leq 1/2$, there exists a solution $u \in V$ of $\mathcal{F}(u) = 0$ satisfying

$$\|u - \hat{u}\|_V \leq \frac{1 - \sqrt{1 - 2\alpha\beta}}{\beta} (=: \rho). \tag{3}$$

The solution u is unique in $\overline{B}(\hat{u}, 2\alpha)$.

Required constants

- α is estimated by

$$\alpha \leq \|\mathcal{F}_{\hat{u}}'^{-1}\|_{\mathcal{L}(V^*,V)} \|\mathcal{F}(\hat{u})\|_{V^*}$$

- β is estimated by

$$\beta \leq \|\mathcal{F}_{\hat{u}}'^{-1}\|_{\mathcal{L}(V^*,V)} L,$$

  where L is a positive number satisfying

$$\left\|F_v' - F_w'\right\|_{\mathcal{L}(V,V^*)} \leq L\|v - w\|_V \text{ for all } v, w \in D.$$

- The most important and difficult part is to estimate the operator norm of $\|\mathcal{F}_{\hat{u}}'^{-1}\|$.
- Several methods for estimating the inverse norm have been developed.

Estimation of $\|\mathcal{F}_{\hat{u}}'^{-1}\|_{\mathcal{L}(V^*,V)}$

Theorem 2

Let $\Phi : V \to V^*$ be the canonical isometric isomorphism. If the point spectrum of $\Phi^{-1}\mathcal{F}_{\hat{u}}'$ (denoted by $\sigma_p(\Phi^{-1}\mathcal{F}_{\hat{u}}'))$ does not contain zero, then the inverse of $\mathcal{F}_{\hat{u}}'$ exists and

$$\left\|\mathcal{F}_{\hat{u}}'^{-1}\right\|_{B(V^*,V)} \leq \mu_0^{-1}, \tag{4}$$

where

$$\mu_0 = \min\left\{|\mu| \ : \ \mu \in \sigma_p\left(\Phi^{-1}\mathcal{F}_{\hat{u}}'\right) \cup \{1\}\right\}. \tag{5}$$

[7] K. Tanaka, A. Takayasu, X. Liu, and S. Oishi, “Verified norm estimation for the inverse of linear elliptic operators using eigenvalue evaluation,” *Japan Journal of Industrial and Applied Mathematics*, vol. 31, no. 3, pp. 665–679, 2014

The eigenvalue problem $\Phi^{-1}\mathcal{F}'_{\hat{u}}u = \mu u$ in V is equivalent to

$$(\nabla u, \nabla v) - \left(F'_{\hat{u}}u, v\right) = \mu\,(u, v)_V \quad \text{for all } v \in V.$$

Since $\mu = 1$ is already known to be in $\sigma\left(\Phi^{-1}\mathcal{F}'_{\hat{u}}\right)$, it suffices to look for eigenvalues $\mu \neq 1$. By setting $\lambda = (1-\mu)^{-1}$, we further transform this eigenvalue problem into

$$\text{Find } u \in V \text{ and } \lambda \in \mathbb{R} \text{ s.t. } (u, v)_V = \lambda\left((\tau + F'_{\hat{u}})u, v\right) \quad \text{for all } v \in V. \tag{6}$$

(6) is an eigenvalue problem, the spectrum of which consists of a sequence $\{\lambda_k\}_{k=1}^{\infty}$ of eigenvalues converging to $+\infty$.

In order to compute K on the basis of Theorem 2, we explicitly enclose the eigenvalue λ that minimizes the corresponding absolute value of $|\mu|\left(= |1 - \lambda^{-1}|\right)$, by considering the following approximate eigenvalue problem

$$\begin{aligned}&\text{Find } u \in V_N \text{ and } \lambda^N \in \mathbb{R}\\ &\qquad \text{s.t. } (u_N, v_N)_V = \lambda^N\left((\tau + F'_{\hat{u}})u_N, v_N\right) \quad \text{for all } v_N \in V_N,\end{aligned} \tag{7}$$

where V_N is a finite-dimensional subspace of V.

Theorem 3 ([7, 8])

Suppose that there exists a positive number C_N^τ *such that*

$$\left\|u_g - P_N^\tau u_g\right\|_V \leq C_N^\tau \|g\|_{L^2(\Omega)} \tag{8}$$

for any $g \in L^2(\Omega)$ *and the corresponding weak solution* $u_g \in V$ *to* $-\Delta u = g$. *Then,*

$$\frac{\lambda_k^N}{\lambda_k^N \left(C_N^\tau\right)^2 \|\tau + f'(\hat{u}(\cdot))\|_{L^\infty(\Omega)} + 1} \leq \lambda_k \leq \lambda_k^N.$$

[7] K. Tanaka, A. Takayasu, X. Liu, and S. Oishi, "Verified norm estimation for the inverse of linear elliptic operators using eigenvalue evaluation," *Japan Journal of Industrial and Applied Mathematics*, vol. 31, no. 3, pp. 665–679, 2014

[8] X. Liu, "A framework of verified eigenvalue bounds for self-adjoint differential operators," *Applied Mathematics and Computation*, vol. 267, pp. 341–355, 2015

L^∞-esitimates

Theorem 4 ([9])

For all $u \in H^2(\Omega)$*,*

$$\|u\|_{L^\infty(\Omega)} \le c_0\|u\|_{L^2(\Omega)} + c_1\|\nabla u\|_{L^2(\Omega)} + c_2\|u_{xx}\|_{L^2(\Omega)}$$

with

$$c_j = \frac{\gamma_j}{|\overline{\Omega}|}\left[\max_{x_0\in\overline{\Omega}} \int_{\overline{\Omega}} |x - x_0|^{2j} dx\right]^{1/2}, \ (j = 0, 1, 2),$$

where u_{xx} *denotes the Hesse matrix and* $\gamma_0,\ \gamma_1,$ *and* γ_2 *are constants.*

Note: explicit values of $\gamma_0,\ \gamma_1,$ and γ_2 are shown in (see [9]).

[9] M. Plum, "Explicit H^2-estimates and pointwise bounds for solutions of second-order elliptic boundary value problems," *Journal of Mathematical Analysis and Applications*, vol. 165, no. 1, pp. 36–61, 1992

L^∞-esitimates

- By substituting $u - \hat{u}$ in the formula, we have

$$\|u - \hat{u}\|_{L^\infty(\Omega)} \le c_0\|u - \hat{u}\|_{L^2(\Omega)} + c_1\|\nabla(u - \hat{u})\|_{L^2(\Omega)} + c_2\|(u - \hat{u})_{xx}\|_{L^2(\Omega)}.$$

- For regular Ω, e.g., polygonal Ω,

$$\|u_{xx}\|_{L^2(\Omega)} = \|\Delta u\|_{L^2(\Omega)}$$

  for all $u \in H^2(\Omega) \cap V$ [10].
- All that's left is calculating each term, but it is not easy in general.

[10] P. Grisvard, *Elliptic problems in nonsmooth domains*, vol. 69. SIAM, 2011

Summary of Section 1

- We presented a verification method the elliptic problem

$$\begin{cases} -\Delta u(x) = f(u(x)), & x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega. \end{cases} \tag{D}$$

  on the basis of Newton-Kantorovich's theorem.
- For the elliptic problem, H_0^1-error estimation can be obtained.
- L^∞-error estimation is also obtained by considering the embedding $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$.

Contents

Objective

We continue to consider the homogeneous Dirichlet problem:

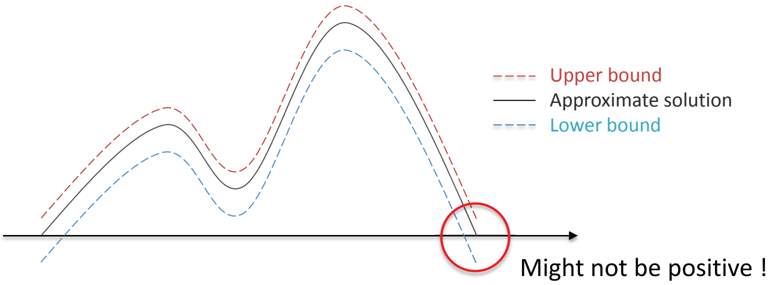
$$\begin{cases} -\Delta u(x) = f(u(x)), & x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega \end{cases} \tag{D}$$

and the corresponding weak form

$$\mathcal{F}(u) = 0 \tag{P}$$

with the same assumption in the previous section.

Positive solution and its enclosure



- It is possible for the exact solution u to be negative in some part, even if approximation $\hat{u}$ is positive.
- On the contrary, u may be positive even when $\hat{u}$ is negative in some part as long as the verified enclosure contains a positive function.
- In essence, it is not necessary to confirm $\hat{u} \geq 0$.

Purpose in Section 2

To prove the positivity of u of (D) only assuming H_0^1-error estimation:

$$\|u - \hat{u}\|_{H_0^1} \leq \rho.$$

- This will be done without L^∞-error estimation.

Previous research

- [11] for odd function $f(t)$
- [12] generalizing this to general f
- [13] further applying this to the best constant for the embedding $H_0^1(\Omega) \hookrightarrow L^p(\Omega)$, namely the case in which $f(t) = t^p$
- The above methods required L^∞-error estimation

$$\|u - \hat{u}\|_{L^\infty} \leq \sigma.$$

- It often needs H^2-regularity of solution u.

[11] K. Tanaka, K. Sekine, M. Mizuguchi, and S. Oishi, "Numerical verification of positiveness for solutions to semilinear elliptic problems," *JSIAM Letters*, vol. 7, pp. 73–76, 2015

[12] K. Tanaka, K. Sekine, and S. Oishi, "Numerical verification method for positivity of solutions to elliptic equations," *RIMS Kôkyûroku*, vol. 2037, pp. 117–125, 2017

[13] K. Tanaka, K. Sekine, M. Mizuguchi, and S. Oishi, "Sharp numerical inclusion of the best constant for embedding $H_0^1(\Omega) \hookrightarrow L^p(\Omega)$ on bounded convex domain," *Journal of Computational and Applied Mathematics*, vol. 311, pp. 306–313, 2017

Important lemma for proving positivity

Lemma 1

Let f satisfy

$$tf(t) \leq \lambda t^2 + \sum_{i=1}^{n} a_i |t|^{p_i+1} \quad \text{for all } \; t \in \mathbb{R} \tag{9}$$

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

$$\sum_{i=1}^{n} a_i C_{p_i+1}^2 \|u\|_{L^{p_i+1}}^{p_i-1} < 1 - \frac{\lambda}{\lambda_1(\Omega)}, \tag{10}$$

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

Remark 1

The inequality (9) *can be reduced to the combination the following inequalities:*

$$f(t) \leq \lambda t + \sum_{i=1}^{n} a_i t^{p_i} \ \text{ for all } \ t \geq 0,$$

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

Therefore, the polynomial $f(t) = \lambda t + \sum_{i=2}^{n(<p^*)} a_i t|t|^{i-1}$ *with* $\lambda < \lambda_1(\Omega)$ *and* $a_i \in \mathbb{R}$ *obviously satisfies the required inequality* (9). *Indeed, for the set of subscripts* Λ_+ *for which* $a_i \geq 0$ $(i \in \Lambda_+)$ *and* $a_i < 0$ (*otherwise*), *we have* $f(t) \leq \lambda t + \sum_{i \in \Lambda_+} a_i t^i$ *and* $-f(-t) \leq \lambda t + \sum_{i \in \Lambda_+} a_i t^i$ *for all* $t \geq 0$.

Proof.

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

$$\begin{aligned}
\|u\|_V^2 \leq & \int_\Omega \left\{ \lambda \left(u(x)\right)^2 + \sum_{i=1}^{n} a_i |u(x)|^{p_i+1} \right\} dx \\
= & \lambda \|u\|_{L^2}^2 + \sum_{i=1}^{n} a_i \|u\|_{L^{p_i+1}}^{p_i+1} \\
\leq & \left\{ \frac{\lambda}{\lambda_1(\Omega)} + \sum_{i=1}^{n} a_i C_{p_i+1}^2 \|u\|_{L^{p_i+1}}^{p_i-1} \right\} \|u\|_V^2 .
\end{aligned}$$

Therefore, (10) ensures $\|u\|_V = 0$.

Theorem for proving positivity

Theorem 5

Let f satisfy

$$-f(-t) \leq \lambda t + \sum_{i=1}^{n} a_i t^{p_i} \quad \text{for all} \quad t \geq 0 \tag{11}$$

for some $\lambda < \lambda_1(\Omega_-)$, nonnegative coefficients $a_1, a_2, \cdots, a_n$, and subcritical exponents $p_1, p_2, \cdots, p_n \in (1, p^*)$. If

$$\sum_{i=1}^{n} a_i C_{p_i+1}^2 \left(\|\hat{u}_-\|_{L^{p_i+1}} + C_{p_i+1}\rho \right)^{p_i-1} < 1 - \frac{\lambda}{\lambda_1(\Omega_-)}, \tag{12}$$

then the verified solution $u \in V$ of D-problem (P) *in $\overline{B}(\hat{u}, \rho)$ is nonnegative.*

Notation: $\Omega_- = \{x \in \Omega : u(x) \leq 0\}, \quad \hat{u}_- := \max\{-\hat{u}, 0\}$

About $\lambda < \lambda_1(\Omega_-)$

- Note that $\Omega_- = \{x \in \Omega : u(x) \leq 0\}$ is information about an exact solution u
- It follows from $\Omega \supset \Omega_-$ that

$$\lambda_1(\Omega) \leq \lambda_1(\Omega_-).$$

  Therefore, when

$$\lambda < \lambda_1(\Omega)$$

  we also have $\lambda < \lambda_1(\Omega_-)$.

  $\Rightarrow$ Hence, in this case, Ω_- is replaceable with Ω.
- The ease of positivity verification depends on the coefficient of linear term λ.

Example 1: $f(t) = \lambda t + t|t|^{p-1}$

- When $\lambda \geq \lambda_1(\Omega)$, (D) has no positive solution
- Therefore, it is sufficient to consider the case in which $\lambda < \lambda_1(\Omega)$

Corollary 1

Let $f(t) = \lambda t + t|t|^{p-1}$, with $\lambda < \lambda_1(\Omega)$ and $p \in (1, p^*)$. If

$$C_{p+1}^2 \left(\|\hat{u}_-\|_{L^{p+1}} + C_{p+1}\rho\right)^{p-1} < 1 - \frac{\lambda}{\lambda_1(\Omega)}, \tag{13}$$

then the verified solution $u \in V$ of (P) *in $\overline{B}(\hat{u}, \rho)$ is positive.*

- For example when $\lambda = 0$, it is reduced to $\|\hat{u}_-\|_{L^{p+1}} \leq C_{p+1}^{\frac{2}{1-p}} - C_{p+1}\rho$.
- If $p = 3$ and $\Omega = (0, 1)^2$, it is reduced to $\|\hat{u}_-\|_{L^{p+1}} \leq 3.15 - 0.319\rho$.
- Furthermore, if $\hat{u} \geq 0$, it is reduced to $\rho \leq 9.86$.

Example 2: $f(t) = \lambda(t - t^3)$

- When $\lambda < \lambda_1(\Omega)$, (D) has no positive solution.
- Therefore, $\lambda_1(\Omega_-)$ should be estimated to satisfy $\lambda < \lambda_1(\Omega_-)$.

Corollary 2

Let $f(t) = \lambda(t - t^3)$, with $\lambda \geq \lambda_1(\Omega)$. If

$$\lambda < \lambda_1(\Omega_-),$$

then the verified solution $u \in V$ of (P) in $\overline{B}(\hat{u}, \rho)$ is positive.

Evaluation for $\lambda_1(\Omega_-)$

- It goes easy if we have an L^∞-error estimate:

$$\|u - \hat{u}\|_{L^\infty} \leq \sigma.$$

  For example, using the method in [14], we can evaluate a lower bound for $\lambda_1(\Omega_-)$.
- We hope to evaluate $\lambda_1(\Omega_-)$ only assuming an H_0^1-error estimate.
- The biggest problem is that the shape of Ω_- is unknown.
- All we know is that $\Omega_- \subset \Omega$ and $|\Omega_-|$ is very "small".

[14] X. Liu and S. Oishi, "Verified eigenvalue evaluation for the laplacian over polygonal domains of arbitrary shape," *SIAM Journal on Numerical Analysis*, vol. 51, no. 3, pp. 1634–1654, 2013

Evaluation for lower bounds

Lemma 2 ([15])

Let $\Omega \subset \mathbb{R}^N$ $(N = 1, 2, 3, \cdots)$ *is a bounded domain, and* λ_k k*-th eiganvalue of* $-\Delta$ *on* Ω*. Then, we have*

$$\lambda_k \geq \frac{4\pi^2 N}{N+2} \left(\frac{k}{B_N |\Omega|} \right)^{\frac{2}{N}}, \tag{14}$$

where $|\Omega|$ *and* B_N *stands for the volume of* Ω *and the unit* N*-ball, respectively.*

[15] P. Li and S.-T. Yau, "On the schrödinger equation and the eigenvalue problem," *Communications in Mathematical Physics*, vol. 88, no. 3, pp. 309–318, 1983

Evaluation for lower bounds

Adapting Lemma 2 to the case in which $N = 2, 3$, we have the following estimations for the first eigenvalue.

Corollary 3

Under the same assumption, we have

$$\lambda_1(\Omega) \geq 2\pi|\Omega|^{-1}, \qquad N = 2,$$

$$\lambda_1(\Omega) \geq \frac{3 \times 6^{\frac{2}{3}}}{5}\pi^{\frac{4}{3}}|\Omega|^{-\frac{2}{3}}, \qquad N = 3.$$

[15] P. Li and S.-T. Yau, “On the schrödinger equation and the eigenvalue problem,” *Communications in Mathematical Physics*, vol. 88, no. 3, pp. 309–318, 1983

Upper bound for $|\Omega_-|$

Prerequisite: $\|u - \hat{u}\|_V \leq \rho$

Theorem 6

Assume that approximate solution $\hat{u}$ is continuous or piecewise continuous over Ω. For a real number m, define

$$\hat{\Omega}_m := \{x \in \Omega : \hat{u}(x) \leq m\}.$$

If

$$\|\hat{u}_+\|_{L^{p+1}(\hat{\Omega}_m)} \geq C_{p+1}\rho$$

for an arbitrarily fixed $p \in [1, p^*)$, then we have

$$|\Omega_-| \leq |\hat{\Omega}_m|.$$

Steps for evaluation of $\lambda_1(\Omega_-)$

1. Select $p \in [1, p^*)$. $p = 1$ is useful for us.
2. For a small $m > 0$, we set $\hat{\Omega}_m := \{x \in \Omega : \hat{u}(x) \leq m\}$ and confirm that

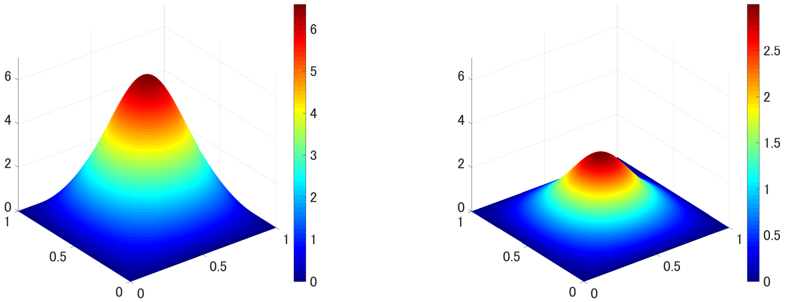
$$\|\hat{u}_+\|_{L^{p+1}(\hat{\Omega}_m)} \geq C_{p+1}\rho.$$

3. Evaluate $\lambda_1(\Omega_-)$ via $|\hat{\Omega}_m|$. For example when $n = 2, 3$, it follows from Corollary 3 that

$$\lambda_1(\Omega_-) \geq 2\pi|\hat{\Omega}_m|^{-1}, \qquad (N = 2)$$

$$\lambda_1(\Omega_-) \geq \frac{3 \times 6^{\frac{2}{3}}}{5}\pi^{\frac{4}{3}}|\hat{\Omega}_m|^{-\frac{2}{3}}, \qquad (N = 3)$$

Application 1: $f(t) = t|t|^{p-1}$



$p = 3, \ \max_{x \in \Omega} \hat{u}(x) \approx 6.6232$ $\qquad$ $p = 5, \ \max_{x \in \Omega} \hat{u}(x) \approx 3.1721$

Figure 1: Solutions for $p = 3, 5$.

Application 1: $f(t) = t|t|^{p-1}$

Table 1: Verification results for $p = 3, 5$.

p	3	5
N	40	40
$\lVert \mathcal{F}_{\hat{u}}'^{-1} \rVert_{\mathcal{L}(V^*,V)}$	1.70325176	2.36317681
$\lVert \mathcal{F}(\hat{u}) \rVert_{V^*}$	$2.64173615 \times 10^{-8}$	$1.92671579 \times 10^{-3}$
L	0.67839778	6.47198581
α	$4.49954173 \times 10^{-8}$	$4.55317005 \times 10^{-3}$
β	1.15548221	15.2944468
ρ	$4.63295216 \times 10^{-8}$	$5.47604979 \times 10^{-3}$
C_{p+1}	0.31830989	0.39585400
$\lVert \hat{u}_- \rVert_{L^{p+1}}$	$4.19109326 \times 10^{-2}$	$4.81952900 \times 10^{-2}$
$C_{p+1}^2 \left(\lVert \hat{u}_- \rVert_{L^{p+1}} + C_{p+1}\rho \right)^{p-1}$	$1.77973446 \times 10^{-4}$	$1.00813027 \times 10^{-6}$

The limits of evaluation

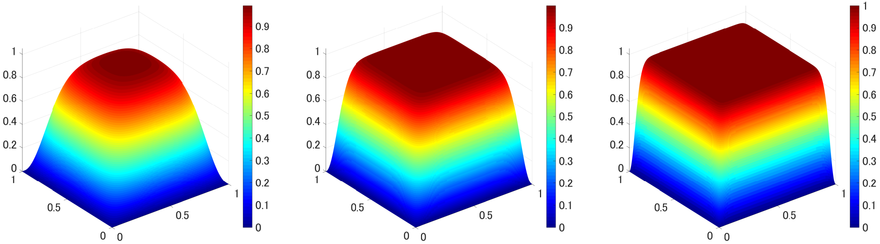
1. When ρ is fixed, how rough can we evaluate $\|\hat{u}_-\|_{L^{p+1}}$?

   When $p = 3 \Rightarrow \|\hat{u}_-\|_{L^{p+1}} \leq 3.15$ then OK.
   When $p = 5 \Rightarrow \|\hat{u}_-\|_{L^{p+1}} \leq 1.59$ then OK.

2. When $\|\hat{u}_-\|_{L^{p+1}} = 0$, how large can we evaluate ρ?

   When $p = 3 \Rightarrow \rho \leq 9.86$ then OK.
   When $p = 5 \Rightarrow \rho \leq 4.01$ then OK.

Application 2: $f(t) = \varepsilon^{-2}(t - t^3)$



$\varepsilon = 0.1$ $\varepsilon = 0.05$ $\varepsilon = 0.025$

Figure 2: Solutions for $\varepsilon = 0.1, 0.05, 0.025$.

Application 2: $f(t) = \varepsilon^{-2}(t - t^3)$

Table 2: Verification results for $\varepsilon = 0.1, 0.05, 0.025$.

ε	0.1	0.05	0.025
N	40	40	60
$\|\mathcal{F}_{\hat{u}}'^{-1}\|_{\mathcal{L}(V^*,V)}$	2.85871420	4.57367687	26.8239159
$\|\mathcal{F}(\hat{u})\|_{V^*}$	$5.57390453 \times 10^{-10}$	$2.15869521 \times 10^{-6}$	$1.99428443 \times 10^{-6}$
L	3.00408573	5.02704780	7.57229904
α	$1.59342000 \times 10^{-9}$	$9.87317430 \times 10^{-6}$	$5.34945174 \times 10^{-5}$
β	8.58782250	22.9920923	$2.03118712 \times 10^{+2}$
ρ	$1.59342002 \times 10^{-9}$	$9.87429519 \times 10^{-6}$	$5.37883476 \times 10^{-5}$
m	2^{-4}	2^{-4}	2^{-4}
$\lambda_1(\Omega_-) \geq$	$2.09235179 \times 10^{+2}$	$1.83828050 \times 10^{+3}$	$2.57359270 \times 10^{+4}$
ε^{-2}	$1.0 \times 10^{+2}$	$4.0 \times 10^{+2}$	$1.6 \times 10^{+3}$

Summary of Section 2

- We proposed a method for proving the positivity of solutions of the elliptic problem

$$\begin{cases} -\Delta u(x) = f(u(x)), & x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega. \end{cases} \tag{D}$$

- We assume an H_0^1-error estimation between u and its approximation $\hat{u}$

$$\|u - \hat{u}\|_V \le \rho.$$

- Our method can be applied provided that $\hat{u}$ is sufficiently near to a nonnegative function and ρ sufficiently small.
- The advantage of this method is no L^∞-error estimation is required.

Contents

Required verification results

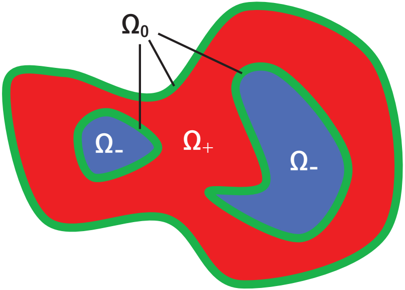
- Let $\hat{u} \in H_0^1(\Omega) \cap L^\infty(\Omega)$ be a numerical computed approximate solution (usually which may have higher regularity in real computations).
- Suppose that one can succeed to prove the existence of u in the forms:

$$\|\nabla(u - \hat{u})\|_{L^2} \leq \rho$$
$$\|u - \hat{u}\|_{L^\infty} \leq \sigma,$$

  using verified numerical computation methods for PDEs.
- σ is important for determining the location of nodal lines.

Notation

- $\overline{u} := \hat{u} + \sigma$ and $\underline{u} := \hat{u} - \sigma$
- $\Omega_+ := \{x \in \Omega : \underline{u}(x) > 0\}$ or its superset,
- $\Omega_- := \{x \in \Omega : \overline{u}(x) < 0\}$ or its superset,
- $\Omega_0 := \Omega \backslash (\Omega_+ \cup \Omega_-)$



Main theorem for verifying #N.D.(u)

Theorem 7

Let f satisfy (9) *for some $\lambda < \lambda_1(\Omega_0)$. Denote $C_{p_i+1} = C_{p_i+1}(\Omega)$. If*

$$\sum_{i=1}^{n} a_i C_{p_i+1}(\Omega_0)^2 \left(\|\hat{u}\|_{L^{p_i+1}(\Omega_0)} + C_{p_i+1}\rho \right)^{p_i-1} < 1 - \frac{\lambda}{\lambda_1(\Omega_0)}, \qquad (15)$$

then the verified solution $u \in V$ of the D-problem (P) *satisfies*

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

where $\#\text{C.C.}(\Omega)$ is the number of connected components of Ω. Note that if Ω_0 is disconnected, (15) *is understood as the set of inequalities for all connected components Ω_0^j $(j = 1, 2, \cdots)$ of Ω_0. If Ω_0 is empty, $\lambda_1(\Omega_0)$ is understood as ∞ so that $\lambda/\lambda_1(\Omega_0) = 0$.*

Remark 2

Sicne $C_{p_i+1}(\Omega_0) \le C_{p_i+1}(\Omega)$, the following simplified inequality is a sufficient for (15) *with replacing $C_{p_i+1}(\Omega_0)$ with $C_{p_i+1}(\Omega)$.*

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

As long as we have $\lambda < \lambda_1(\Omega)$, this further simplified 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 $\lambda_1(\Omega_0) \ge \lambda_1(\Omega)$; this is confirmed by considering extension outside Ω_0.

Allen-Cahn equation

As an important problem, we consider the stationary problem of Allen-Cahn equation:

$$\begin{cases} -\Delta u(x) = \varepsilon^{-2}(u(x) - u(x)^3), & x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega, \end{cases} \tag{AC}$$

which is equivalent to (D) with the nonlinearity $f(t) = \varepsilon^{-2}(t - t^3)$.

Application to Allen-Cahn equation

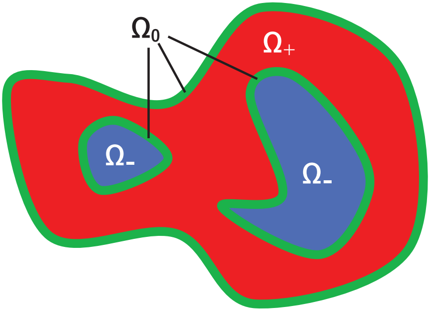
Corollary 4

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

$$\varepsilon^{-2} < \lambda_1(\Omega_0), \tag{16}$$

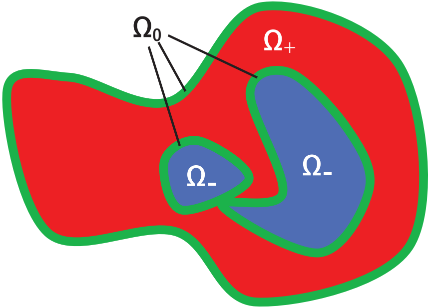
then the verified solution $u \in V$ *of D-problem* (P) *satisfies*

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



$$\varepsilon^{-2} < \lambda_1 \rightarrow \begin{cases} \text{P.N.D}(u) = 1 \\ \text{N.N.D}(u) = 2 \\ \text{N.D}(u) = 3 \end{cases}$$

$$\varepsilon^{-2} \geq \lambda_1 \rightarrow \text{unknown}$$



$\varepsilon^{-2} < \lambda_1$

$$\to \begin{cases} \text{P.N.D}(u) = 1 \\ 1 \leq \text{N.N.D}(u) \leq 2 \\ 2 \leq \text{N.D}(u) \leq 3 \end{cases}$$

$\varepsilon^{-2} \geq \lambda_1 \to$ unknown

Numerical examples

We consider

$$\begin{cases} -\Delta u(x) = \varepsilon^{-2}(u(x) - u(x)^3), & x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega, \end{cases} \tag{AC}$$

with a unit square $\Omega = (0, 1)^2$. To obtain "good" approximate solutions, we constructed approximate solutions $\hat{u}$ using a Legendre polynomial basis.

To get verified inclusions,

$$\|\nabla(u - \hat{u})\|_{L^2} \leq \rho$$

and

$$\|u - \hat{u}\|_{L^\infty} \leq \sigma,$$

we used the method described in [16].

[16] M. Plum, "Existence and multiplicity proofs for semilinear elliptic boundary value problems by computer assistance," *Jahresbericht der Deutschen Mathematiker Vereinigung*, vol. 110, no. 1, pp. 19–54, 2008

Sign-changing solutions

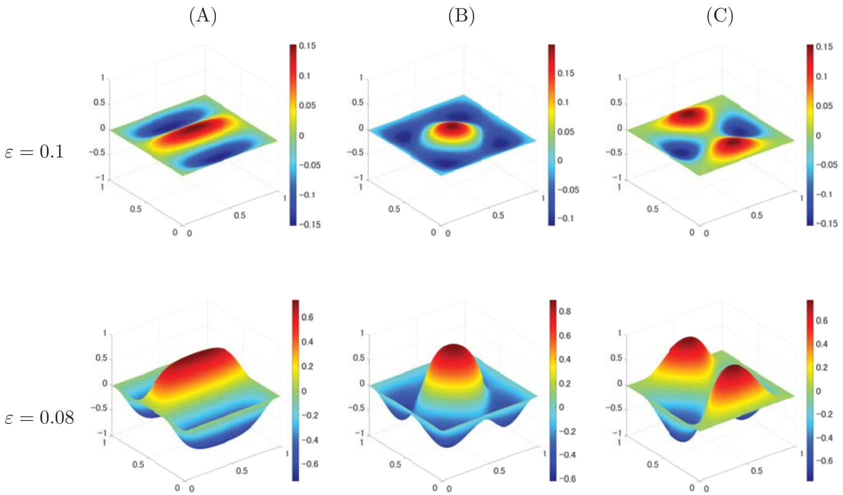


Figure 3: Verified solutions of (AC).

Sign-changing solutions

$\varepsilon = 0.06$

$\varepsilon = 0.04$

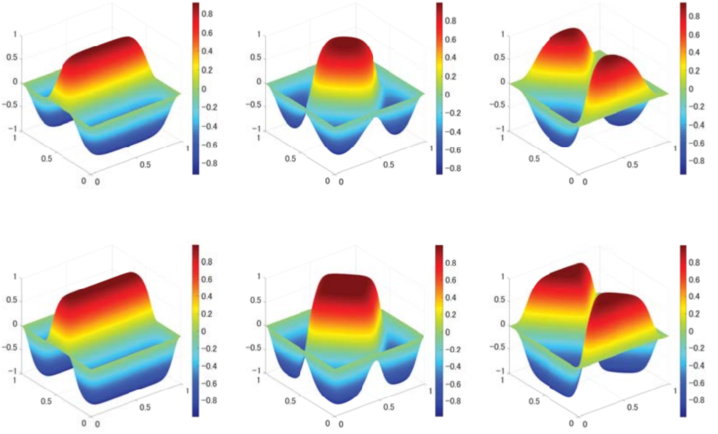


Figure 4: Verified solutions of (AC).

Table 3: Verification results of sign-changing solutions to (AC).

ID	ε	N	ρ	σ	#P.N.D.	#N.N.D.	#N.D.
(A)	0.1	100	3.96e-14	1.45e-13	1	1 – 2	2 – 3
	0.08	100	5.03e-13	1.03e-11			
	0.06	100	6.81e-08	3.11e-06			
	0.04	150	3.90e-06	4.98e-04			
(B)	0.1	100	8.74e-15	3.12e-14	1	1	2
	0.08	100	4.08e-15	5.46e-14			
	0.06	100	3.75e-13	1.39e-11			
	0.04	120	1.14e-07	1.44e-05			
(C)	0.1	80	8.74e-15	3.12e-14	1 – 2	1 – 2	2 – 4
	0.08	80	1.17e-12	1.86e-11			
	0.06	80	8.55e-09	3.29e-07			
	0.04	120	5.68e-07	7.13e-05			

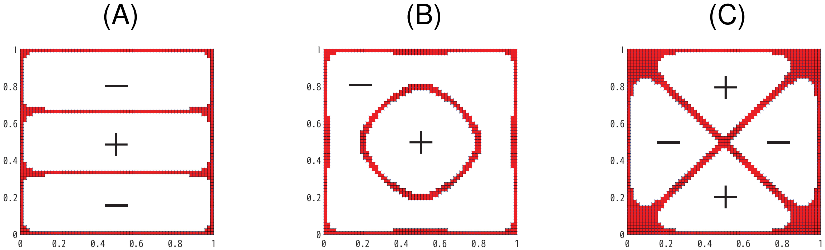


Figure 5: Verified nodal lines of the solutions (A), (B), and (C) for $\varepsilon = 0.08$. We confirmed $(\hat{u} + \sigma)(\hat{u} - \sigma) \leq 0$ on red squares. For ease of viewing, these were drawn with rough accuracy by dividing the domain Ω into 2^{12} smaller congruent squares and implementing interval arithmetic on each of them. For each solution, our method proved that there exists no nodal domain of u in Ω_0, the union of the red squares. Meanwhile, the sign of u is strictly determined in the blanks.

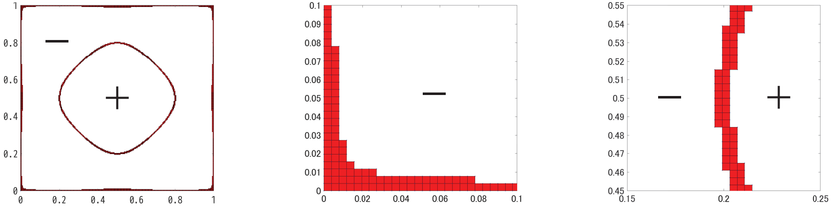
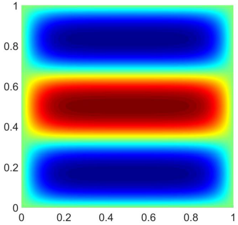


Figure 6: Accurate inclusion of nodal line of solution (B) with $\varepsilon = 0.08$ (left), and its magnifications (center and right). These were drawn by dividing the domain Ω into 2^{16} smaller congruent squares and implementing interval arithmetic on each of them. In the blanks, the sign of u is strictly determined.

Refinement the estimate of #N.D.(u)

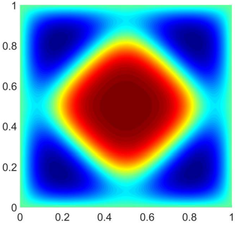
(A)



$1 \leq \#\mathrm{N.N.D}(u) \leq 2$

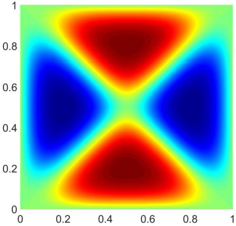
$\Rightarrow \#\mathrm{N.N.D}(u) = 2$

(B)



$\#\mathrm{N.D}(u) = 2$

(C)



$2 \leq \#\mathrm{N.D}(u) \leq 4$

$\Rightarrow 3 \leq \#\mathrm{N.D}(u) \leq 4$

Summary for Section 3

- We proposed a rigorous numerical method for analyzing the sing-change structure of solutions to the elliptic problem

$$\begin{cases} -\Delta u(x) = f(u(x)), & x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega. \end{cases} \tag{P}$$

- The required assumption is the error estimations between u and its approximation $\hat{u}$ in the form:

$$\|\nabla(u - \hat{u})\|_{L^2} \leq \rho,$$
$$\|u - \hat{u}\|_{L^\infty} \leq \sigma.$$

- We showed the application to Allen-Cahn equation.

Contents

Extension to other boundary conditions

We extend our theorems to the mixed boundary value problem

$$\begin{cases} -\Delta u(x) = f(u(x)), & x \in \Omega, \\ u(x) = 0, & x \in \Gamma_D, \\ \frac{\partial u}{\partial n}(x) = 0, & x \in \Gamma_N, \end{cases} \tag{M}$$

where $\Gamma_D, \Gamma_N \subset \partial\Omega$ satisfy $\Gamma_D \cap \Gamma_N = \emptyset$ and $\Gamma_D \cup \Gamma_N = \partial\Omega$.

Extended notation

- We extend the solution space to $V := \{u \in H^1(\Omega) : u = 0 \text{ on } \partial\Gamma_D\}$.
- The inner product endowed with V should be changed depending on boundary 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 boundary conditions.
- To avoid confusion, we call (P) corresponding to (M) (with assuming $\Gamma_N = \partial\Omega$) as *N-problem*, and call (P) corresponding to (M) (with assuming $\Gamma_D \neq \emptyset$ and $\Gamma_N \neq \emptyset$) as *M-problem*.

Extended notation

- 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 by

$$\|u\|_{L^{p+1}(\Omega)} \leq C_{p+1} \|u\|_{V(\Omega,\Gamma_D)} \quad \text{for all } u \in V, \tag{17}$$

where $p \in [1, \infty)$ when $N = 1, 2$ and $p \in [1, p^*]$ when $N \geq 3$.

- In the following definition (18), we assume $\Gamma_D \neq \emptyset$. Expecting this special case is enough 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

$$\lambda_1(\Omega, \Gamma_D) := \inf_{v \in V \setminus \{0\}} \frac{\|v\|^2_{V(\Omega,\Gamma_D)}}{\|v\|^2_{L^2(\Omega)}}. \tag{18}$$

Extended theorem

Theorem 8

Let f satisfy (9) *for some $\lambda < \min_j\{\lambda_1(\Omega_0^j, \partial\Omega_0^j \backslash \Gamma_N)\}$. Denote $C_{p_i+1} = C_{p_i+1}(\Omega, \partial\Omega\backslash\Gamma_N)$, $C^j_{p_i+1} = C_{p_i+1}(\Omega_0^j, \partial\Omega_0^j\backslash\Gamma_N)$, and $\lambda_1^j = \lambda_1(\Omega_0^j, \partial\Omega_0^j\backslash\Gamma_N)$. If we have*

$$\sum_{i=1}^{n} a_i (C^j_{p_i+1})^2 \left(\|\hat{u}\|_{L^{p_i+1}(\Omega_0^j)} + C_{p_i+1}\rho \right)^{p_i-1} < 1 - \frac{\lambda}{\lambda_1^j}, \tag{19}$$

for each j, then the verified solution $u \in V$ of (M) *satisfies,*

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

where the first eigenvalue is understood as ∞ when Ω_0^j is empty.

Contents