Implementation of Hopf and Double-Hopf Continuation Using Bordering Methods

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We discuss the computational study of curves of Hopf and double-Hopf points in the software package CONTENT developed at CWI, Amsterdam. These are important points in the numerical study of dynamical systems characterized by the occurrence of one or two conjugate pairs of pure imaginary eigenvalues in the spectrum of the Jacobian matrix. The bialternate product of matrices is extensively used in three codes for the numerical continuation of curves of Hopf points and in one for the continuation of curves of double-Hopf points. In the double-Hopf and two of the single-Hopf cases this is combined with a bordered matrix method. We use this software to find special points on a Hopf curve in a model of chemical oscillations and by computing a Hopf and a double-Hopf curve in a realistic model of a neuron.

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1. INTRODUCTION

Consider a dynamical system depending on parameters,

$$\dot{u} = F(u, \alpha), \quad u, F(u) \in \mathbb{R}^n, \ \alpha \in \mathbb{R}^m,$$
 (1)

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whose equilibria satisfy the nonlinear system of equations

$$F(u, \alpha) = 0. (2)$$

Typically, the behavior of solutions of (1) depends qualitatively on the parameters. CONTENT [Kuznetsov et al. 1997] is an interactive software environment for the computational study of dynamical systems. CONTENT 1.4 is freely available via anonymous login on ftp.cwi.nl in the directory /pub/CONTENT (it is strongly advised to read the README file in this directory before attempting to install CONTENT). Currently, there are versions of CONTENT for SGI Irix 5.x/6.x, Sun OS 5.x, DEC OSF1 3.2, IBM R6000 AIX 4, and HP-UX 7000, as well as for PC Linux Red Hat 4.x (Motif 2.0 should be installed) and PC MS-WINDOWS 95/NT (Borland C++ 5.0 is required).

CONTENT allows the simulation of orbits of (1) by numerical integration, the continuation of solutions to (2), and the computation of special solutions to (1) such as periodic orbits. It automatically detects bifurcations and computes normal form coefficients at found points. CONTENT further allows to continue equilibrium bifurcations in ODEs and detect further degeneracies. It also supports continuation of equilibria and cycles in iterated maps, and continuation of the solutions to certain boundary-value problems on the unit interval [Kuznetsov et al. 1996].

A basic element of CONTENT is a predictor-corrector continuation code to compute implicitly defined curves like branches of solutions to (2) if a parameter is freed. The code allows to detect, locate, and pathfollow numerically several types of bifurcation points, basically by adding other equations to the system (2), freeing an appropriate number of parameters, and using the same continuation code. The resulting extended system of equations is called the defining system and is automatically generated in CONTENT.

An important feature of CONTENT is its ability to employ first, second, and third derivatives of the right-hand side of (1). In fact, the user can choose one of three ways to compute the derivatives: symbolic (automatic generation using C++ [Levitin 1995]), numerical (finite differences), and by a user-provided routine. We will routinely use first and second derivatives, occasionally also third derivatives of F.

In the present article we discuss the implementation into CONTENT of two algorithms for the numerical continuation of Hopf curves and one for the continuation of double-Hopf curves. We recall that a Hopf point is a solution point to (2) where the Jacobian matrix F_u has a pair of eigenvalues $\pm i\omega_0$, $\omega_0 > 0$. It is a double-Hopf point if there are two such pairs. The presence of Hopf points or double-Hopf points has profound implications for the dynamic behavior of (1) for nearby parameter values; e.g., see Kuznetsov [1995]. In particular, periodic orbits appear generically near single-Hopf points, while homoclinic, quasiperiodic, and chaotic motions exist near double-Hopf points.

For the bordered matrix methods the main mathematical result is the following.

Proposition 1. Let

$$M = \left(\begin{array}{cc} A & B \\ C^T & D \end{array}\right)$$

be a nonsingular $(n + m) \times (n + m)$ block matrix with $A \in \mathbb{R}^{n \times n}$, $B, C \in \mathbb{R}^{n \times m}$, $D \in \mathbb{R}^{m \times m}$. Let the inverse

$$M^{-1} = \left(\begin{array}{cc} P & Q \\ R^T & S \end{array}\right)$$

be decomposed similarly. Let $p \leq \min(n, m)$. Then A has rank deficiency p if and only if S has rank deficiency p.

For a proof we refer to Govaerts and Pryce [1989]. In the case where $m \ll n$ and p small we will typically use this result to express that A has a desired rank deficiency.

The essential tool in the present approach to Hopf points is the bialternate matrix product or biproduct. If A is an $n \times n$ matrix (typically $A = F_u$) and I_n denotes the $n \times n$ identity matrix then the biproduct $2 A \odot I_n$ is an $m \times m$ matrix with m = n(n-1)/2. Its rows and columns are both induced by pairs (i, j) with i > j, and the biproduct is formally defined by

$$(2A\odot I_n)_{(i,j),(k,l)} = \left\{egin{array}{ll} -a_{il} & ext{if } k=j \ a_{ik} & ext{if } k
eq i ext{ and } l=j \ a_{jl} & ext{if } k=i ext{ and } l=j \ a_{jl} & ext{if } k=i ext{ and } l
eq j \ -a_{jk} & ext{if } l=i \ 0 & ext{otherwise} \end{array}
ight.$$

The pairs (i, j) and (k, l) are ordered lexicographically. For example, if A is a general 3×3 matrix then

$$2A \odot I_3 = \left(egin{array}{cccc} a_{11} + a_{22} & a_{23} & -a_{13} \ a_{32} & a_{11} + a_{33} & a_{12} \ -a_{31} & a_{21} & a_{22} + a_{33} \end{array}
ight).$$

For our purposes the main results about biproducts are as follows:

PROPOSITION 2. If A has eigenvalues $\lambda_1, \ldots, \lambda_n$, then $2A \odot I_n$ has eigenvalues $(\lambda_i + \lambda_j)_{1 \leq j < i \leq n}$. If λ can be written as $\lambda_i + \lambda_j$ with j < i in a unique way, then λ is an algebraically and geometrically simple eigenvalue of $2A \odot I_n$.

COROLLARY 1. $2A\odot I_n$ is singular if and only if A has a zero-sum pair of eigenvalues.

In particular, $2A \odot I_n$ is singular at a Hopf point. But it is also singular if there are two real eigenvalues with sum zero. This is called a neutral-saddle case. Also, there is an intermediate case where A has two zero eigenvalues. This is called a BT (Bogdanov-Takens) point; it is another important case in the dynamical study of (1).

From a mathematical point of view, the matrices with exactly one pair of zero-sum eigenvalues form a codimension 1 manifold in the space of all matrices, defined by (for example) the condition that the determinant of the biproduct matrix is zero. The algorithms in CONTENT actually compute curves with zero-sum pairs of eigenvalues; the distinction between Hopf, BT, and neutral saddle is essentially an afterthought. Points with two zero-sum pairs of eigenvalues are not in this manifold but on its boundary. We have the following result.

Proposition 3. If A has exactly two different zero-sum pairs of eigenvalues then 0 is an eigenvalue of $2A \odot I_n$ with algebraic and geometric multiplicity 2. In particular, $2A \odot I_n$ has rank deficiency 2.

A double-Hopf point is a special case of this; the algorithm in CONTENT computes points with two zero-sum pairs of eigenvalues, and the specialization (double-Hopf, Hopf-neutral saddle, etc.) is done afterward.

Proposition 2 and Corollary 1 are classic. A proof of Proposition 3 is given in Govaerts et al. [1997].

We note that the bialternate product was introduced in 1900 by Stéphanos [1990] and recently revived as a computational tool in Guckenheimer et al. [1997] and Kuznetsov [1995].

2. CONTINUATION OF SINGLE-HOPF CURVES

2.1 Standard Method for Hopf Curve

In the standard implementation, a Hopf curve is defined as a one-dimensional manifold Γ in \mathbb{R}^{2n+3} endowed with coordinates (u, v, κ, α) where $u, v \in \mathbb{R}^n$, $\kappa \in \mathbb{R}$, $\alpha \in \mathbb{R}^2$ have to satisfy

$$\begin{cases} F(u, \alpha) = 0 \\ (F_u^2(u, \alpha) + \kappa I_n)v = 0 \\ \langle v, v \rangle - 1 = 0 \\ \langle L, v \rangle = 0. \end{cases}$$
 (3)

This defining system was introduced in Holodniok and Kubiček [1984] and Roose and Hlavaček [1985]. We note that actually the computed points are Hopf points only if $\kappa > 0$; for $\kappa = 0$ we have BT-points, and for $\kappa < 0$ we have neutral saddles.

In (3) L is a constant vector whose choice is in principle arbitrary; it is only required that L is not orthogonal to the null-eigenspace of the matrix

 $F_u^2 + \kappa I_n$. The last condition in (3) is necessary to make the choice of v locally unique.

The following test functions are computed along the standard Hopf curve to detect and process Hopf singularities:

$$\begin{cases} \psi_1 = \frac{1}{2\omega_0} \operatorname{Re}[\langle p, \, C(q, \, q, \, \bar{q}) \rangle - 2\langle p, \, B(q, \, A^{-1}B(q, \, \bar{q}) \rangle \\ + \langle p, \, B(\bar{q}, \, (2i\omega_0 I_n - A)^{-1}B(q, \, q)) \rangle], \\ \psi_2 = \kappa, \\ \psi_3 = \det(A), \\ \psi_4 = \det(2A_{|N^c} \odot I_{n-2}) \end{cases}$$

Here $A = F_u(u, \alpha)$; the complex vectors $p, q \in \mathbb{C}^n$ satisfy

$$A q = i \omega_0 q$$
, $A^T p = -i \omega_0 p$, $\langle q, q \rangle = \langle p, q \rangle = 1$,

$$\langle \operatorname{Re} q, \operatorname{Im} q \rangle = 0, \quad (4)$$

where $\langle p, q \rangle = \bar{p}^T q$ is the standard scalar product in \mathbb{C}^n (also used in \mathbb{R}^n), and the multilinear functions B(q, p) and C(p, q, r) are defined by

$$B_i(q, p) = \sum_{j,k=1}^n \left. \frac{\partial^2 F_i(u, \alpha_0)}{\partial u_j \partial u_k} \right|_{(u_0, \alpha_0)} q_j p_k \tag{5}$$

and

$$C_i(p, q, r) = \sum_{i, k, l=1}^n \frac{\partial^3 F_i(u, \alpha_0)}{\partial u_j \partial u_k \partial u_l} \Big|_{\substack{(u_0, \alpha_0) \\ (u_0, \alpha_0)}} p_j q_k r_l$$
 (6)

for $i=1,\,2,\,\ldots$, n. The test function ψ_1 is only defined when the critical eigenvalues are imaginary, i.e., $\kappa=\omega_0^2>0$. In this case, one can use v to compute q. Namely, the vector $q=q_R+iq_I\in\mathbb{C}^n$ with

$$q_R = v, \ q_I = -\frac{1}{\omega_0 ||v||} Av$$

is obviously a critical eigenvector of A corresponding to $i\omega_0$. An extra normalization makes it satisfying (4). In the literature ψ_1 is known as the first Lyapunov coefficient; its sign distinguishes sub- and supercritical Hopf bifurcations. The above formula for ψ_1 is derived using the center manifold reduction in Kuznetsov [1995, Sect. 5.4].

manifold reduction in Kuznetsov [1995, Sect. 5.4]. In the definition of ψ_4 $N^C \subset \mathbb{R}^n$ is the orthogonal complement of the two-dimensional singular space of A^T that corresponds to the critical eigenvalues. This is an invariant subspace of A; the eigenvalues of $A|_{N^C}$ are the eigenvalues of A other than the critical ones.

The following singularities can be detected and located as regular zeros of the above-defined test functions:

- —Generalized Hopf: $\psi_1 = 0$;
- —Bogdanov-Takens: $\psi_2 = \psi_3 = 0$;
- —Zero-Hopf: $\psi_3 = 0, \ \psi_2 \neq 0;$
- —Double Hopf: $\psi_4 = 0$.

Again, these singularities strongly influence the dynamic behavior of (1). We note that Generalized Hopf is the bifurcation where the first Lyapunov coefficient vanishes; this is sometimes called a degenerate Hopf or Bautin bifurcation. We refer to Kuznetsov [1995] for details.

2.2 Bordered Squared Jacobian Method for Hopf Curve

Here the Hopf curve is defined as a one-dimensional manifold in \mathbb{R}^{n+3} endowed with coordinates (u, κ, α) where $u \in \mathbb{R}^n$, $\kappa \in \mathbb{R}$, $\alpha \in \mathbb{R}^2$ have to satisfy

$$\begin{cases} F(u, \alpha) = 0 \\ g_{ij1} = 0 \\ g_{ij2} = 0 \end{cases}$$
 (7)

where $g_{ij} = g_{ij}(u, \alpha)$ are components of the matrix G obtained by solving a nonsingular system with two right-hand sides

$$\begin{pmatrix} F_u^2 + \kappa I_n & B_1 & B_2 \\ \hline C_1^T & 0 & 0 \\ \hline C_2^T & 0 & 0 \end{pmatrix} \begin{pmatrix} V \\ G \end{pmatrix} = \begin{pmatrix} O \\ I_2 \end{pmatrix}. \tag{8}$$

This system is based on the ideas in Chu et al. [1994] and Werner [1996]; B_1 , B_2 , C_1 , C_2 are vectors in \mathbb{R}^n . By Proposition 1, G has rank defect 2 in a Hopf point which translates to four conditions:

$$g_{11} = 0$$
, $g_{12} = 0$, $g_{21} = 0$, $g_{22} = 0$

Two of these are chosen as defining equations. The test functions are the same as in the standard Hopf curve, and the same singularities can be detected.

2.3 Bordered Biproduct Method for Hopf Curve

The bordered biproduct Hopf curve is specified by the following defining functions,

$$\begin{cases} F(u, \alpha) = 0 \\ g_{11}g_{22} - g_{12}g_{21} = 0, \end{cases}$$

where $g_{ij} = g_{ij} (u, \alpha) (i, j = 1, 2)$ are the components of the matrix

$$G = \left(\begin{array}{cc} g_{11} & g_{12} \\ g_{21} & g_{22} \end{array}\right)$$

obtained from solving

$$\begin{pmatrix} \frac{2 F_u \odot I_n & W_1 & W_2}{V_1^T} & d_{11} & d_{12} \\ V_2^T & d_{21} & d_{22} \end{pmatrix} \begin{pmatrix} V \\ G \end{pmatrix} = \begin{pmatrix} O \\ I_2 \end{pmatrix}, \tag{9}$$

where V_1 , V_2 , W_1 , $W_2 \in \mathbb{R}^m$, d_{11} , d_{12} , d_{21} , $d_{22} \in \mathbb{R}$, m = n(n-1)/2 are constant quantities chosen so that the matrix in (9) is nonsingular.

The equation $g_{11}g_{22} - g_{12}g_{21} = 0$ means that G has rank defect one. By Proposition 1 then $2 F_u \odot I_n$ also has rank defect one, which is the condition for a zero-sum pair of eigenvalues by Corollary 1.

If the derivatives G_z (z one of the state variables or parameters) are to be computed symbolically, then we also solve

$$(W^{T} G) \begin{pmatrix} \frac{2 F_{u} \odot I_{n} & W_{1} & W_{2}}{V_{1}^{T} & d_{11} & d_{12}} \\ V_{2}^{T} & d_{21} & d_{22} \end{pmatrix} = (O I_{2}),$$

$$(10)$$

where $W \in \mathbb{R}^{m \times 2}$. Then indeed

$$G_z = -W^T (2F_{uz} \odot I_n) V.$$

Along the biproduct Hopf curve, the following test functions are computed:

$$\begin{cases} \psi_1 = \frac{1}{2\omega_0} \operatorname{Re}[\langle p, \, C(q, \, q, \, \bar{q}) \rangle - 2\langle p, \, B(q, \, A^{-1}B(q, \, \bar{q}) \rangle \\ + \langle p, \, B(\bar{q}, \, (2i\,\omega_0 I_n - A)^{-1}B(q, \, q)) \rangle], \\ \psi_2 = \frac{\langle v, \, Av \rangle \langle w, \, Aw \rangle - \langle w, \, Av \rangle \langle v, \, Aw \rangle}{\langle v, \, v \rangle \langle w, \, w \rangle - \langle v, \, w \rangle^2}, \\ \psi_3 = \det(A), \\ \psi_4 = g_{22} \end{cases}$$

Here $A = F_u(u, \alpha)$; two real vectors $v, w \in \mathbb{R}^n$ are such that $Q = v \wedge w$ where \wedge denotes the wedge product and Q is a right singular vector of $2A \odot I_n$. We recall that the wedge product $v \wedge w$ of two vectors in \mathbb{R}^n is a vector in $\mathbb{R}^{n(n-1)/2}$ indexed by pairs (i, j) where $1 \leq j < i \leq n$ such that $(v \wedge w)_{(i,j)} = v_j w_i - v_i w_j$. In the present case, v, w span the two-dimensional eigenspace that corresponds to the zero-sum pair of eigenvalues. This is an invariant subspace of A, and by some easy computations one verifies that $\psi_2(=\kappa)$ is the product of the two zero-sum eigenvalues.

The complex vectors $p, q \in \mathbb{C}^n$ satisfy (4), and the multilinear functions B(p, q) and C(p, q, r) are defined by (5) and (6). The test function ψ_1 is identical to the first test function evaluated along the standard Hopf curve. It is only defined when the critical eigenvalues are imaginary, i.e., $\psi_2 = \omega_0^2 > 0$. In this case, one can use v to compute q. Namely, the vector $q = q_R + iq_I \in \mathbb{C}^n$ with

$$q_R = \frac{v}{\|v\|}, \ q_I = -\frac{1}{\omega_0 \|v\|} A v$$

is a critical eigenvector of A corresponding to $i\omega_0$. An extra normalization makes it satisfying (4).

The same singularities as in Section 2.1 can be detected and located as regular zeros of the above-defined test functions:

- —Generalized Hopf: $\psi_1 = 0$;
- —Bogdanov-Takens: $\psi_2 = \psi_3 = 0$;
- —Zero-Hopf: $\psi_3 = 0$, $\psi_2 \neq 0$;
- —Double-Hopf: $\psi_4 = 0$.

2.4 Bifurcation, Continuation, and Auxiliary Data

The computation of single-Hopf curves generically requires two free parameters. The continuation code in CONTENT can be used to continue Hopf curves defined by the three systems: the Standard Hopf (I) system, the Squared Jacobian Hopf (II) system, and the Bordered Biproduct Hopf (III) system. Conceptually we distinguish between bifurcation, continuation, and auxiliary data. The bifurcation data are the same for all Hopf curves. These are

$$(u, \alpha, \kappa, v, L)$$

where u contains the state variables, α the parameters, κ is the product of the zero-sum eigenvalues, and v is a nonzero vector in the eigenspace of the zero-sum eigenvalues. Finally, L is a vector not orthogonal to this eigenspace; in practice it is an approximation to a vector in the eigenspace orthogonal to v. The continuation data are the unknowns in the set of defining equations and thus depend on the computational method. In addition, each method may have its own auxiliary data, i.e., quantities that are fixed in the defining equations for one or more continuation steps (prediction and correction) but may still have to be adapted.

For type (I) the continuation data are

$$(u, \alpha, \kappa, v),$$

and L is an auxiliary vector.

For type (II) the continuation data are

$$(u, \alpha, \kappa)$$
,

while $B_1,\,B_2,\,C_1,\,C_2$ are auxiliary vectors and $(i_1,j_1),\,(i_2,j_2)$ are auxiliary integer numbers.

For type (III), the continuation data are simply

$$(u, \alpha),$$

but this method has more auxiliary data, namely $V_1,\ V_2,\ W_1,\ W_2\in\mathbb{R}^m$ and $D\in\mathbb{R}^{2\times 2}$ where

$$D = \left(\begin{array}{cc} d_{11} & d_{12} \\ d_{21} & d_{22} \end{array} \right).$$

Each type has a Starter routine where the continuation and auxiliary data are generated that are needed in the Hopf defining condition or test functions. Also, the tangent vector to the curve at the starting point is computed. This information is then passed to the continuation code (Continuer).

The Continuer computes successive points on the Hopf curve and evaluates a number of test functions. If it detects a sign change of a test function, it locates its zero within given accuracy using bisections. In such a way, higher degeneracies or bifurcations on the Hopf curve are computed.

After a fixed number of steps (chosen by the user but typically one) during continuation, the auxiliary data are refreshed. This is done by the Adapter routine.

2.5 Implementation of the Standard Hopf Method

In the Starter the initial values of u, α , v, L are read from the stored data. In the Adapter the vector L is adapted as a vector in the singular space of $F_u^2 + \kappa I_n$ and orthogonal to V = v; the aim is to avoid that L ever becomes orthogonal to the singular space, since this would make the defining system for standard Hopf singular.

2.6 Implementation of the Squared Jacobian Hopf Method

In the Starter the initial values of u, α , κ are read from the stored data, and the auxiliary data B_1 , B_2 , C_1 , C_2 , (i_1, j_1) , (i_2, j_2) are generated. The auxiliary data are updated in the Adapter. The process of generating and updating the auxiliary data is basically the same as in the double-Hopf case; indeed, in both cases we express that a matrix has rank defect two. We refer to Sections 4.2 and 4.3 for details.

2.7 Implementation of the Bordered Biproduct Hopf Method

2.7.1 Starter. The initial values of u, α are read from the stored data. Then we distinguish between two cases. If $m \ge 2$, i.e., $n \ge 3$, then the

bordering vectors V_1 , $V_2 \in \mathbb{R}^m$ are initially chosen as follows:

$$V_1 = (0, \ldots, 0, 1, 0)^T$$
 $V_2 = (0, \ldots, 0, 1)^T$,

while the bordering columns W_1 , $W_2 \in \mathbb{R}^m$ are chosen as vectors of the type

$$(0, 0, \ldots, 0, 1, 0, \ldots, 0, 0)^T$$

where the position of the 1 is determined by the row indices of the two rows with minimal pivot elements in the LU-decomposition with complete pivoting of the matrix $2 F_u \odot I_n$. Initially, $d_{ij} = 0$, i, j = 1, 2. This choice guarantees that the bordered matrix

$$\begin{pmatrix}
\frac{2 F_u \odot I_n & W_1 & W_2}{V_1^T & d_{11} & d_{12}} \\
V_2^T & d_{21} & d_{22}
\end{pmatrix}$$
(11)

is nonsingular if 2 F_u \odot I_n has rank defect at most two (at least for practical purposes, assuming that the ill conditioning of $2F_u$ \odot I_n translates into the appearance of small pivot elements). To improve the condition of (11) before continuation is started, V_1 , V_2 , W_1 , W_2 and d_{11} , d_{12} , d_{21} , d_{22} are once adapted, as is described in the next section.

In the case m = 1, i.e., n = 2, we put

$$V_1 = (1), \quad V_2 = (0), \quad W_1 = (1), \quad W_2 = (0)$$

and

$$d_{11} = d_{12} = d_{21} = 0, \quad d_{22} = 1.$$

Indeed, the matrix

$$\left(egin{array}{cccc} 2 \ F_u \odot I_2 & 1 & 0 \ 1 & 0 & 0 \ 0 & 0 & 1 \end{array}
ight)$$

is always nonsingular.

2.7.2 Adapter. During continuation, the borders are adapted to make (11) as well conditioned as possible. This is done in the following way. We want V_1 to be a right singular vector of $2 F_u \odot I_n$, and assume that (11) is still nonsingular in the actual point. So we solve

$$\begin{pmatrix} 2 F_u \odot I_n & W_1 & W_2 \\ V_1^T & d_{11} & d_{12} \\ V_2^T & d_{21} & d_{22} \end{pmatrix} (\xi_1^{(0)} \xi_2^{(0)}) = \begin{pmatrix} O \\ I_2 \end{pmatrix}.$$
 (12)

Let $(\alpha \beta)$ denote the row in

$$\left(\begin{array}{ccc} \xi_{1,m+1}^{(0)} & \xi_{2,m+1}^{(0)} \\ \xi_{1,m+2}^{(0)} & \xi_{2,m+2}^{(0)} \end{array}\right)$$

containing the largest of the four entries (in absolute value). The new values for V_1 are then the first m components of a normalized version of $\xi_1^{(1)}$ with

$$\xi_1^{(1)} = -\beta \xi_1^{(0)} + \alpha \xi_2^{(0)}$$
.

By this construction V_1 is a right singular vector of $2 F_u \odot I_n$.

The adaptation of W_1 is done similarly with the matrix (11) in (12) replaced by its transpose. So W_1 is adapted to become a normalized left singular vector of $2 F_u \odot I_n$. We set $d_{11} = d_{22} = 0$. Now consider

$$M_{1} = \begin{pmatrix} 2 F_{u} \odot I_{n} & W_{1} \\ V_{1}^{T} & 0 \end{pmatrix}.$$
 (13)

This matrix is nonsingular if $2 F_u \odot I_n$ has rank defect 1, i.e., in every single-Hopf point. We will border it choosing V_2 , W_2 , d_{21} , d_{12} in such a way that (11) is as well conditioned as possible in this case. Since the condition for nonsingularity of (11) is

$$(V_2^T d_{21}) M_1^{-1} {W_2 \choose d_{12}} \neq 0, (14)$$

we first solve

$$M_1 \begin{pmatrix} V_2^{(n)} \\ d_{21}^{(n)} \end{pmatrix} = \begin{pmatrix} W_2 \\ d_{12} \end{pmatrix} \tag{15}$$

and then normalize

$$egin{pmatrix} V_2^{(n)} \ d_{21}^{(n)} \end{pmatrix}$$

to provide the new V_2 , d_{21} . Then we solve

$$M_{1}^{T} \begin{pmatrix} W_{2}^{(n)} \\ d_{12}^{(n)} \end{pmatrix} = \begin{pmatrix} V_{2} \\ d_{21} \end{pmatrix}$$
 (16)

and normalize

$$\left(egin{array}{c} W_2^{(n)} \ d_{12}^{(n)} \end{array}
ight)$$

to provide the new W_2 , d_{12} .

We note two things. First, if the computed point is actually close to a double-Hopf point, i.e., to a point where $2 \ F_u \odot I_n$ has rank defect two, then

$$egin{pmatrix} V_2 \ d_{21} \end{pmatrix}$$

tends to the right singular vector of M_1 , i.e., V_2 tends to a right singular vector of 2 $F_u \odot I_n$ orthogonal to V_1 , and d_{21} tends to zero. Similarly, W_2 tends to a left singular vector of 2 $F_u \odot I_n$ orthogonal to W_1 , and d_{12} tends to zero. Hence (11) will remain nonsingular even at double-Hopf points, and our defining system for Hopf points is still defined (though it becomes singular because a double-Hopf point is generically an intersection of two curves of single-Hopf points). This is the main reason for using a bordering with two additional rows and columns instead of one.

Second, since M_1 has full rank in single-Hopf, points it follows from Propositions 1 and 2 that $g_{22} \neq 0$. Hence we will use g_{22} as a test function for the detection of double-Hopf or other points with two zero-sum pairs of eigenvalues. We note that by Propositions 1 and 3 all components of G must vanish if F_u has two zero-sum pairs of eigenvalues.

3. EXAMPLES

3.1 LP Neuron Model

As a first example model we used the LP (Lateral Pyloric) neuron model of the stomatogastric ganglion of the crab Cancer Borealis, described in Govaerts et al. [1997]. We do not repeat the (very complicated) complete description here. It is given in the easily accessible paper [Govaerts et al. 1997] and typing it in from paper would be an error-prone task anyway; a code can be obtained from the authors if desired. We just recall that the model has 13 state variables, and we consider three free parameters (the model contains a large number of other parameters which will be fixed in our implementation). We started from a Hopf point with coordinates given in Table I and continued using the bordered biproduct method (the Hopf point itself was found by path-following a curve of equilibria, starting from a point with values suggested by experiments and measurements).

A projection of the resulting Hopf curve on the (I_{ext}, \bar{g}_{Af}) —space is shown in Figure 1 which was drawn by CONTENT. The parameters I_{ext} and \bar{g}_{Af} were freed and $\bar{g}_{K(eg)}$ was held fixed.

On this curve, we detected one zero-Hopf point (denoted as ZH) and one double-Hopf and four Hopf-neutral saddle points (both indicated with DH). The critical eigenvalue at the zero-Hopf point is 40.28604585i. The two pairs of complex eigenvalues causing the double-Hopf point are $\pm 40.32075i$

	state	value	param	value
1	v	-37.375628	I_{ext}	0.962394
2	h	0.09414726	$ar{ar{g}}_{Af}$	3.3467726
3	Ca	0.17133200	$ar{ar{g}}_{K(Ca)}$	5
4	a_{Ca_1}	0.02257790		
5	a_{Ca_2}	0.00020707		
6	b_{Ca_I}	0.17107233		
7	n	0.32563857		
8	$a_{K(Ca)}$	0.00174379		
9	$b_{K(Ca)}$	0.7778751		
10	a_A	0.58698691		
11	b_{Af}	0.01623749		
12	b_{As}	0.01623749		
13	a_h	0.00234855		

Table I. A Hopf Point in the LP-Neuron Model

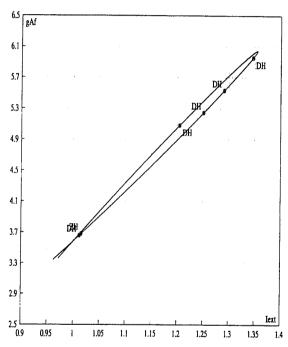


Fig. 1. A double-Hopf point on a Hopf curve.

and $\pm 0.063568i$. In Figure 1 the double-Hopf point is the one very close to the zero-Hopf point (but distinct from it: see Figure 3 for a zoom-in).

3.2 A Chemical Model

The second example is a chemical model given by the following equations:

$$\begin{cases} \dot{x} = 2q_{1}z^{2} - 2q_{5}x^{2} - q_{3}xy \\ \dot{y} = q_{2}z - q_{6}y - q_{3}xy \\ \dot{s} = q_{4}z - kq_{4}s, \end{cases}$$

	state	value	param	value
1	\boldsymbol{x}	0.07792759	q_{1}	2.5
2	y	0.2330654	q_2	1.040992
3	s	0.4921479	q_3	10
4			q_4	0.0675
5			$q_{\it 5}$	1
. 6			$q_{\it 6}$	0.1
7			k	0.4

Table II. A Hopf Point in a Chemical Model

where z = 1 - x - y - s (see Bykov et al. [1978] and Khibnik et al. [1987]). This system is used as an example in Khibnik et al. [1993]. Starting from the point with coordinates given in Table II, we obtained a (closed) Hopf curve.

The notation GH indicates a generalized Hopf (or Bautin) point, and BT is an abbreviation denoting a Bogdanov-Takens point. Note that the part of the Hopf curve to the right from the BT points corresponds to neutral saddles.

4. CONTINUATION OF DOUBLE-HOPF CURVES

The computation of double-Hopf curves generically requires three free parameters, say $\alpha = (\alpha_1, \alpha_2, \alpha_3)$. In this section, we describe the implementation in CONTENT of this computation using a doubly bordered biproduct matrix.

4.1 Defining System

The Jacobian matrix F_u has two pairs of purely imaginary eigenvalues at a double-Hopf point, so by Proposition 3 the biproduct matrix $2 F_u \odot I_n$ has rank defect two. We border it with two additional rows and columns to make it nonsingular.

The double-Hopf curve will be specified by the following defining functions:

$$\begin{cases}
F(u, \alpha) = 0 \\
g_{i_1j_1} = 0 \\
g_{i_2j_2} = 0
\end{cases}$$
(17)

with $g_{ij} = g_{ij}(u, \alpha)$ components of the matrix G obtained by solving

$$\begin{pmatrix}
\frac{2 F_u \odot I_n & W_1 & W_2}{V_1^T} & 0 & 0 \\
V_2^T & 0 & 0
\end{pmatrix}
\begin{pmatrix}
V \\
G
\end{pmatrix} = \begin{pmatrix}
O \\
I_2
\end{pmatrix}.$$
(18)

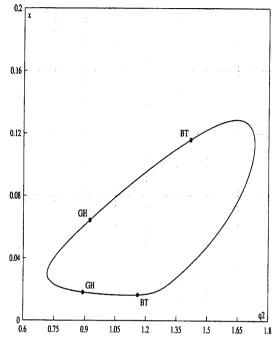


Fig. 2. A Hopf curve in a chemical model.

By Proposition 3, G has rank defect two in a double-Hopf point, which translates to four conditions:

$$g_{11} = 0$$
, $g_{12} = 0$, $g_{21} = 0$, $g_{22} = 0$

Two of these are chosen as defining functions. So the continuation data are u, α with V_1 , V_2 , W_1 , W_2 and (i_1, j_1) , (i_2, j_2) as auxiliary data (the analogue of the 2×2 matrix D in Section 2 is a zero matrix).

We note again that (17) actually defines points with two zero-sum pairs of eigenvalues; distinction between double-Hopf, Hopf-neutral saddle, etc., is done in the postprocessing.

Symbolic derivatives of $g_{i_1j_1}$, $g_{i_2j_2}$, if desired, can be computed as in Section 2.2.

4.2 Starter

The initial values for u, α are read from the stored data. The initial choice of V_1 , V_2 , W_1 , W_2 is obtained from pivot information as in Section 2.5.1 in the case $m \geq 2$ (the case m = 1 is impossible, since we need at least four state variables). To decide the choice of (i_1, j_1) , (i_2, j_2) we first perform an LU-decomposition with complete pivoting of

$$\left(egin{array}{ccccc} F_u^T & 0 & 0 & 0 \ & \vdots & \vdots & \vdots \ F_{lpha_1}^T & 0 & 0 & 0 \ F_{lpha_2}^T & 0 & 0 & 0 \ F_{lpha_3}^T & 0 & 0 & 0 \end{array}
ight).$$

Let p_1 , p_2 , p_3 be the rows in which the three smallest pivots appear, and set $F_z = [F_u, F_\alpha]$. Now solve

$$\begin{pmatrix} F_z \\ e_{p_1}^T \\ e_{p_2}^T \\ e_{p_3}^T \end{pmatrix} (V_1 \ V_2 \ V_3) = \begin{pmatrix} O \\ I_3 \end{pmatrix}. \tag{19}$$

Here e_{p_i} is the (p_i) th unit vector; by construction the matrix in the left-hand side of (19) is generically well conditioned (we assume that F_z has full rank n), and

$$V_N = (V_1 \ V_2 \ V_3)$$

is a base for the three-dimensional singular space of F_z .

Now we compute the derivatives $(g_{ij})_z$ with z either a state variable or a parameter. In this way, we obtain four vectors G_{11z} , G_{12z} , G_{21z} , and G_{22z} in \mathbb{R}^{n+3} that contain these derivatives. The tangent vector to the double-Hopf curve is necessarily in the space spanned by V_N and orthogonal to all vectors G_{ijz} . We project the four of them orthogonally onto the span of V_N and obtain

$$\begin{cases} G_{11}^{*} = V_{N}(V_{N}^{T} V_{N})^{-1} V_{N}^{T} G_{11z} \\ G_{12}^{*} = V_{N}(V_{N}^{T} V_{N})^{-1} V_{N}^{T} G_{12z} \\ G_{21}^{*} = V_{N}(V_{N}^{T} V_{N})^{-1} V_{N}^{T} G_{21z} \\ G_{22}^{*} = V_{N}(V_{N}^{T} V_{N})^{-1} V_{N}^{T} G_{22z} \end{cases}$$

$$(20)$$

So in the absence of roundoff and truncation errors the four vectors in (20) span only a two-dimensional space. We choose two index pairs so that the corresponding vectors span this space in a numerically optimal way. First we compute $||G_{11}^*||$, $||G_{12}^*||$, $||G_{21}^*||$, and $||G_{22}^*||$; the largest norm gives the first index pair (i_1, j_1) . After that, $G_{i_1 j_1}^*$ is normalized.

To find the second index pair (i_2, j_2) , we project G_{ij}^* onto the orthogonal complement of $G_{i,j}^*$ for all $(i,j) \neq (i_1,j_1)$, i.e.,

$$G_{ij}^{**} = G_{ij}^* - \langle G_{ij}^*, G_{ij_1}^* \rangle G_{ij_1}^* \text{ with } (i, j) \neq (i_1, j_1).$$

Again norms are calculated, and the index with largest norm gives (i_2, j_2) . To improve the performance, the Adapter is called before starting the continuation.

4.3 Adapter

The adaptation of V_1 , V_2 , W_1 , W_2 is easier than in Section 2.5.2. Indeed, the vectors $\xi_1^{(0)}$, $\xi_2^{(0)}$ now span the two-dimensional right singular space of 2 $F_u \odot I_n$. So we orthogonalize and normalize them to form the new V_1 , V_2 . Adaptation of W_1 , W_2 is done similarly. This procedure is optimal in the

	state	value	param	value
1	υ	-37.23289	I_{ext}	1.011663
2	h	0.09175642	$ar{ar{g}}_{Af}$	3.655107
3	Ca	0.1718781	$\bar{g}_{K(Ca)}$	5
4	a_{Ca_1}	0.0230323	311(34)	
5	a_{Ca_2}	0.0002113377		
6	b_{Ca_I}	0.168557		
7	n	0.3274851		
8	$a_{K(Ca)}$	0.001795097		
9	$b_{K(Ca)}$	0.7773248		
10	a_A	0.589148		
11	b_{Af}	0.01586182		
12	b_{As}	0.01586182		
13	a_h	0.002319861		

Table III. A Double-Hopf Point in the LP-Neuron Model

sense that the big square matrix in (18) has minimal condition number if the original problem was "reasonably" scaled, i.e., so that 1 is in or near the interval that contains the m-2 largest singular values of 2 $F_u \odot I_n$. The choice for (i_1,j_1) and (i_2,j_2) is adapted in the same way as in the Starter, except that for the calculation of V_N the three bottom rows of the matrix (19) are replaced by $(g_{i_1j_1})_z$, $(g_{i_2j_2})_z$ and the tangent vector to the curve.

5. EXAMPLE: LP NEURON MODEL

On the Hopf curve of Figure 1, a double-Hopf point was detected with coordinates given in Table III.

We use this point to start continuation of a double-Hopf curve, indicated as a dashed line in Figure 3. In fact, Figure 3 is a zoom-in on Figure 1 near the zero-Hopf (ZH) point. It shows also that the double-Hopf and zero-Hopf points in Figure 1 do not intersect itself at the double-Hopf point.

6. COMPARISON WITH OTHER SOFTWARE

LOCBIF2 [Khibnik et al. 1993] and AUTO97 [Doedel et al. 1997] are probably the best-known codes that allow to compute curves of Hopf bifurcation points.

The algorithm in AUTO97 (and its many predecessors since about 1980) is close to our Standard Hopf method but uses the imaginary part of the Hopf eigenvalue as an unknown of the problem. More precisely, the defining system used in AUTO for the continuation of the Hopf bifurcation is given by the following 3n + 2 equations in \mathbb{R}^{3n+3} endowed with coordinates $(u, v, w, \omega, \alpha)$:

$$\begin{cases} F(u, \alpha) = 0 \\ F_u(u, \alpha)v + \omega w = 0 \\ F_u(u, \alpha)w - \omega v = 0, \\ \langle v, v_0 \rangle + \langle w, w_0 \rangle - 1 = 0 \\ \langle v, w_0 \rangle - \langle v_0, w \rangle = 0 \end{cases}$$
(21)

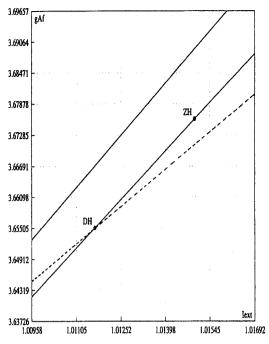


Fig. 3. Zoom-in of Figure 1.

where $q_0 = v_0 + iw_0$ is the critical eigenvector at the previous computed point in the curve. It is assumed that $\omega > 0$. Therefore, AUTO does not compute curves of points with zero-sum eigenvalues but only Hopf curves. Thus, using (21), AUTO could not pass a Bogdanov-Takens point where $\omega = 0$ and detect it regularly.

The algorithm in LOCBIF2 computes curves of points with zero-sum eigenvalues using the defining system

$$\begin{cases} F(u, \alpha) = 0 \\ \Delta_{n-1}(u, \alpha) = 0 \end{cases}$$
 (22)

where Δ_{n-1} is the Hurwitz determinant of order n-1 associated to the characteristic polynomial of $F_u(u,\alpha)$. Thus, it is conceptually closer to our Bordered Biproduct Hopf method. It has the advantage that it does not use the biproduct matrix. Our experience with Example 1 shows that problems with n=13, m=n(n-1)/2=78 can still be handled efficiently with the Bordered Biproduct Hopf method, but for larger values of n the method slows down considerably. On the other hand, the method in LOCBIF2 computes and differentiates numerically the coefficients of the characteristic polynomial of the Jacobian matrix, and this makes it less robust because of scaling problems.

For the double-Hopf case our method is to the best of our knowledge the first implemented code. LOCBIF2 allows to detect double-Hopf points as self-crossing points of the defining equations (22) but cannot path-follow double-Hopf points (see Khibnik et al. [1993, p. 50, p. 64] for more information). No other standard package considers double-Hopf points.

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