Rigorous verification of saddle-node bifurcations in ODEs

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Abstract

In this paper, we introduce a general method for the rigorous verification of saddle-node bifurcations in ordinary differential equations. The approach is constructive in the sense that we obtain precise and explicit bounds within which the saddle-node bifurcation occurs. After introducing a set of sufficient generic conditions, an algorithm to verify rigorously the conditions is introduced. The approach is applied to prove existence of some saddle-node bifurcations in the Hodgkin-Huxley model.

Key words. Saddle-node bifurcation, rigorously verified numerics
Contraction Mapping Theorem, Hodgkin-Huxley model

1 Introduction

Parameter dependent models in the form of nonlinear vector fields are ubiquitous in physics, biology, finance and chemistry. As one varies the parameters, one can reach a point in parameter space where the dynamics of the solutions undergo a dramatic change. This phenomenon is called a bifurcation. For realistic nonlinear models, identifying a set of parameters at which a bifurcation occurs almost always requires a complicated analysis. In fact, this identification process is not exact in general and therefore inevitably results in some uncertainties. Taking into account these uncertainties, verifying rigorously the presence of a bifurcation becomes almost impossible using standard pen and paper analysis. The goal of the present paper is to propose a general rigorous verification method for one of the simplest possible bifurcation: the saddle-node bifurcation. The idea is to introduce a set of sufficient generic conditions and then present an algorithm that can verify rigorously (possibly with the help of a computer program and interval arithmetic) the conditions.

Before proceeding with the presentation of our method, it is important to realize that the proposed approach is by no means the first attempt to present a rigorous verification method for bifurcations in differential equations. Using a Krawczyk-based interval validation method, a computer-assisted approach is proposed in [1] to study turning points, symmetry breaking bifurcation points and hysteresis points. Double turning points have being studied in [2, 3], period doubling bifurcations were tackled in [4] and cocoon bifurcations were considered in [5]. Steady states bifurcations in partial differential equations have recently been addressed [6]. An approach to prove rigorously a weaker (topological) notion of bifurcations for steady states of nonlinear partial differential equations is proposed in [7].

While our approach is similar to the work presented in [1], we believe that the verification method that we propose is different. Indeed, instead of using the Krawczyk-based interval validation method, we use the radii polynomial approach (first introduced in [8])

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which provide, in the context of differential equations, an efficient means of determining a domain on which the contraction mapping theorem is applicable. The advantage of the radii polynomial approach is twofold. First, most of the estimates are done analytically and generally, hence providing explicit formulas that can give insights into the problems under study. Second, costly computations involving interval arithmetic can be postponed to the very end of the proofs, hence reducing significantly the computational cost (e.g. see [8, 9]).

The paper is organized as follows. In Section 2, we introduce the definition of a saddle-node bifurcation and the sufficient generic conditions for a saddle-node bifurcation to occur. In Section 3, we introduce the radii polynomial approach in finite dimension to solve rigorously nonlinear equations. In particular, we show how to enclose rigorously eigenvalues of interval matrices. In Section 4, we introduce the rigorous verification method for saddle-node bifurcations. In particular we introduce Algorithm 5 to verify rigorously the bifurcations. In Section 5, we apply the method to prove existence of saddle-node bifurcations in the Hodgkin-Huxley equation.

2 Definitions and sufficient generic conditions

Given a C^1 function $f\colon \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$, consider the parameter dependent vector field

$$\dot{x} \stackrel{\text{def}}{=} \frac{dx}{dt} = f(x,\lambda), \qquad \lambda \in \mathbb{R}. \tag{2.1}$$

Definition 1. *A* saddle-node *for* (2.1) *is a point* $(\tilde{x},\tilde{\lambda}) \in \mathbb{R}^n \times \mathbb{R}$ *such that*

1. $f(\tilde{x},\tilde{\lambda}) = 0$
2. 0 *is an eigenvalue of* $D_x f(\tilde{x},\tilde{\lambda})$ *with algebraic multiplicity one and all other eigenvalues have non-zero real parts.*

Definition 2. Given $f\colon \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ a *saddle-node bifurcation* occurs at the saddle-node $(\tilde{x},\tilde{\lambda}) \in \mathbb{R}^n \times \mathbb{R}$ if the following conditions are met.

1. There exists a smooth curve $g\colon (-\delta,\delta) \to \mathbb{R}^n \times \mathbb{R}$ denoted by $s \mapsto (g_1(s), g_2(s))$ such that $g(0) = (\tilde{x},\tilde{\lambda})$ and $f(g_1(s), g_2(s)) = 0$.
2. The curve defined by g has a *quadratic tangency* with $\mathbb{R}^n \times \{\tilde{\lambda}\}$ at $(\tilde{x},\tilde{\lambda})$, that is
$$g_2(0) = \tilde{\lambda}, \quad g_2'(0) = 0, \quad \text{and} \quad g_2''(0) \neq 0.$$
3. If $s \neq 0$ then $D_x f(g_1(s), g_2(s))$ is hyperbolic, that is $Re(\sigma) \neq 0$ for all the eigenvalues σ of $D_x f(g_1(s), g_2(s))$, and if $\sigma(s)$ is the eigenvalue of $D_x f(g_1(s), g_2(s))$ that satisfies $\sigma(0) = 0$, then $\sigma'(0) \neq 0$.

The following result is proved in Theorem 8.12 in [10] and provides sufficient generic conditions for a saddle-node bifurcation to occur in the n-dimensional setting. The main idea of the proof is to use a Lyapunov-Schmidt reduction.

Theorem 1 (Saddle-node bifurcation theorem). *Assume* $f\colon \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ *is* C^1, $(\tilde{x},\tilde{\lambda}) \in \mathbb{R}^n \times \mathbb{R}$ *is a saddle-node, and the kernel of* $D_x f(\tilde{x},\tilde{\lambda})$ *is spanned by the non-zero vector* $\tilde{v} \in \mathbb{R}^n$. *If*

$$D_\lambda f(\tilde{x},\tilde{\lambda}) \neq 0 \quad \text{and} \quad D_x^2 f(\tilde{x},\tilde{\lambda})(\tilde{v},\tilde{v}) \neq 0$$

and both are not in the range of $D_x f(\tilde{x},\tilde{\lambda})$, *then there is a saddle-node bifurcation at* $(\tilde{x},\tilde{\lambda})$. *Moreover, among all* C^∞ *one parameter families that have a saddle-node, those that undergo a saddle-node bifurcation form an open and dense subset.*

The saddle-node bifurcation theorem provides sufficient generic conditions for the existence of a saddle-node bifurcation. This process begins by finding a saddle-node, that is a point $(\tilde{x}, \tilde{\lambda})$ such that (i) $f(\tilde{x}, \tilde{\lambda}) = 0$; (ii) $\dim \ker D_x f(\tilde{x}, \tilde{\lambda}) = 1$; and (iii) all non-zero eigenvalues of $D_x f(\tilde{x}, \tilde{\lambda})$ have non-zero real parts. In order to verify assumptions (i) and (ii), we first compute $(x, \lambda, v) \in \mathbb{R}^{2n+1}$ such that $f(x, \lambda) = D_x f(x, \lambda) v = 0 \in \mathbb{R}^n$. For a realistic nonlinear model f, this task is in general impossible using pen-and-paper standard techniques. To solve this problem, we use the radii polynomial approach (see Section 3) to solve general finite dimensional systems of nonlinear equations. In this process, we show how to use this approach to rigorously enclose the eigenvalues of matrices with interval entries, as we will need to show that all non-zero eigenvalues of $D_x f(\tilde{x}, \tilde{\lambda})$ have non-zero real parts.

3 Solving rigorously systems of nonlinear equations

Throughout this section we make use of the *sup norm* on $\mathbb{R}^m$, i.e., given $x = (x_1, \ldots, x_m) \in \mathbb{R}^m$ define

$$\|x\|_\infty \stackrel{\text{def}}{=} \max_{k=1,\ldots,m} \{|x_k|\}.$$

In this norm the closed ball of radius r centered at x is denoted by

$$\overline{B_r(x)} \stackrel{\text{def}}{=} \{y \in \mathbb{R}^m \mid \|x - y\|_\infty \leq r\}.$$

The next result is strongly influenced by the presentation of Yamamoto in [11].

Theorem 2. *Let $U \subset \mathbb{R}^m$ be an open set and let $T = (T_1, \ldots, T_m) \in C^1(U, \mathbb{R}^m)$, where $T_k \colon \mathbb{R}^m \to \mathbb{R}$. Let $\bar{x} \in U$. Assume that $Y = (Y_1, \ldots, Y_m) \in \mathbb{R}^n$ and $Z(r) = (Z_1(r), \ldots, Z_m(r)) \in \mathbb{R}^m$ provide the following bounds:*

$$|T_k(\bar{x}) - \bar{x}_k| \leq Y_k \quad \text{and} \quad \sup_{b,c \in \overline{B_r(0)}} |DT_k(\bar{x} + b)c| \leq Z_k(r) \tag{3.1}$$

for all $k = 1, \ldots, m$. If $\|Y + Z(r)\|_\infty < r$, then $T \colon \overline{B_r(\bar{x})} \to \overline{B_r(\bar{x})}$ is a contraction mapping with contraction constant

$$\kappa \stackrel{\text{def}}{=} \frac{\|Z(r)\|_\infty}{r} < 1.$$

In particular, there exists a unique $\tilde{x} \in \overline{B_r(\bar{x})}$ such that $T(\tilde{x}) = \tilde{x}$.

Proof. The mean value theorem applied to T_k implies that for any $x, y \in \overline{B_r(\bar{x})}$ there exists $z \in \{tx + (1-t)y \mid t \in [0,1]\} \subset \overline{B_r(\bar{x})}$ such that

$$T_k(x) - T_k(y) = DT_k(z)(x - y).$$

Thus,

$$|T_k(x) - T_k(y)| = \left| DT_k(z) \frac{r(x-y)}{\|x-y\|_\infty} \right| \frac{\|x-y\|_\infty}{r} \leq Z_k(r) \frac{\|x-y\|_\infty}{r}. \tag{3.2}$$

Setting $y = \bar{x}$ and noting that $\|x - y\|_\infty \leq r$, (3.2) yields

$$|T_k(x) - T_k(\bar{x})| \leq Z_k(r).$$

By the triangle inequality

$$|T_k(x) - \bar{x}_k| \leq |T_k(x) - T_k(\bar{x})| + |T_k(\bar{x}) - \bar{x}_k| \leq Z_k(r) + Y_k \leq \|Y + Z(r)\|_\infty < r.$$

That proves that $T(\overline{B_r(\bar{x})}) \subseteq \overline{B_r(\bar{x})}$.

From (3.2), it follows that

$$\|T(x) - T(y)\|_\infty \leq \|Z(r)\|_\infty \frac{\|x-y\|_\infty}{r}.$$

By assumption $\|Z(r)\|_\infty \leq \|Y + Z(r)\|_\infty < r$. Therefore T is a contraction on $\overline{B_r(\bar{x})}$ with a contraction constant $\kappa = \frac{\|Z(r)\|_\infty}{r} < 1$, and hence, by the contraction mapping theorem there exists a unique $\tilde{x} \in \overline{B_r(\bar{x})}$ such that $T(\tilde{x}) = \tilde{x}$. □

Observe that Theorem 2 does not prescribe a specific value of r. In fact, to emphasize the freedom to choose r we introduce the following concept.

Definition 3. *Given $T \in C^1(U, \mathbb{R}^m)$, $U \subset \mathbb{R}^m$ open, and vectors $Y, Z(r) \in \mathbb{R}^m$ satisfying* (3.1) *the associated* radii polynomials *$p_k(r)$, $k = 1, \ldots, m$ are given by*

$$p_k(r) \stackrel{\text{def}}{=} Y_k + Z_k(r) - r. \tag{3.3}$$

Using the radii polynomials we restate Theorem 2 in the form in which we make primary use of it.

Corollary 3. *Let $U \subset \mathbb{R}^m$ be open, $F \in C^1(U, \mathbb{R}^m)$ and $A\colon \mathbb{R}^m \to \mathbb{R}^m$ be an invertible linear map. Define $T\colon U \to \mathbb{R}^m$ by*

$$T(x) \stackrel{\text{def}}{=} x - AF(x).$$

Let $\bar{x} \in U$, let $Y, Z(r) \in \mathbb{R}^m$ satisfy (3.1), *and let $p_k(r)$, $k = 1, \ldots, m$ be the associated radii polynomials. If there exists $r > 0$ such that $p_k(r) < 0$, for all $k = 1, \ldots, m$, then there exists a unique $\tilde{x} \in \overline{B_r(\bar{x})}$ such that $F(\tilde{x}) = 0$.*

Proof. Suppose that $r > 0$ is such that $p_k(r) < 0$ for all $k = 1, \ldots, m$. Hence,

$$\|Y + Z(r)\|_\infty = \max_{k=1,\ldots,m} \{(Y + Z(r))_k\} < r.$$

From Theorem 2 there exists a unique $\tilde{x} \in \overline{B_r(\bar{x})}$ such that $T(\tilde{x}) = \tilde{x}$ and therefore by invertibility of A, such that $F(\tilde{x}) = 0$. □

The *radii polynomial approach* consists of constructing the radii polynomials as defined in (3.3), and then verifying the hypothesis of Corollary 3. In practice, $\bar{x} \in U$ is a numerical approximation obtained using an iterative numerical scheme (e.g. Newton's method) and the matrix A is chosen as an approximate inverse of $DF(\bar{x})$. The matrix A can even be considered as the exact inverse if one is willing to spend the computational effort.

3.1 Computation of eigenvalues and eigenvectors

As became clear in Definition 1, verifying that a point $(\tilde{x}, \tilde{\lambda})$ is a saddle-node requires showing that 0 is an eigenvalue of $D_x f(\tilde{x}, \tilde{\lambda})$ with algebraic multiplicity one and all other eigenvalues have non-zero real parts. We can achieve such task by computing the sets of all eigenvalues of $D_x f(\tilde{x}, \tilde{\lambda})$. In this section, we show how to adapt the radii polynomial approach to do this. We essentially mimic the presentation of [12]. Consider the problem of rigorously determining solutions (μ, v) of the equation

$$Mv = \mu v, \tag{3.4}$$

for a given matrix $M \in \mathbb{C}^{n\times n}$ under the assumption that an approximate eigenpair $(\bar{\mu}, \bar{v})$ has been determined numerically. In particular, we show how the radii polynomial approach can be used to obtain these quantities rigorously. For sake of simplicity we do not present how to verify generalized eigenvectors.

Recall from Section 3 that radii polynomials provide a domain of existence of a unique zero of a function. In this case the most obvious function is

$$\tilde{F}(\mu, v) \stackrel{\text{def}}{=} Mv - \mu v$$

where $\tilde{F}\colon \mathbb{C}^{n+1} \to \mathbb{C}^{n+1}$. However, given a solution $(\tilde{\mu}, \tilde{v})$ of (3.4) and any $\theta \in \mathbb{C} \setminus \{0\}$, $(\tilde{\mu}, \theta\tilde{v})$ is also a solution. This implies that the solution $(\tilde{\mu}, \tilde{v})$ is not *isolated*, i.e. that there is no neighborhood of $(\tilde{\mu}, \tilde{v})$ in $\mathbb{C}^{n+1}$ on which $(\tilde{\mu}, \tilde{v})$ is the unique solution to $\tilde{F}(\tilde{\mu}, \tilde{v}) = 0$. To address this issue, we introduce the notion of a *phase condition* which will ensure that solutions are isolated. Observe that uniqueness fails along a two dimensional parameter space $\mathbb{C} \setminus \{0\}$, thus one expects to obtain uniqueness by reducing by two the dimension of the space on which the function $\tilde{F}$ acts. With this in mind we choose a phase condition that involves fixing one of the components of v to be a given constant.

To be more precise, suppose that an approximate eigenpair of M has been computed, that is $(\bar{\mu}, \bar{v})$ such that $M\bar{v} \approx \bar{\mu}\bar{v}$. Choose k such that

$$|\bar{v}_k| = \max\{|\bar{v}_j| \mid j = 1, \ldots, n\}$$

and define $F : \mathbb{C}^n \to \mathbb{C}^n$ by

$$F(x) \stackrel{\text{def}}{=} M \begin{bmatrix} v_1 \\ \vdots \\ \bar{v}_k \\ \vdots \\ v_n \end{bmatrix} - \mu \begin{bmatrix} v_1 \\ \vdots \\ \bar{v}_k \\ \vdots \\ v_n \end{bmatrix} \tag{3.5}$$

where $x = (\mu, v_1, v_2, \ldots, v_{k-1}, v_{k+1}, \ldots, v_n)$. By definition, a solution x of $F(x) = 0$ corresponds to an eigenpair (μ, v) of M with the eigenvalue μ given by the first component of x and the eigenvector $v = (v_1, \ldots, v_{k-1}, \bar{v}_k, v_{k+1}, \ldots, v_n)$.

Continuing to follow the radii polynomial approach we define the operator $T : \mathbb{C}^n \to \mathbb{C}^n$ by

$$T(x) = x - AF(x), \tag{3.6}$$

where A is a numerical inverse of $DF(\bar{x})$. We assume that A is invertible, which can be verified with interval arithmetic. For the purpose of constructing the necessary bounds for the radii polynomials we make use of the norm $||x||_\infty = \max_{i=1,\ldots,n}\{|x_i|\}$.

To simplify the expression of $DF(\bar{x})$ we introduce the following notation. Given a matrix $B \in \mathbb{C}^{n\times m}$, we let $(B)_{\hat{k}}$ denote the $n \times (m-1)$ matrix obtained by deleting the k-th column of B. At $\bar{x} = (\bar{\mu}, \bar{v}_1, \bar{v}_2, \ldots, \bar{v}_{k-1}, \bar{v}_{k+1}, \ldots, \bar{v}_n)$

$$DF(\bar{x}) = \left[\begin{array}{c|c} -\bar{v}_1 & \\ \vdots & \\ -\bar{v}_k & (M - \bar{\mu} I_n)_{\hat{k}} \\ \vdots & \\ -\bar{v}_n & \end{array}\right]. \tag{3.7}$$

To apply the radii polynomial result, i.e. Corollary 3, we need to obtain the bounding vectors Y and $Z(r)$. Since $T(\bar{x}) - \bar{x} = -AF(\bar{x})$, let

$$Y \stackrel{\text{def}}{=} |AF(\bar{x})| \in \mathbb{R}^n_+, \tag{3.8}$$

where the absolute values are taking component-wise. To obtain a bound $Z(r)$ satisfying (3.1) we note that

$$\begin{aligned} DT(\bar{x}+b)c &= (I - ADF(\bar{x}+b))\, c \\ &= (I - ADF(\bar{x}))c + A[(DF(\bar{x}) - DF(\bar{x}+b))c] \end{aligned}$$

which implies that

$$|DT(\bar{x}+b)c| \ll |(I - ADF(\bar{x}))c| + |A[(DF(\bar{x}) - DF(\bar{x}+b))c]|, \tag{3.9}$$

where $\ll$ denotes component-wise inequalities. Observe that

$$DF(\bar{x}+b) = \left[\begin{array}{c|c} -\bar{v}_1 - b_2 & \\ \vdots & \\ -\bar{v}_{k-1} - b_k & \\ -\bar{v}_k & (M - (\bar{\mu} + b_1)I_n)_{\hat{k}} \\ -\bar{v}_{k+1} - b_{k+1} & \\ \vdots & \\ -\bar{v}_n - b_n & \end{array}\right]$$

Thus,

$$DF(\bar{x}) - DF(\bar{x}+b) = \left[\begin{array}{c|c} b_2 & \\ \vdots & \\ b_k & \\ 0 & b_1(I_n)_{\hat{k}} \\ b_{k+1} & \\ \vdots & \\ b_n & \end{array}\right].$$

Define

$$Z(r) = rZ_0 + r^2 Z_1, \tag{3.10}$$

where

$$Z_0 \stackrel{\text{def}}{=} |I_n - A \cdot DF(\bar{x})|\mathbb{1}_n, \quad Z_1 \stackrel{\text{def}}{=} 2|A|(\mathbb{1}_n - e_k), \tag{3.11}$$

where $\mathbb{1}_n \in \mathbb{R}^n$ is the vector whose entries are all equal to 1, and where e_k the k-th element of the canonical basis of $\mathbb{R}^n$. Returning to (3.9), it is left to the reader to check that

i) $\displaystyle\sup_{c \in B(r)} |(I - ADF(\bar{x}))c| \ll rZ_0$

ii) $\displaystyle\sup_{b,c \in B(r)} |A[(DF(\bar{x}) - DF(\bar{x}+b))c]| \ll r^2 Z_1.$

This combined with (3.8) guarantees that (3.1) is satisfied. Therefore, by Corollary 3, if there exists $r > 0$ such that

$$p_k(r) \stackrel{\text{def}}{=} Y_k + Z_k(r) - r < 0,$$

then we have proven the existence of an eigenpair $(\tilde{\mu}, \tilde{v})$ for M within radius r of the numerical approximation $(\bar{\mu}, \bar{v})$.

4 Rigorous verification of a saddle-node bifurcation

Theorem 1 provides a sufficient condition to verify the existence of a saddle-node bifurcation. The process begins by finding a saddle-node, that is a point $(\tilde{x}, \tilde{\lambda})$ such that (i) $f(\tilde{x}, \tilde{\lambda}) = 0$; (ii) $\dim \ker D_x f(\tilde{x}, \tilde{\lambda}) = 1$; and (iii) all non-zero eigenvalues of $D_x f(\tilde{x}, \tilde{\lambda})$ have non-zero real parts. Assumptions (i) and (ii) are verified rigorously and simultaneously using the radii polynomial approach of Section 3 by computing $(x, \lambda, v) \in \mathbb{R}^{2n+1}$ satisfying $f(x, \lambda) = D_x f(x, \lambda) v = 0 \in \mathbb{R}^n$. As the eigenvectors come in family, we must impose a phase condition to isolate the solutions. Since an eigenvector v associated to the zero eigenvalue must be real, the phase condition $\|v\|^2 - 1 = 0$ isolates the solutions. Denote $X = (x, \lambda, v) \in \mathbb{R}^{2n+1}$, and look for X such that

$$F(X) \stackrel{\text{def}}{=} \begin{pmatrix} f(x,\lambda) \\ \|v\|^2 - 1 \\ D_x f(x,\lambda) v \end{pmatrix} = 0. \tag{4.1}$$

Assume that using the radii polynomial approach of Section 3, we found a ball in $\mathbb{R}^{2n+1}$ enclosing a unique solution $\tilde{X} = (\tilde{x}, \tilde{\lambda}, \tilde{v})$ of (4.1). The kernel of $D_x f(\tilde{x}, \tilde{\lambda})$ must be one dimensional, as otherwise we would not have an isolated solution in $\mathbb{R}^{2n+1}$. To complete the rigorous verification that $(\tilde{x}, \tilde{\lambda})$ is a saddle-node, we must verify that all non-zero eigenvalues of $D_x f(\tilde{x}, \tilde{\lambda})$ have non-zero real parts. This can be achieved by using the theory of Section 3.1. At this point, the matrix $D_x f(\tilde{x}, \tilde{\lambda})$ contains the errors inherited from the computation of $(\tilde{x}, \tilde{\lambda})$ only known to exist within a ball of small radius r. In this case, the bounds defined (3.11) will be computed with the interval matrix $M = D_x f(\tilde{x}, \tilde{\lambda})$ in (3.7). Using the theory of Section 3.1 as stated, assuming that the k-th eigenvalue of $D_x f(\tilde{x}, \tilde{\lambda})$ is contained in the ball $B_k \in \mathbb{C}$, if there exists a unique $j \in \{1, \dots, n\}$ such that $0 \in B_j$ and if $B_k \cap i\mathbb{R} = \emptyset$ for all $k \neq j$, then we can conclude that $(\tilde{x}, \tilde{\lambda})$ is a saddle-node point.

Now, define

$$u_1 \stackrel{\text{def}}{=} D_\lambda f(\tilde{x}, \tilde{\lambda}) \quad \text{and} \quad u_2 \stackrel{\text{def}}{=} D_x^2 f(\tilde{x}, \tilde{\lambda})(\tilde{v}, \tilde{v}). \tag{4.2}$$

From Theorem 1, to show that there is a saddle-node bifurcation at $(\tilde{x}, \tilde{\lambda})$, it remains to verify that $u_1, u_2 \neq 0$ and that u_1 and u_2 are not in the range of $D_x f(\tilde{x}, \tilde{\lambda})$. The following results provides an elegant way of verifying these assumptions.

Lemma 4. *Let $D : \mathbb{R}^n \to \mathbb{R}^n$ a linear transformation with $\dim(\ker(D)) = 1$. Then $\ker D^T = \langle w \rangle$, for some $w \in \mathbb{R}^n \setminus \{0\}$. Also, u is in the range of D if and only if $u \cdot w = 0$.*

Proof. By the rank-nullity theorem, $\text{rank}(D) \stackrel{\text{def}}{=} \dim(\text{image}(D)) = n - \dim(\ker(D)) = n - 1$. Since $\text{rank}(D) = \text{rank}(D^T)$ the rank-nullity theorem implies that $\dim(\ker(D^T)) = 1$. Hence, there is a non-zero vector $w \in \mathbb{R}^n$ such that $\ker D^T = \langle w \rangle$.

Now, if $u \in \mathbb{R}^n$ is in the range of D, there exists $y \in \mathbb{R}^n$ such that $u = Dy$, and then $u \cdot w = w^T u = w^T(Dy) = (w^T D) y = (D^T w)^T y = 0$. This implies that

$$\text{image}(D) \subset (\ker(D^T))^\perp = (\langle w \rangle)^\perp \stackrel{\text{def}}{=} \{u \in \mathbb{R}^n \mid u \cdot w = 0\}. \tag{4.3}$$

Conversely, assume $u \cdot w = 0$, that is $u \in (\langle w \rangle)^\perp = (\ker(D^T))^\perp$. Since $(\ker(D^T))^\perp$ is an $(n-1)$-dimensional subspace and $\dim(\text{image}(D)) = n - 1$, we use (4.3) to get $\text{image}(D) = (\ker(D^T))^\perp$. Hence, $u \in (\ker(D^T))^\perp = \text{image}(D)$, that is u is in the range of D. □

Let $D \stackrel{\text{def}}{=} D_x f(\tilde{x}, \tilde{\lambda})$. From the previous lemma, two last explicit steps remain to verify the last hypotheses of Theorem 1: (iv) compute rigorously a non-zero vector w such that $\ker D^T = \langle w \rangle$ (possibly using the radii polynomial approach); (v) verify that u_1, u_2 as defined by (4.2) satisfy $u_1 \cdot w \neq 0$ and $u_2 \cdot w \neq 0$ (possibly with interval arithmetic).

Let us now introduce how to use the radii polynomial approach to compute rigorously a non-zero vector w such that $\ker D^T = \langle w \rangle$. At this point, it is known rigorously that $\dim \ker(D) = 1$, which implies that $\operatorname{rank}(D) = \operatorname{rank}(D^T) = n-1$. Therefore, when looking for a non-zero w satisfying $D^T w = 0$, we can get rid of one row of D^T without changing the solution space. Now the question is which equation to get rid of? As usual, we use a numerical approximation to answer that question. Assume that $\bar{v} \neq 0$ satisfies $D\bar{v} \approx 0$. Let k the component of $\bar{v}$ with the largest magnitude, that is

$$|\bar{v}_k| = \max_{i=1,\dots,n} \{|\bar{v}_i|\} \neq 0.$$

Denote by $C_1, \dots, C_n$ the columns of D and $R_1, \dots, R_n$ the corresponding rows of D^T that is $R_i = C_i^T$ for $i = 1, \dots, n$. Then since $D\bar{v} \approx 0$,

$$C_k \approx \frac{1}{\bar{v}_k} \sum_{\substack{i=1\\ i\neq k}}^{n} \bar{v}_i C_i \Longrightarrow R_k = C_k^T \approx \frac{1}{\bar{v}_k} \sum_{\substack{i=1\\ i\neq k}}^{n} \bar{v}_i C_i^T = \frac{1}{\bar{v}_k} \sum_{\substack{i=1\\ i\neq k}}^{n} \bar{v}_i R_i.$$

Since the k-th row R_k of D^T is a linear combination of the other rows, we get rid of it, or equivalently we get rid of the k-th column C_k of D. Denote $M \overset{\text{def}}{=} \left(D_{\hat{k}}\right)^T$, with $D_{\hat{k}}$ the $n \times (n-1)$ matrix defined by D without its k-th column C_k. A non-zero unit vector w such that $\ker D^T = \langle w \rangle$ is an isolated solution of

$$g(w) \overset{\text{def}}{=} \begin{pmatrix} \|w\|^2 - 1 \\ Mw \end{pmatrix} = 0, \tag{4.4}$$

which we solve using the radii polynomial approach as introduced in Section 3. Finally, using Lemma 4, we can show that the vectors u_1 and u_2 defined in (4.2) are not in the range of $D = D_x f(\tilde{x}, \tilde{\lambda})$ by verifying (with interval arithmetic) that

$$u_1 \cdot w \neq 0 \quad \text{and} \quad u_2 \cdot w \neq 0. \tag{4.5}$$

Condition (4.5) immediately implies that $u_1, u_2 \neq 0$.

We summarize the work we have done in an algorithm.

Algorithm 5. *The following steps are sufficient to verify the existence of a saddle-node bifurcation at a point* $(\tilde{x}, \tilde{\lambda})$.

(a) *Compute* $(\tilde{x}, \tilde{\lambda})$ *such that* $f(\tilde{x}, \tilde{\lambda}) = 0$ *and* $\dim \ker D_x f(\tilde{x}, \tilde{\lambda}) = 1$. *This can be achieved by finding a ball in* $\mathbb{R}^{2n+1}$ *enclosing a unique solution* $\tilde{X} = (\tilde{x}, \tilde{\lambda}, \tilde{v})$ *of* (4.1). *This can be done using the radii polynomial approach as introduced in Section 3.*

Let $D \overset{\text{def}}{=} D_x f(\tilde{x}, \tilde{\lambda})$.

(b) *Show that all non-zero eigenvalues of* D *have non-zero real parts. This can be achieved as follows: using the radii polynomial approach, as introduced in Section 3.1, show that the set of eigenvalues of* D*, denoted by* $\sigma(D)$*, satisfies*

- $\sigma(D) \subset \bigcup_{j=1}^{n} B_j$*, for some small balls* $B_j \in \mathbb{C}$,
- $0 \in B_k$ *for a unique* $k \in \{1, \dots, n\}$,
- $B_j \cap i\mathbb{R} = \emptyset$*, for all* $j \in \{1, \dots, n\}$ *such that* $j \neq k$.

(c) *Compute a non-zero vector* w *such that* $\ker D^T = \langle w \rangle$. *This can be done by computing an isolated solution of* (4.4) *using the radii polynomial approach of Section 3.*

(d) *Defining the vectors* u_1 *and* u_2 *as in* (4.2)*, verify that* $u_1 \cdot w \neq 0$ *and that* $u_2 \cdot w \neq 0$. *This step can be achieved using interval arithmetic.*

5 Saddle-node bifurcations in the Hodgkin-Huxley model

The Hodgkin-Huxley model for the action potential of a space-clamped squid axon is defined by the four dimensional vector field

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \end{pmatrix} = \begin{pmatrix} -20 - 120x_2^3x_3\left(x_1 - 25.1\ln(\frac{23}{1350}(550-\lambda))\right) - 36x_4^4\left(x_1 - 25.1\ln(\frac{\lambda}{400})\right) - 0.3(x_1+24.3) \\ \frac{9}{25}(1-x_2)\frac{x_1-\Delta(\lambda)+35}{1-\exp\left(-\frac{x_1-\Delta(\lambda)+35}{10}\right)} - \frac{72}{5}x_2\exp\left(-\frac{x_1-\Delta(\lambda)+60}{18}\right) \\ \frac{63}{250}(1-x_3)\exp\left(-\frac{x_1-\Delta(\lambda)+60}{20}\right) - \frac{18}{5}x_3\frac{1}{\exp\left(-\frac{x_1-\Delta(\lambda)+30}{10}\right)+1} \\ \frac{9}{250}(1-x_4)\frac{x_1-\Delta(\lambda)+50}{1-\exp\left(-\frac{x_1-\Delta(\lambda)+50}{10}\right)} - \frac{9}{20}x_4\exp\left(-\frac{x_1-\Delta(\lambda)+60}{80}\right) \end{pmatrix} \tag{5.1}$$

where

$$\Delta(\lambda) \stackrel{\text{def}}{=} 9.32\ln(\frac{11}{10} - \frac{\lambda}{500}).$$

The variable x_1 is the membrane potential, x_2 is the activation of a sodium current, x_3 is the activation of a potassium current, x_4 is the inactivation of the sodium current and the parameter λ is the external potassium concentration.

Using a standard pseudo-arclength continuation technique [13], we obtain the bifurcation diagram of Figure 1. From this numerical simulation, we can conjecture the existence of two saddle-node bifurcations at $\lambda \approx 426.42$ and at $\lambda \approx 53.61$.

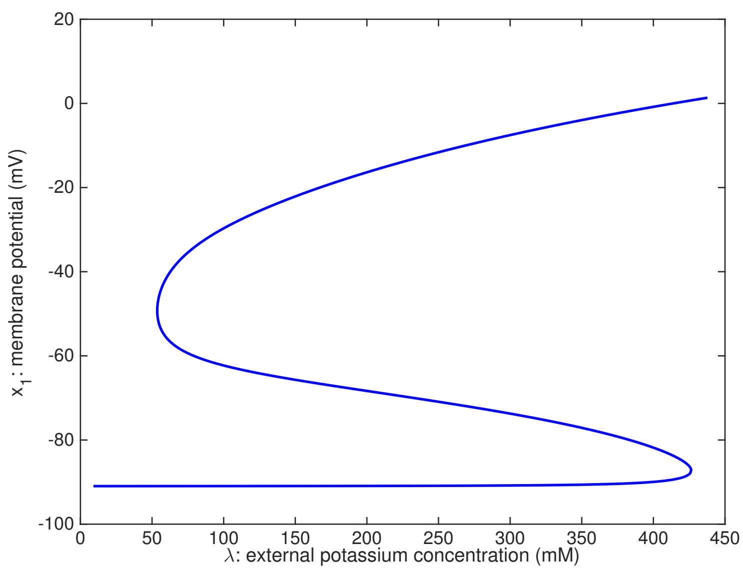

Figure 1: A branch of equilibria which undergoes two saddle-node bifurcations.

Denote by $f(x,\lambda)$ the right-hand side of (5.1). Let $X = (x,\lambda,v) \in \mathbb{R}^9$, and define $F : \mathbb{R}^9 \to \mathbb{R}^9$ as in (4.1). Applying Newton's method to problem (4.1), we compute two approximate solutions

$$\bar{X}_1 \stackrel{\text{def}}{=} \begin{pmatrix} -87.2515605439908 \\ 0.0089034888748 \\ 0.9231857631959 \\ 0.1363687823857 \\ 426.4159725555050 \\ 0.9998982043007 \\ 0.0011653907919 \\ -0.0105518817291 \\ 0.0095331365494 \end{pmatrix} \quad \text{and} \quad \bar{X}_2 \stackrel{\text{def}}{=} \begin{pmatrix} -49.270516282150226 \\ 0.170894916154782 \\ 0.241946685250340 \\ 0.487852905937695 \\ 53.607108413683697 \\ 0.999427022035232 \\ 0.016569867126847 \\ -0.025152384230317 \\ 0.015441006985167 \end{pmatrix} \tag{5.2}$$

corresponding to the two possible saddle-node points.

Theorem 6. *There is a saddle-node bifurcation at a point*

$$(\tilde{x}_1, \tilde{\lambda}_1) \in \overline{B_{r_1}(\bar{x}_1, \bar{\lambda}_1)}, \qquad r_1 \stackrel{\text{def}}{=} 1.715 \times 10^{-12},$$

where $(\bar{x}_1, \bar{\lambda}_1) \in \mathbb{R}^5$ *is given by the first five components of* $\bar{X}_1$ *in* (5.2).

Theorem 7. *There is a saddle-node bifurcation at a point*

$$(\tilde{x}_2, \tilde{\lambda}_2) \in \overline{B_{r_2}(\bar{x}_2, \bar{\lambda}_2)}, \qquad r_2 \stackrel{\text{def}}{=} 2.034 \times 10^{-12},$$

where $(\bar{x}_2, \bar{\lambda}_2) \in \mathbb{R}^5$ *is given by the first five components of* $\bar{X}_2$ *in* (5.2).

The proofs of Theorem 6 and Theorem 7 are both obtained by applying Algorithm 5. We therefore verify steps (a), (b), (c) and (d) of the algorithm.

Proof. (a) Let $\bar{X}$ one of the two points $\bar{X}_1$ or $\bar{X}_2$ given in (5.2). We already have that $F(\bar{X}) \approx 0$, with F given by (4.1). Note that

$$D_X F(\bar{X}) = \begin{pmatrix} D_x f(\bar{x}, \bar{\lambda}) & D_\lambda f(\bar{x}, \bar{\lambda}) & 0 \\ 0 & 0 & 2\bar{v}^T \\ D_x \left(D_x f(\bar{x}, \bar{\lambda}) \bar{v} \right) & D_x D_\lambda f(\bar{x}, \bar{\lambda}) v & D_x f(\bar{x}, \bar{\lambda}) \end{pmatrix}. \tag{5.3}$$

Using INTLAB in MATLAB [14], compute the exact inverse $A = D_X F(\bar{X})^{-1}$. Note that in practice, the so obtained A will have interval entries. Define $T : \mathbb{R}^9 \to \mathbb{R}^9$ by

$$T(X) = X - AF(X).$$

Using interval arithmetic, compute the upper bound Y such that $\left| AF(\bar{X}) \right| \ll Y$.

Now, thanks to the (perfect) choice of A

$$DT(\bar{X} + b)c = -A \left(DF(\bar{X} + b) - DF(\bar{X}) \right) c.$$

Defining $h : [0, 1] \to \mathbb{R}^9$ by $h(s) = D_X F(\bar{X} + sb)c$, $h(1) - h(0) = \left(D_X F(\bar{X} + b) - D_X F(\bar{X}) \right) c$. For each $k \in \{1, \ldots, 9\}$, there exists $s_k \in [0, 1]$ such that

$$\left(D_X F_k(\bar{X} + b) - D_X F_k(\bar{X}) \right) c = h_k(1) - h_k(0) = h_k'(s_k) = D_X^2 F_k(\bar{X} + s_k b)(b, c).$$

Now, let $\tilde{b}, \tilde{c} \in \overline{B_1(0)}$ such that $b, c \in \overline{B_r(0)}$ are given by $b = \tilde{b} r$ and $c = \tilde{c} r$. In this case,

$$\left(D_X F_k(\bar{X} + b) - D_X F_k(\bar{X}) \right) c = D_X^2 F_k(\bar{X} + s_k b)(\tilde{b}, \tilde{c}) r^2.$$

Set $r^* = 10^{-4}$ an a-priori upper bound for the left point of the existence interval of the radii polynomials. We will have to show a-posteriori that $r \leq r^*$. Denote by $\mathbf{b}^* = [-r^*, r^*]^9$ a vector in $\mathbb{R}^9$ whose entries are given by the interval $[-r^*, r^*]$. Denote by $\mathbf{X}^* = \bar{X} + \mathbf{b}^*$ a vector in $\mathbb{R}^9$ with its k-th entry given by the interval $[\bar{X}_k - r^*, \bar{X}_k + r^*]$. Denote by $\boldsymbol{\delta} = [-1, 1]^9$ a vector in $\mathbb{R}^9$ whose entries are given by the interval $[-1, 1]$. Then, for each $b, c \in \overline{B_r(0)}$, it is left to the reader to verify that

$$\left| A \left(DF(\bar{X} + b) - DF(\bar{X}) \right) c \right| \in \left| A D_X^2 F(\mathbf{X}^*)(\boldsymbol{\delta}, \boldsymbol{\delta}) \right|.$$

Using interval arithmetic, compute $Z_1 \in \mathbb{R}^9$ such that

$$\left| A D_X^2 F(\mathbf{X}^*)(\boldsymbol{\delta}, \boldsymbol{\delta}) \right| \ll Z^{(2)}.$$

Using the previous bounds, define the radii polynomials $p_k(r) = Z_k^{(2)} r^2 - r + Y_k$. For each of the point $\bar{X}_1$ and $\bar{X}_2$ given in (5.2), we computed the radii polynomials and obtained the existence intervals

$$I_1 = \left[1.715 \times 10^{-12} \ , \ 8.052 \times 10^{-6} \right] \quad \text{and} \quad I_2 = \left[2.034 \times 10^{-12} \ , \ 1.974 \times 10^{-5} \right],$$

respectively. Since $8.052 \times 10^{-6}, 1.974 \times 10^{-5} < r^* = 10^{-4}$, then the existence intervals are valid. Let $r_1 \stackrel{\text{def}}{=} 1.715 \times 10^{-12}$ and $r_2 \stackrel{\text{def}}{=} 2.034 \times 10^{-12}$. Recall (5.2), then by Corollary 3, there exists a unique $\tilde{X}_1 = (\tilde{x}_1, \tilde{\lambda}_1, \tilde{v}_1) \in \overline{B_{r_1}(\bar{X}_1)}$ such that $F(\tilde{X}_1) = 0$ and there exists a unique $\tilde{X}_2 = (\tilde{x}_2, \tilde{\lambda}_2, \tilde{v}_2) \in \overline{B_{r_2}(\bar{X}_2)}$ such that $F(\tilde{X}_2) = 0$. Hence, for $j = 1, 2$, $f(\tilde{x}_j, \tilde{\lambda}_j) = 0$ and the kernel of $D_x f(\tilde{x}_j, \tilde{\lambda}_j)$ must be one dimensional, as otherwise we would not have that $\tilde{X}_j$ isolated solution in $\mathbb{R}^9$.

(b) Choose $j \in \{1, 2\}$ and let $I \stackrel{\text{def}}{=} I_j$ the existence interval associated to $\bar{X} \stackrel{\text{def}}{=} \bar{X}_j$. Let r the smallest radius of the existence interval I. Define $\mathbf{B} = \overline{B_r\left((\bar{x}, \bar{\lambda})\right)} \subset \mathbb{R}^5$, that is

$$\mathbf{B} = \prod_{k=1}^{4} \left[\bar{x}_k - r, \bar{x}_k + r \right] \times \left[\bar{\lambda} - r, \bar{\lambda} + r \right].$$

Let $D \stackrel{\text{def}}{=} D_x f(\tilde{x}, \tilde{\lambda})$ and $\mathbf{D} \stackrel{\text{def}}{=} D_x f(\mathbf{B})$ a 4×4 interval matrix computed with interval arithmetic. Note that $D \subset \mathbf{D}$. Using the radii polynomial approach as introduced in Section 3.1, we now show that $\sigma(\mathbf{D}) \subset \bigcup_{j=1}^{n} B_j$, for some small balls $B_j \in \mathbb{C}$. The only modification from the theory of Section 3.1 is that we now have a matrix whose entries are intervals. Hence, the bounds Y in (3.8) and the bounds Z_0, Z_1 in (3.11) have to bound all possible error coming from $\mathbf{D}$. Interval arithmetic can be used to do this. Using the above procedure and INTLAB, we proved that the eigenvalues of $D_x f(\tilde{x}_1, \tilde{\lambda}_1)$ are enclosed in $\cup_{j=1}^{4} B_j$, where

$$\begin{aligned}
B_1 &= \left\{ z \in \mathbb{C} \ : \ |z + 32.02633660454969| \leq 3.394274197807681 \times 10^{-11} \right\} \\
B_2 &= \left\{ z \in \mathbb{C} \ : \ |z - 9.305978062941147 \times 10^{-16}| \leq 1.069542699059249 \times 10^{-11} \right\} \\
B_3 &= \left\{ z \in \mathbb{C} \ : \ |z + 0.9317141708275124| \leq 9.975910428070430 \times 10^{-12} \right\} \\
B_4 &= \left\{ z \in \mathbb{C} \ : \ |z + 0.5558951614569074| \leq 1.774408327300926 \times 10^{-12} \right\}.
\end{aligned}$$

Therefore, we obtain that $0 \in B_k$ for the unique $k = 2 \in \{1, 2, 3, 4\}$, and that $B_j \cap i\mathbb{R} = \emptyset$, for all $j \in \{1, 3, 4\}$. This shows that $(\tilde{x}_1, \tilde{\lambda}_1)$ is a saddle-node. We repeated the same procedure to show that $(\tilde{x}_2, \tilde{\lambda}_2)$ is also a saddle-node.

(c) Let

$$\bar{w}_1 \stackrel{\text{def}}{=} \begin{pmatrix} 0.019179161523012 \\ 0.001671623761223 \\ 0.000309560202397 \\ 0.999814617621566 \end{pmatrix} \quad \text{and} \quad \bar{w}_2 \stackrel{\text{def}}{=} \begin{pmatrix} -0.009242057198078 \\ -0.253654297666144 \\ -0.937890513625427 \\ 0.236506799280007 \end{pmatrix}, \tag{5.4}$$

numerical approximations satisfying $D_x f(\bar{x}_1, \bar{\lambda_1})^T \bar{w}_1 \approx 0$ and $D_x f(\bar{x}_2, \bar{\lambda_2})^T \bar{w}_2 \approx 0$.

Choose $j \in \{1, 2\}$, let $D = D_x f(\tilde{x}_j, \tilde{\lambda_j})$ and $\bar{w} = \bar{w}_j$. Based on D, construct the 3×4 matrix M as above in order to define the problem $g(w) = 0$ as in(4.4). Using the radii polynomial approach of Section 3 applied on (4.4), we showed the existence of (i) $\tilde{w}_1 \in \overline{B_{7.246\times 10^{-13}}(\bar{w}_1)}$ such that $D_x f(\tilde{x}_1, \tilde{\lambda_1})\tilde{w}_1 = 0$ and (ii) $\tilde{w}_2 \in \overline{B_{1.595\times 10^{-11}}(\bar{w}_2)}$ such that $D_x f(\tilde{x}_2, \tilde{\lambda_2})\tilde{w}_2 = 0$.

(d) For $j = 1, 2$, define

$$u_1^{(j)} = D_\gamma f(\tilde{x}_j, \tilde{\lambda}_j) \quad \text{and} \quad u_2^{(j)} = D_x^2 f(\tilde{x}_j, \tilde{\lambda}_j)(\tilde{v}_{,j}\, \tilde{v}_j).$$

With interval arithmetic, we showed that for both $j = 1, 2$, $u_1^{(j)} \cdot \tilde{w}_j \neq 0$ and $u_2^{(j)} \cdot \tilde{w}_j \neq 0$. All steps are performed in the MATLAB code `proofs.m` available at [15]. This concludes the proofs of Theorem 6 and Theorem 7. □

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