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A verified continuation algorithm for solution curve of nonlinear elliptic equations

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Abstract—In this article, a verified numerical continuation method is proposed for a nonlinear operator equation. Numerical continuation method calculates solution curve of parameterized nonlinear equation approximately. Although the verified numerical computation yields point wise proofs of the solution curve, continuous branch following is difficult to be proved. On the basis of the implicit function theorem, a smooth solution branch of Ambrosetti-Prodi's type problem is obtained by our verified continuation approach.

1. Introduction

Let $\mathbb{R}$ be the set of real numbers. V is assumed to be a Hilbert space. In this article, we consider to find $(u,\lambda) \in V\times\mathbb{R}$ such that

$$G(u,\lambda) = 0 \text{ in } V. \tag{1}$$

Here, G is a nonlinear map from $V\times\mathbb{R}$ to V. The aim of this article is to pursue the solution path of parameterized nonlinear operator equation explicitly. The solution path is the set of equilibria: $\mathcal{E} = \{(u,\lambda)\in V\times\mathbb{R} : G(u,\lambda) = 0\}$. Numerical continuation method, which calculates the solution curve of parameterized nonlinear equation approximately, is known as an efficient approach for the problem (1). There are several techniques of getting a solution branch numerically. It is difficult to prove the existence of exact solution around the approximate solution due to some computational errors of approximation.

On the other hand, verified computations of nonlinear operator equation [1, 2, 3] etc. enable us to figure out all errors in computation explicitly. Methods of verified computations have been developed over the last two decades. For a fixed λ, we can prove the existence and local uniqueness of the exact solution with computer-assistance. Although the verified computation yields point wise proofs of the solution path, continuous branch following is still difficult to be proved. This article propose a method of smooth continuation for the parameterized nonlinear operator equation (1) on the basis of the implicit function theorem. We call the proposed method as verified continuation method.

2. Notation and formulation

Let Ω be a bounded polygonal or polyhedral domain in $\mathbb{R}^d$ $(d = 1,2,3)$. We denote the usual Lebesgue and Sobolev spaces on Ω by $L^2(\Omega)$ and $H^1(\Omega) = W^{1,2}(\Omega)$. The L^2 inner product is denoted by

$$(\mathrm{u},\mathrm{v})_{L^2} := \int_\Omega \mathrm{u}^T\mathrm{v}dx \ \text{ for } \mathrm{u},\mathrm{v}\in L^2(\Omega)^d.$$

Let us set a function space $V := \{v\in H^1(\Omega) : v = 0 \text{ on } \partial\Omega\}$. Here, $v = 0$ on $\partial\Omega$ is in the trace sense. We endow a inner product with $(u,v)_V := (\nabla u,\nabla v)_{L^2}$ for $u,v\in V$.

In this article, we consider the following parameterized nonlinear elliptic problem:

$$\begin{cases} -\Delta u = f(u,\lambda) & \text{in } \Omega, \\ u|_{\partial\Omega} = 0, \end{cases} \tag{2}$$

where $f : H_0^1(\Omega)\times\mathbb{R}\to L^2(\Omega)$ is assumed to be Fréchet differentiable with respect to u and λ. Let λ be a real parameter. The variational formulation of the problem (2) is given as: Find $(u,\lambda)\in V\times\mathbb{R}$ such that

$$(\nabla u,\nabla v)_{L^2} - (f(u,\lambda),v)_{L^2} = 0,\ \forall v\in V.$$

From the Riesz representation theorem, we can define a nonlinear operator $G : V\times\mathbb{R}\to V$ by

$$(G(u,\lambda),v)_V := (\nabla u,\nabla v)_{L^2} - (f(u,\lambda),v)_{L^2},\ \forall v\in V.$$

Then, the problem (2) is described by the operator equation (1) equivalently. The partial Fréchet derivative of G corresponding to u at $(u_0,\lambda_0)\in V\times\mathbb{R}$ is denoted by $G_u[u_0,\lambda_0] : V\to V$. For $v\in V$, it satisfies

$$(G_u[u_0,\lambda_0]v,w)_V := (\nabla v,\nabla w)_{L^2} - (f_u[u_0,\lambda_0]v,w)_{L^2},\ \forall w\in V,$$

where $f_u[u_0,\lambda_0]$ is the partial Fréchet derivative of f with respect to u at (u_0,λ_0). Furthermore, the partial Fréchet derivative of G with λ at (u_0,λ_0) is denoted by $G_\lambda[u_0,\lambda_0] : \mathbb{R}\to V$. For $\mu\in\mathbb{R}$,

$$(G_\lambda[u_0,\lambda_0]\mu,w)_V := -\mu(f_\lambda[u_0,\lambda_0],w)_{L^2},\ \forall w\in V,$$

where $f_\lambda[u_0,\lambda_0]$ is the partial Fréchet derivative of f with λ at (u_0,λ_0).

Consider a regular triangulation of Ω. The Lagrange finite element space $V_h \subset V$ will be used to find the approximate solution of (2). The function in V_h is a continuous function over the domain and its restriction on each element is a polynomial of a certain degree. Let P_h be the operator to project V onto V_h with the inner product $(\cdot,\cdot)_V$. It satisfies

$$(u - P_h u, v_h)_V = 0, \ \forall v_h \in V_h.$$

Assuming that the following a priori error estimate holds

$$\|u - P_h u\|_V \le M_h \|\Delta u\|_{L^2}, \ \ \|u - P_h u\|_{L^2} \le M_h^2 \|\Delta u\|_{L^2}.$$

The error constant M_h depends only on the mesh size h, the degree of polynomial, and the solution singularity.

3. Simple parameter continuation

This part is devoted to explaining a parameter continuation algorithm. Numerical continuation methods compute a family or path of solutions of (1) in the finite dimensional space $V_h \times \mathbb{R}$. Suppose that we are given an approximate solution $(u_0, \lambda_0) \in V_h \times \mathbb{R}$ of (1). The idea of simple parameter continuation is to find a solution at $\lambda = \lambda_0 + \delta\lambda$ for a small perturbation $\delta\lambda$. Then, we can follow the solution path step by step.

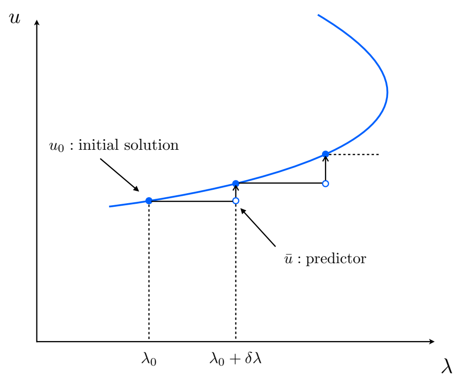

Figure 1: Simple parameter continuation

This is also called the predictor-corrector method which proceeds in two steps. First, we predict the rough approximation of solution at λ. Second, the corrector step refines the initial approximation by using Newton's method. For a given λ and an initial guess $\bar{u} \in V_h$ of the solution $u(\lambda)$, we iterate the following steps until $\|\delta u\| < \varepsilon$ is satisfied for a small $\varepsilon > 0$,

$$\begin{aligned} &(G_u[\bar{u}, \lambda]\delta u, v_h)_V = -(G(\bar{u}, \lambda), v_h)_V, \ \forall v_h \in V_h, \\ &\bar{u} = \bar{u} + \delta u. \end{aligned} \tag{3}$$

When it stops, the solution $u(\lambda)(= \bar{u})$ is determined on the basis of Newton's method. It is well known that the procedure will converges quadratically when the initial guess is sufficiently close to the solution. In particular, the simple parameter continuation uses the previous solution u_0 as the predictor in the next step. Then, the corrector step compute the solution $u(\lambda)$ by the Newton iterations, see Figure 1.

Algorithm 1 (Simple parameter continuation) *Given a known solution $(u_0, \lambda_0) \in V_h \times \mathbb{R}$, we compute the solution at nearby value $\lambda = \lambda_0 + \delta\lambda$ as follows:*

1. *Determine the predictor $\bar{u} = u_0$ by the solution at λ_0.*
2. *Refine the initial guess by Newton's iteration (3) until convergence.*
3. *Use $(u(\lambda), \lambda) \in V_h \times \mathbb{R}$ as the new initial entry (u_0, λ_0) and go back to Step 1.*

Suppose that $(u(\lambda), \lambda)$ is obtained for each fixed λ. The original problem (1) is transformed into

$$\text{Find } u \in V \text{ such that } F(u) = 0 \text{ in } V. \tag{4}$$

$F : V \to V$ is assumed to be the Fréchet differentiable mapping with respect to u. Let $\hat{u} := u(\lambda) \in V_h$ be the approximate solution to (4). The Fréchet derivative of F at $\hat{u}$ is denoted by $F_u[\hat{u}] : V \to V$. In order to verify the existence and local uniqueness of the exact solution in the neighborhood of $\hat{u}$, we consider to apply the Newton-Kantorovich theorem.

Theorem 1 (Newton-Kantorovich)
Assuming the Fréchet derivative $F_u[\hat{u}] : V \to V$ is nonsingular and satisfies

$$\|F_u[\hat{u}]^{-1} F(\hat{u})\|_V \le \alpha,$$

for a certain positive α. Then, let

$$\overline{B}(\hat{u}, 2\alpha) := \{v \in V : \|v - \hat{u}\|_V \le 2\alpha\}$$

be a closed ball centered at $\hat{u}$ with radius 2α. Let also $D \supset \overline{B}(\hat{u}, 2\alpha)$ be an open ball in V. We assume that for a certain positive ω, it holds:

$$\|F_u[\hat{u}]^{-1}(F_u[v] - F_u[w])\|_{V,V} \le \omega \|v - w\|_V, \quad \forall v, w \in D.$$

If $\alpha\omega \le \frac{1}{2}$ holds, then there is a solution $u \in V$ of (4) satisfying

$$\|u - \hat{u}\|_V \le \rho := \frac{1 - \sqrt{1 - 2\alpha\omega}}{\omega}.$$

Furthermore, the solution u is unique in $\overline{B}(\hat{u}, \rho)$.

Corollary 2 *To apply the Newon-Kantorovich theorem, we calculate three constants below explicitly.*

$$\|F_u[\hat{u}]^{-1}\|_{V,V} \le C_1, \tag{5}$$

$$\|F(\hat{u})\|_V \le C_{2,h},$$

$$\|F_u[v] - F_u[w]\|_{V,V} \le C_3\|v - w\|_V, \quad \forall v, w \in D \subset V.$$

The constants C_1, $C_{2,h}$ and C_3 yield

$$\|F_u[\hat{u}]^{-1}F(\hat{u})\|_V \le C_1C_{2,h},$$

and

$$\|F_u[\hat{u}]^{-1}(F_u[v] - F_u[w])\|_{V,V} \le C_1C_3\|v - w\|_V.$$

Therefore, if the condition $C_1^2C_{2,h}C_3 \le 1/2$ is confirmed by verified numerical computations, then the existence and local uniqueness of the solution are proved numerically based on the Newton-Kantorovich theorem.

Then, for each point $u(\lambda)$, we can validate the existence and local uniqueness of exact solution. Although the verified computation yields point wise proofs of the solution path, continuous branch following is still difficult to be proved.

4. A verified continuation method

In this section, we propose a method of verifying continuous solution curve of parameterized nonlinear operator equation (1). On the basis of *radii polynomials*, there are one existing method to compute continuous solution path [4]. Through the method derives precise estimate, it deeply depends on base functions of approximation. It is difficult to apply the method to the finite element method. The basic tool for the verified continuation is the implicit function theorem. First, we note some assumptions which need to prove the implicit function theorem. We fix $(u_0, \lambda_0) \in V_h \times \mathbb{R}$. Assuming $G_u[u_0, \lambda_0]$ is nonsingular and satisfies

$$\|G_u[u_0, \lambda_0]^{-1}\|_{V,V} \le b_0.$$

$G_\lambda[u_0, \lambda_0]$ is bounded by

$$\|G_\lambda[u_0, \lambda_0]\|_{\mathbb{R},V} \le K_0.$$

Furthermore, it follows that

$$\|G(u_0, \lambda_0)\|_V \le \rho_0.$$

Setting $r_0 > 2b_0\rho_0$ and $\varepsilon > 0$, let us define

$$B(u_0, r_0) := \{v \in V : \|v - u_0\|_V \le r_0\}$$

and

$$B(\lambda_0, \varepsilon) := \{\lambda \in \mathbb{R} : |\lambda - \lambda_0| \le \varepsilon\}.$$

Suppose that there exist constants $M, N \ge 0$ satisfying

$$\|G_u[v, \lambda] - G_u[w, \lambda]\|_{V,V} \le M\|v - w\|_V$$

and

$$\|G_\lambda[v, \lambda] - G_\lambda[w, \lambda]\|_{\mathbb{R},V} \le N\|v - w\|_V$$

for $\forall\lambda \in B(\lambda_0, \varepsilon)$ and $\forall v, w \in B(u_0, r_0)$. Under the assumption above, the implicit function theorem for verified continuation is obtained as below.

Theorem 3 (Implicit function theorem) *Let b_0, K_0, ρ_0, r_0, M, and N satisfy the previous inequalities. In addition, we obtain a constant denoted by*

$$K(\varepsilon) = \sup_{(u,\lambda)\in B(u_0,r_0)\times B(\lambda_0,\varepsilon)} \|D_\lambda[u, \lambda]\|_{\mathbb{R},V}$$

If

$$r_0 - 2b_0\rho_0 \ge 2b_0K(\varepsilon)\varepsilon \;\; and \;\; b_0(Mr_0 + N\varepsilon) < 1$$

holds, then there uniquely exists $u(\lambda) \in B(u_0, r_0)$ satisfying (1) for $\forall\lambda \in B(\lambda_0, \varepsilon)$.

The implicit function theorem is computable because the radii of balls r_0 and ε explicitly. This theorem is also called the *constructive* implicit function theorem. On the basis of the implicit function theorem and verified computation using Newton-Kantorovich's theorem, we propose a procedure of verified continuation algorithm. The algorithm uses the simple parameter continuation mentioned in the previous section.

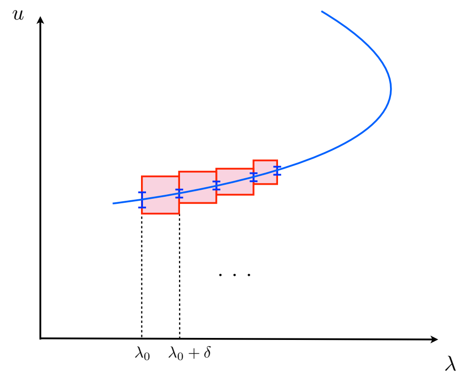

Figure 2: Existence of continuous solution path

Algorithm 2 (Verified parameter continuation) *Given a known solution $(u_0, \lambda_0) \in V_h \times \mathbb{R}$ and $\delta > 0$, we validate the solution existence in the interval $[\lambda_0, \lambda_0 + \delta]$ as follows:*

1. *Verify the exact solution around (u_0, λ_0) by Newton-Kantorovich's theorem. If the verification fails, then the algorithm ends in failure.*
2. *Put a small perturbation $\delta > 0$ and determine a predictor $\bar{u} = u_0$.*
3. *Compute $u(\lambda_0 + \delta/2) \in V_h$ as a corrector by Newton's iterations.*
4. *Prove the existence of exact solution in the box: $B(u_0, r_0) \times B(\lambda_0, \delta/2)$ using the implicit function theorem. If the theorem is not obtained, go to Step 6.*

5. *Update $u_0 = u(\lambda_0 + \delta)$ and $\lambda_0 = \lambda_0 + \delta$, go back to Step 1.*

6. *Update $\delta = \delta/2$ and go back to Step 3.*

The algorithm verifies the existence and local uniqueness of exact solution of (1) in each box $B(u_0, r_0) \times B(\lambda_0, \delta/2)$. For every step, boxes will connect each other, see Figure 2. Then, we prove a continuous solution path uniquely. The continuation method may fail at some step because of the existence of singularities on the solution curve (e.g. folds or bifurcation point). Near the singular points there exist more than one solution and the implicit function theorem is not valid. In that case, another technique of continuation is needed.

5. Application to Ambrosetti-Prodi problem

The verified continuation algorithm is applicable to the Ambrosetti-Prodi type problem:

$$\begin{cases} -\Delta u = g(u) + \lambda h(x) & \text{in } \Omega, \\ u|_{\partial\Omega} = 0. \end{cases} \tag{6}$$

As a typical example of the Ambrosetti-Prodi type problem, we consider $g(u) = u^2$ and $h(x) = 1$. The domain Ω is the unit square $\Omega = (0,1)^2$. All computations are carried out on a Cent OS 6.3, 3.10GHz Intel Xeon E5-2687W. We use MATLAB2012a with INTLAB version 6 [5].

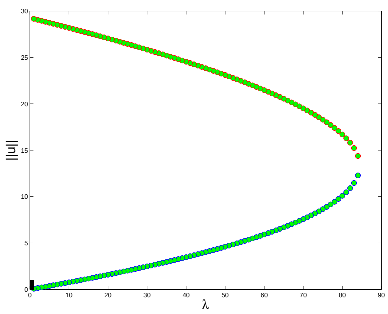

Figure 3: Point wise proof of (2)

The verified computation in [3] proves that the exact solution of (6) uniquely exists in the neighborhood of its approximation. Figure 3 shows the point wise existence proof of the exact solution. Sufficient condition of Newton-Kantorovich's theorem is satisfied on each point. The shape of the solution path can also be expected in Figure 3. It seems to have a fold point around $\lambda \approx 84$.

Furthermore, the verified continuation method yields a continuous solution path in several boxes in Figure 4. Because of the singularities on the fold point, the continuation method is failed. The upper branch is failed at $\lambda_1 = 83.138437$. The lower branch is available to pursue until $\lambda_2 = 83.217876$. Then, there exist at least two solution of (6) in the case of $\lambda \leq \lambda_1$. The fold point is difficult to treat only by the simple continuation method. Pseudo-arclength continuation is proposed by H.B. Keller to overcome this difficulties. Using the method, we will construct another verified continuation method in future.

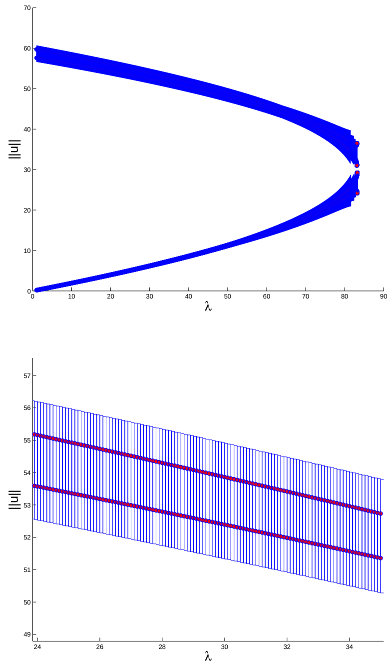

Figure 4: Continuous solution path

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