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COMPUTING HOPF BIFURCATIONS I*

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Abstract. This paper addresses the problems of detecting Hopf bifurcations in systems of ordinary differential equations and following curves of Hopf points in two-parameter families of vector fields. The established approach to this problem relies upon augmenting the equilibrium condition so that a Hopf bifurcation occurs at an isolated, regular point of the extended system. We propose two new methods of this type based on classical algebraic results regarding the roots of polynomial equations and properties of Kronecker products for matrices. In addition to their utility as augmented systems for use with standard Newton-type continuation methods, they are also particularly well adapted for solution by computer algebra techniques for vector fields of small or moderate dimension.

Key words. Hopf bifurcation, resultant, bialternate product

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1. Introduction.

Consider the n-dimensional system of ordinary differential equations defined by

$$\dot{x} = f(x, \alpha) \tag{1}$$

where $x = x(t) \in \mathbb{R}^n$ and $f : \mathbf{U} \to \mathbb{R}^n$ is a C^2-smooth function, defined on a subset $\mathbf{U} \subset \mathbb{R}^n$, which depends upon a vector of parameters, $\alpha \in \mathbb{R}^k$. An *equilibrium* of this system is a point $x \in \mathbb{R}^n$ with the property that $f(x, \alpha) = 0$. As the parameters α are varied, equilibrium points can undergo bifurcation [14]. There are two types of elementary bifurcations that occur in generic one-parameter families of systems: saddle nodes and Hopf bifurcations. At a saddle-node bifurcation, the Jacobian derivative evaluated at an equilibrium point possesses a simple zero eigenvalue. Similarly, a necessary condition for Hopf bifurcation is the presence of a pure imaginary eigenvalue pair in the spectrum of $D_x f$. One would like robust algorithms for the calculation of parameter values where one of these bifurcations occurs in parameterized families of vector fields. In the case of saddle-node bifurcations, one may obtain the bifurcation locus by augmenting the equation $f(x, \alpha) = 0$ with a procedure to calculate equilibrium points where $D_x f$ has numerical rank $(n-1)$. An inflated system for the detection of saddle nodes has been previously proposed using $\det(D_x f)$ as the augmenting equation [1, 20]. To treat Hopf bifurcations in a similar manner, one requires explicit equations that determine whether the n-square matrix $D_x f$ has a pair of pure imaginary eigenvalues. This paper examines procedures for locating Hopf bifurcations

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based on the singularity of matrices obtained from algebraic transformations of the Jacobian matrix at an equilibrium.

Previous investigators have proposed a variety of approaches to the determination of Hopf bifurcation points, which may be divided into two broad classes. A typical *indirect* method employs a numerical algorithm for computing the spectrum of the Jacobian at each point along a path of equilibria and then interpolating to locate parameter values at which a pair of eigenvalues cross the imaginary axis. For vector fields of small dimension, the unsymmetric QR factorization algorithm is widely advocated, while for larger problems Krylov subspace techniques are fast and provide adequate accuracy in few iterations [21, 8]. In a *direct* method, equations which characterize the Hopf point augment the usual equilibrium condition and standard techniques are used to solve for roots of the resulting system. Algorithms frequently used in practice solve explicitly for the purely imaginary eigenvalues together with a normalized basis of the corresponding eigenspace [12, 23, 24, 16]. Such an approach may be viewed as simultaneously solving for an equilibrium point and an eigensubspace by an iterative method. In this sense, transition from indirect to direct methods has replaced the use of highly stable and robust linear algebra techniques for spectral computations with root-finding algorithms which are only locally convergent. Such a strategy has a drawback. The minimal dimension of the inflated system increases to at least $2n + 1$, which may decrease the performance expected from the algorithm used to solve the resulting nonlinear system of equations and increase the demand for good initial values and small stepsizes. A side effect of these methods is that they produce more information than required—the detection of a pair of purely imaginary eigenvalues—at a significant computational cost.

The purpose of this paper is to examine the algebraic structure of Hopf bifurcation computations and to use the insight gained to construct direct methods that rely upon minimally augmented systems for the computation of Hopf bifurcations. Our methods are based on the algebraic properties of polynomial resultants and matrix symmetric products. This algebraic theory has been applied to many areas of applied mathematics, in particular to develop criticality conditions in Lyapunov stability analysis and root location [3]. The primary focus here is to develop a theoretical basis for algorithms to study Hopf bifurcation in multiparameter vector fields of modest dimensions where a complete and detailed description of the dynamics is a reasonable objective. Our experience in this context suggests the approach may prove fruitful for three reasons: First, the bifurcation analysis for a multiparameter dynamical system typically proceeds through a number of phases, the earliest aimed at providing a gross decomposition of the product space of phase and parameter variables into regions of greater or lesser interest. Criteria for Hopf bifurcation that can be easily evaluated based on the fixed point Jacobian alone, without requiring the details of its spectrum, lead to fast algorithms for "scanning" the parameter space for candidate regions of interest. Second, recent developments in computer algebra techniques and the widespread availability of powerful computing machines require reassessment of mathematical algorithms normally reserved exclusively for problems of very small dimension. Application of computer algebra methods to problems in dynamical systems has already proved effective in normal form computation, center-manifold reduction, and perturbation analysis [22]. It is clear that approaches to computing Hopf bifurcations that require the use of iterative algorithms or direct evaluation of the eigenvalues are unsuitable for use with symbolic methods. If, instead, the Hopf condition is expressed in terms of functions of the Jacobian, then, for some problems, application of symbolic methods

become feasible. Third, steady progress in computer hardware and software evolution promises to continue the trend toward very fast, very robust methods for the solution of linear algebra problems. It seems desirable to exploit reliable methods for matrix manipulation in exchange for reducing the size or difficulty inherent in the solution of nonlinear equations, even if the required penalty is an increase in the dimension of the matrices involved. For some problems, especially those with a special structure, this approach may yield algorithms that are more effective than those in widespread use. A companion paper to this one [15] studies the implementation of these methods on three examples. Detailed comparisons with other algorithms are discussed there, though we make a few comments about these comparisons in the final section of this paper.

Methods for detecting Hopf bifurcation based on algebraic techniques have appeared in the literature, and the present paper complements and extends those results in a number of ways. In particular, the program *LINLBF* by Khibnik and his coworkers [18] incorporates a method for following curves of Hopf bifurcations based on the resultant of two polynomials which is similar to that described here. Our subresultant condition described in section 2 provides a way of discriminating between Hopf points and other resonant saddle points and can be used by either method. We describe three formally different forms of the resultant criteria that lead to matrix formulations with distinctly different properties and prove that they are equivalent. The development of augmented systems based on tensor products is new, although the important classical role occupied by tensors in the study of stability criteria for ordinary differential equations is very suggestive. Our proof that Hopf bifurcations are isolated solutions to the augmented equations in a neighborhood that does not contain a degenerate point applies to augmented systems based on either resultants or tensor products.

In the next section we recall the algebraic preliminaries required to express the necessary Hopf condition in terms of the singular set for certain algebraic functions of either the Jacobian at an equilibrium point or its associated characteristic polynomial. We present two new methods for following curves of Hopf bifurcation points in two-parameter families and discuss the variations which arise due to the various ways singularity of a matrix may be measured. Concluding remarks, comments about the performance of our algorithms, and a discussion of methods for extending this approach to bifurcation points of greater degeneracy are collected together in section 4.

2. Hopf algorithms using polynomial resultants. We seek explicit criteria that specify whether an $n \times n$ matrix, with coefficients that may depend upon parameters, has a pair of pure imaginary eigenvalues. In this section we develop the desired necessary conditions expressed in terms of the corresponding characteristic polynomial for the matrix.

Let $\mathbf{J}$ be the Jacobian matrix for f, and denote its characteristic polynomial by

$$p(\lambda) = c_0 + c_1\lambda + \cdots + c_{n-1}\lambda^{n-1} + \lambda^n.$$

Clearly, p has the nonzero root pair $\{\lambda, -\lambda\}$ if and only if λ is a common root of the two equations $p(\lambda) + p(-\lambda)$ and $p(\lambda) - p(-\lambda)$. Making the substitution $z = \lambda^2$ and rearranging, we construct two new polynomials. If n is even, let

$$\begin{aligned} r_e(z) &= c_0 + c_2 z + c_4 z^2 + \cdots + c_{n-2} z^{\frac{n-2}{2}} + z^{\frac{n}{2}}, \\ r_o(z) &= c_1 + c_3 z + c_5 z^2 + \cdots + c_{n-1} z^{\frac{n-2}{2}} \end{aligned} \tag{2a}$$

while if n is odd, set

$$\begin{aligned} r_e(z) &= c_0 + c_2 z + c_4 z^2 + \cdots + c_{n-3} z^{\frac{n-3}{2}} + c_{n-1} z^{\frac{n-1}{2}}, \\ r_o(z) &= c_1 + c_3 z + c_5 z^2 + \cdots + c_{n-2} z^{\frac{n-3}{2}} + z^{\frac{n-1}{2}}. \end{aligned} \tag{2b}$$

Then p has a nonzero root pair $\{\lambda, -\lambda\}$ if there exists a z that satisfies

$$\begin{pmatrix} r_e(z) \\ r_o(z) \end{pmatrix} = \mathbf{0}. \tag{3}$$

Two polynomials have a common root if and only if they share a common factor. Since r_e and r_o are univariate polynomials with the degree of r_o less than or equal to the degree of r_e, the *Euclidean algorithm* may be used to answer this question. We compute a sequence of polynomials $P_0 = r_e, P_1 = r_o, P_2, \ldots, P_k$ with the property that P_{i+1} is the remainder of dividing P_{i-1} by P_i. Thus, one requires that the degrees of the P_i are strictly decreasing and that there are polynomials Q_i, $i = 1, \ldots, k$ such that $P_{i-1} = Q_i P_i + P_{i+1}$. The sequence terminates when a P_k is found that divides P_{k-1}. It is easy to verify by induction that the P_i are all in the ideal generated by r_e and r_o in the polynomial ring $R[z]$ which implies that there are polynomials A_i and B_i with $P_i = A_i r_e + B_i r_o$. If r_e and r_o have no common factor, then the repeated divisions will produce a P_k that is a nonzero constant. On the other hand, if r_e and r_o do have a common factor, then their greatest common denominator appears as P_k which divides P_{k-1}. In this way the Euclidean algorithm may be used to determine whether or not two polynomials share a common root.

The Euclidean algorithm is closely related to a collection of determinants constructed from the coefficients of two polynomials. For n even, let the *Sylvester matrix* of the pair of equations (2a) and (2b) be the $(n-1)\times(n-1)$ matrix given by

$$\mathcal{S} = \left[\begin{array}{ccccccccc} c_0 & c_2 & \cdots & c_{n-2} & 1 & 0 & 0 & \cdots & 0 \\ 0 & c_0 & c_2 & \cdots & c_{n-2} & 1 & 0 & \cdots & 0 \\ \vdots & & & & & & & & \vdots \\ 0 & \cdots & \cdots & 0 & c_0 & c_2 & \cdots & c_{n-2} & 1 \\ c_1 & c_3 & \cdots & c_{n-1} & 0 & 0 & \cdots & \cdots & 0 \\ 0 & c_1 & c_3 & \cdots & c_{n-1} & 0 & \cdots & \cdots & 0 \\ \vdots & & & & & & & & \vdots \\ 0 & \cdots & \cdots & 0 & c_1 & c_3 & \cdots & \cdots & c_{n-1} \end{array}\right] \begin{array}{l} \left.\begin{array}{l} \\ \\ \\ \\ \end{array}\right\} \tfrac{n-2}{2} \text{ rows} \\ \left.\begin{array}{l} \\ \\ \\ \\ \end{array}\right\} \tfrac{n}{2} \text{ rows} \end{array}$$

while if n is odd, this matrix is defined to be

$$\mathcal{S} = \left[\begin{array}{ccccccccc} c_0 & c_2 & \cdots & c_{n-3} & c_{n-1} & 0 & 0 & \cdots & 0 \\ 0 & c_0 & c_2 & \cdots & c_{n-3} & c_{n-1} & 0 & \cdots & 0 \\ \vdots & & & & & & & & \vdots \\ 0 & \cdots & \cdots & 0 & c_0 & c_2 & \cdots & c_{n-3} & c_{n-1} \\ c_1 & c_3 & \cdots & c_{n-2} & 1 & 0 & \cdots & \cdots & 0 \\ 0 & c_1 & c_3 & \cdots & c_{n-2} & 1 & 0 & \cdots & 0 \\ \vdots & & & & & & & & \vdots \\ 0 & \cdots & \cdots & 0 & c_1 & c_3 & \cdots & c_{n-1} & 1 \end{array}\right] \begin{array}{l} \left.\begin{array}{l} \\ \\ \\ \\ \end{array}\right\} \tfrac{n-1}{2} \text{ rows} \\ \left.\begin{array}{l} \\ \\ \\ \\ \end{array}\right\} \tfrac{n-1}{2} \text{ rows} \end{array} .$$

The determinant $\mathcal{R}_{\mathcal{S}} = \det(\mathcal{S})$ is a polynomial in the coefficients of p referred to as the *Sylvester resultant* of r_e and r_o. The Sylvester matrix is singular (equivalently,

$\mathcal{R}_{\mathcal{S}} = 0$) if and only if the polynomials r_e and r_o share a common root. The computation of the Sylvester resultant is usually performed through the construction of a *pseudoremainder sequence* for the pair of polynomials. Modulo units in the ring of coefficients of the polynomials, the terms of the pseudoremainder sequence are the intermediate terms produced by the Euclidean algorithm. Explicit formulas for the coefficients of these intermediate terms can be defined in terms of determinants of appropriate submatrices of $\mathcal{S}$, called *subresultants*. We shall use the subresultants that correspond to a linear remainder term from the Euclidean algorithm. The coefficients of the linear remainder may be obtained by considering determinants of two $(n-3)\times(n-3)$ submatrices of $\mathcal{S}$. For $i = 0, 1$ let $\mathcal{S}_i$ denote the matrix obtained from $\mathcal{S}$ by deleting the rows 1 and $\frac{n}{2}$ and the columns 1 and $i+2$. Thus, for n even, $\mathcal{S}_0$ is obtained from the Sylvester matrix by removing the boxed entries shown below.

$$\mathcal{S}_0 = \begin{bmatrix} \boxed{\begin{matrix} c_0 & c_2 & \cdots & c_{n-2} & 1 & 0 & 0 & \cdots \end{matrix}} & 0 \\ 0 & \boxed{\begin{matrix} c_0 & c_2 & \cdots & c_{n-2} & 1 & 0 & \cdots \end{matrix}} & 0 \\ \vdots & & & & & & & \vdots \\ 0 & \cdots & \boxed{\begin{matrix} 0 & c_0 & c_2 & \cdots & c_{n-2} & 1 \end{matrix}} & 0 \\ 0 & \cdots & \cdots & \boxed{\begin{matrix} 0 & c_0 & c_2 & \cdots & c_{n-2} \end{matrix}} & 1 \\ \boxed{\begin{matrix} c_1 & c_3 & \cdots & c_{n-1} & 0 & 0 & \cdots & \cdots \end{matrix}} & & & & & & & 0 \\ 0 & \boxed{\begin{matrix} c_1 & c_3 & \cdots & c_{n-1} & 0 & \cdots & \cdots \end{matrix}} & 0 \\ \vdots & & & & & & & \vdots \\ 0 & \cdots & \boxed{\begin{matrix} 0 & c_1 & c_3 & \cdots & \cdots & c_{n-1} \end{matrix}} & 0 \\ 0 & \cdots & \cdots & \boxed{\begin{matrix} 0 & c_1 & c_3 & \cdots & \cdots & c_{n-1} \end{matrix}} \end{bmatrix}.$$

The relationship between the characteristic polynomial and its corresponding matrices $\mathcal{S}$, $\mathcal{S}_0$, and $\mathcal{S}_1$ leads to the following result.

THEOREM 2.1. *Let $\mathcal{S}$ be the Sylvester matrix for the polynomials r_e and r_o in* (2a) *and* (2b). *Then* **J** *has precisely one pair of pure imaginary eigenvalues if*

$$\mathcal{R}_{\mathcal{S}} = 0 \quad \textit{and} \quad \det(\mathcal{S}_0)\cdot\det(\mathcal{S}_1) > 0.$$

If $\mathcal{R}_{\mathcal{S}} \neq 0$ or $\det(\mathcal{S}_0)\cdot\det(\mathcal{S}_1) < 0$, then $p(\lambda)$ has no purely imaginary roots.

Proof. From the elementary properties of resultants [5, Chap. 3, Prop. 8 and 9], $\mathcal{R}_{\mathcal{S}} = 0$ if and only if r_e and r_o share a common factor in $\mathbb{R}[z]$. Suppose that $\det(\mathcal{S}_0)\cdot\det(\mathcal{S}_1) \neq 0$. Then this common factor is linear and, by Loos [19], it has the explicit form

$$\det(\mathcal{S}_0) + \det(\mathcal{S}_1)z = h_1(z)\cdot r_e(z) + h_2(z)\cdot r_o(z)$$

for two polynomials $h_1, h_2 \in \mathbb{R}[z]$. The solution of $\det(\mathcal{S}_0) + \det(\mathcal{S}_1)z = 0$ results in a common complex root $\hat{z}$ of r_e and r_o which is unique, real, and negative if $\det(\mathcal{S}_0)\cdot\det(\mathcal{S}_1) > 0$. ∎

If $\det(\mathcal{S}) = \det(\mathcal{S}_0)\cdot\det(\mathcal{S}_1) = 0$, then $p(\lambda)$ may have more than one pair of pure imaginary roots, a case which may be resolved by computing higher subresultants.

When the conditions of the theorem are satisfied, the magnitude of the shared root $\hat{z}$ is given by

$$|\hat{z}| = \sqrt{\det(\mathcal{S}_1)/\det(\mathcal{S}_0)}$$

which, in the case of Hopf bifurcation, can be related directly to the period of the limit cycle created at the bifurcation point. An efficient method of evaluating all subresultants (including the determinants of $\mathcal{S}$, $\mathcal{S}_0$, and $\mathcal{S}_1$) is the *generalized polynomial remainder sequences* algorithm due to Habicht, Brown, and Collins. For a detailed discussion, see Loos [19].

In the case of (2a) and (2b), the determinant of the Sylvester matrix can be expressed explicitly in terms of the eigenvalues of $\mathbf{J}$, according to the following result.

THEOREM 2.2. *Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the roots of the polynomial $p(\lambda)$ and let $\mathcal{S} = (s_{ij})$ be the $(n-1)\times(n-1)$ Sylvester matrix of the associated pair (r_e, r_o). If $m = \binom{\lfloor (n+1)/2 \rfloor}{2} + \binom{n}{2}$, then*

$$\mathcal{R}_{\mathcal{S}} \quad = \quad (-1)^m \cdot \prod_{1 \le i < j \le n} (\lambda_i + \lambda_j).$$

Proof. We note that

$$\prod_{1 \le i < j \le n} (\lambda_i + \lambda_j)$$

and the Sylvester resultant $\mathcal{R}_{\mathcal{S}}$ are symmetric polynomials in $\lambda_1, \ldots, \lambda_n$. They can be rewritten uniquely as polynomials in the coefficients $c_0, \ldots, c_{n-1}$ of the polynomial

$$p(\lambda) = \prod_{i=1}^{n} (\lambda - \lambda_i) = \lambda^n + \sum_{i=0}^{n-1} c_i \lambda^i.$$

We denote these two polynomials by $\mathrm{prod}(c_0, \ldots, c_{n-1})$ and $\mathrm{res}(c_0, \ldots, c_{n-1})$, respectively. Both polynomials have integer coefficients, and res is irreducible [26] in $\mathbf{Z}[c_0, \ldots, c_{n-1}]$.

The polynomials prod and res define the same hypersurface in the affine space $\mathbf{C}^n$. Namely, a point $(c_0, \ldots, c_{n-1})$ lies in this hypersurface if and only if the polynomial

$$\lambda^n + \sum_{i=0}^{n-1} c_i \lambda^i$$

has a quadratic factor of the form $\lambda^2 - \mu$. Hence there exists an integer s such that $\mathrm{prod} = s \cdot \mathrm{res}$ in $\mathbf{Z}[c_0, \ldots, c_{n-1}]$.

In order to show $s = (-1)^m$, we apply the classical algorithm for rewriting symmetric functions in terms of elementary symmetric functions. We begin by noting that the lexicographic leading term of

$$\prod_{1 \le i < j \le n} (\lambda_i + \lambda_j)$$

equals $\lambda_1^{n-1} \lambda_2^{n-2} \cdots \lambda_{n-1}^1 \lambda_n^0$. There is a unique monomial in the elementary symmetric functions $(-1)^{n-i} c_i$ which has the same leading term, namely,

$$(-1)^{n-1} \cdot c_1 \cdot (-1)^{n-2} c_2 \cdot \ \cdots \cdot (-c_{n-1}) \quad = \quad (-1)^{\binom{n}{2}} \cdot c_1 c_2 c_3 \cdots c_{n-1}.$$

Therefore the monomial $c_1c_2c_3\cdots c_{n-1}$ occurs with coefficient $(-1)^{\binom{n}{2}}$ in prod. However, the same monomial occurs with coefficient $(-1)^{1+2+\cdots+\lfloor(n-1)/2\rfloor}$ in the expansion of res = det($\mathcal{S}$), as can be verified from the definition of the matrix $\mathcal{S}$. The desired factor s is the quotient of these two coefficients. This quotient equals $(-1)^m$ and the proof of Theorem 2.2 is complete. □

We note that Theorem 2.1 imposes two requirements on the characteristic polynomial of $\mathbf{J}$: a singularity condition for the resultant matrix and an inequality involving subresultants. There are many classical results on root location in systems of polynomial equations. For example, the well-known Routh–Hurwitz criterion for stability matrices determines whether all the eigenvalues of a matrix have nonpositive real parts. We describe two other criteria for a polynomial to have a factor of the form $x^2-\mu$ that are appealing alternatives to the calculation of the Sylvester resultant. For ease of exposition, we consider the case where $n\geq 2$ is even in the discussion that follows; similar results for the case where n is odd follow analogously.

Let $\mathcal{M}$ denote the space of all real $\frac{n}{2}$-square matrices and charpoly : $\mathcal{M}\to\mathbb{R}_{\frac{n}{2}}[x]$ the map that associates an element of $\mathcal{M}$ to its characteristic polynomial. If $\mathcal{N}\subset\mathcal{M}$ is the dense subset of matrices with simple eigenvalues, then the equivalence relation $A\sim B$ defined by the condition that charpoly(A) = charpoly(B) for $A,B\in\mathcal{N}$ induces a partition of $\mathcal{N}$ into similarity classes. For each equivalence class in this partition, a useful representative element is a matrix that displays the coefficients of the associated characteristic polynomial along a row or down a column; such an element is called a *companion* matrix. Notice that for n even, r_e is a monic polynomial. Thus, we may take

$$\mathcal{C}_{r_e}=\begin{bmatrix}0&0&0&\cdots&0&-c_0\\1&0&0&\cdots&0&-c_2\\0&1&0&\cdots&0&-c_4\\\vdots&&&&\vdots&\vdots\\0&0&0&\cdots&1&-c_{n-2}\end{bmatrix}$$

as the representative element of $[\mathcal{C}_{r_e}]$, since charpoly($\mathcal{C}_{r_e}$) = r_e. Moreover, for each $A\in[\mathcal{C}_{r_e}]$ there exists a (nonsingular) matrix W such that

$$\mathcal{C}_{r_e}W=WA.$$

Recall that a matrix polynomial of degree k with elements in $\mathcal{M}$ is an expression of the form

$$q(\mathbf{M})=a_k\mathbf{M}^k+a_{k-1}\mathbf{M}^{k-1}+\cdots+a_1\mathbf{M}+a_0\mathbf{I},$$

where $q:\mathcal{M}\to\mathcal{M}$, $\mathbf{M}\in\mathcal{M}$, the coefficients a_i are scalars, and $\mathbf{I}$ is the unit matrix. An alternative expression for $\mathcal{R}_{\mathcal{S}}$ is given by the following theorem [3, Sect. 1.2].

THEOREM 2.3. *For r_o and r_e defined as above, let $r_o(\mathcal{C}_{r_e})\equiv\mathcal{C}$ if n is even and $r_e(\mathcal{C}_{r_o})\equiv\mathcal{C}$ if n is odd. If $\mathcal{R}_{\mathcal{C}}$ is used to denote* det($\mathcal{C}$)*, then*

$$\mathcal{R}_{\mathcal{C}}=\mathcal{R}_{\mathcal{S}}.$$

Thus, the vanishing of $\mathcal{R}_{\mathcal{C}}$ provides an alternative to the condition $\mathcal{R}_{\mathcal{S}}=0$ given in Theorem 2.1 but involves a matrix of smaller dimension. To develop a third equivalent criterion, we consider the *Bezout* resultant. Again, for n even, consider the two

polynomials specified by (2a). We define the brackets

$$[i,j] = \det \begin{bmatrix} c_{2i} & c_{2j} \\ c_{2i+1} & c_{2j+1} \end{bmatrix}$$

where $0 \le i,j \le \frac{n}{2}$ and we take $c_n = 1, c_{n+1} = 0$. The *Bezout* matrix $\mathcal{B}$ corresponding to the polynomial pair (r_e, r_o) is an $\frac{n}{2}$-dimensional square, symmetric matrix with entries constructed as sums of bracket products in the coefficients c_i as follows: for $1 \le i \le j \le \frac{n}{2}$ set

$$\begin{aligned} k_{min} &= \max\left(0, i+j-\frac{n}{2}-1\right), \\ k_{max} &= i-1. \end{aligned} \tag{4}$$

Then,

$$(\mathcal{B})_{ij} = \sum_{k=k_{min}}^{k_{max}} [i+j-k-1, k] = (\mathcal{B})_{ji}\,. \tag{5}$$

The only modification required in this definition for the case of n odd is that c_n has the value prescribed by the characteristic polynomial p and c_{n+1} is taken to be unity.

The Sylvester and Bezout matrices are intimately related (see Theorem 1.13 of Barnett [3] and note that, in his notation, $\det(T_1) = 1$) which leads to the following theorem.

THEOREM 2.4. *For the Bezout matrix corresponding to the polynomial pair (r_e, r_o), let $\mathcal{R}_\mathcal{B}$ denote* $\det(\mathcal{B})$. *Then we have*

$$\mathcal{R}_\mathcal{B} = (-1)^n\, \mathcal{R}_\mathcal{S}. \tag{6}$$

Moreover, the coefficients of the linear remainder term from the Euclidean algorithm may be expressed as determinants of certain Bezout submatrices, in analogy to the subresultants defined for the Sylvester form. Consider two submatrices, $\mathcal{B}_i$ for $i = 0, 1$, obtained by deleting the first column and the ith row of $\mathcal{B}$. Then the *Bezout subresultants* formed from the determinants of $\mathcal{B}_0$ and $\mathcal{B}_1$, together with (6), may be used to specify the hypersurface of n-square matrices with a purely imaginary eigenvalue pair. Since we have not found the particular relationship given in the following theorem described in the literature, we provide a sketch of the proof.

THEOREM 2.5. *Let $\mathcal{B}$ be the Bezout matrix for the polynomials r_e and r_o in* (2a) *and* (2b). *Then* $\mathbf{J}$ *has precisely one pair of pure imaginary eigenvalues if*

$$\mathcal{R}_\mathcal{B} = 0 \quad \textit{and} \quad \det(\mathcal{B}_0)\cdot\det(\mathcal{B}_1) > 0.$$

If $\mathcal{R}_\mathcal{B} \neq 0$ or $\det(\mathcal{B}_0)\cdot\det(\mathcal{B}_1) < 0$, then $p(\lambda)$ has no purely imaginary roots.

Proof. The Bezout matrix $\mathcal{B}$ is a symmetric $m \times m$ matrix where $m = \lfloor \frac{n}{2} \rfloor$. By Barnett [4, Sect. 1.5] it satisfies the following identity in the indeterminates w and z:

$$\begin{aligned} (1, w, w^2, \ldots, w^{m-1}) \cdot \mathcal{B} \cdot (1, z, z^2, \ldots, z^{m-1})^T \\ = \quad \frac{r_e(w)\, r_o(z) - r_e(z)\, r_o(w)}{w - z}. \end{aligned} \tag{7}$$

Suppose that $\det(\mathcal{B}) = 0$ but $\det(\mathcal{B}_0)\cdot\det(\mathcal{B}_1) \neq 0$. Then r_e and r_o have a common complex root, say w_0. From (7) we conclude

$$(1, w_0, w_0^2, \ldots, w_0^{m-1}) \cdot \mathcal{B} \cdot (1, z, z^2, \ldots, z^{m-1})^T = 0 \tag{8}$$

for all $z \in \mathbf{C}$. If we substitute m distinct values for z and invert the corresponding Vandermonde matrix, then we see that (8) implies that $(1, w_0, w_0^2, \ldots, w_0^{m-1}) \cdot \mathcal{B}$ is the zero vector. Now, by our assumptions, the Bezout matrix has rank $m-1$. The unique (up to scaling) vector in its kernel is computed by Cramer's rule. For some nonzero constant c we find

$$\begin{aligned}(1, w_0, w_0^2, \ldots, w_0^{m-2}, w_0^{m-1}) \\ = c \cdot ((-1)^m \det(\mathcal{B}_{m-1}), \ldots, \det(\mathcal{B}_2), -\det(\mathcal{B}_1), \det(\mathcal{B}_0)).\end{aligned}$$

This implies $w_0 \cdot \det(\mathcal{B}_1) + \det(\mathcal{B}_0) = 0$. Hence w_0 is negative if and only if $\det(\mathcal{B}_0) \cdot \det(\mathcal{B}_1)$ is positive. Our proof is complete because w_0 is the only common root of r_e and r_o (otherwise $\operatorname{rank}(\mathcal{B}_0) < m-1$). □

Thus, we have three distinct but equivalent methods of computing the singularity condition necessary to establish that the Jacobian has a pair of purely imaginary eigenvalues: one (Sylvester) related directly to the sufficiency condition, one (Companion) small in dimension compared to n, and, finally, one (Bezout) which is not only small but has a symmetric structure. We illustrate the ideas presented above concerning polynomial resultants with the following example.

Example. Consider the case $n = 6$. Then (2a) and (2b) become

$$\begin{aligned}p(\lambda) &= c_0 + c_1\lambda + \cdots + c_5\lambda^5 + \lambda^6, \\ r_e(z) &= c_0 + c_2 z + c_4 z^2 + z^3, \\ r_o(z) &= c_1 + c_3 z + c_5 z^2.\end{aligned}$$

The Sylvester matrix and the two relevant submatrices, $\mathcal{S}_0$ and $\mathcal{S}_1$, are given by

$$\mathcal{S} = \begin{bmatrix} c_0 & c_2 & c_4 & 1 & 0 \\ 0 & c_0 & c_2 & c_4 & 1 \\ c_1 & c_3 & c_5 & 0 & 0 \\ 0 & c_1 & c_3 & c_5 & 0 \\ 0 & 0 & c_1 & c_3 & c_5 \end{bmatrix},$$

$$\mathcal{S}_0 = \begin{bmatrix} c_2 & c_4 & 1 \\ c_3 & c_5 & 0 \\ c_1 & c_3 & c_5 \end{bmatrix}, \quad \mathcal{S}_1 = \begin{bmatrix} c_0 & c_4 & 1 \\ c_1 & c_5 & 0 \\ 0 & c_3 & c_5 \end{bmatrix}.$$

By Theorem 2.1, p has a pair of purely imaginary roots if and only if

$$\begin{aligned}\mathcal{R}_{\mathcal{S}} = {c_0}^2{c_5}^2 + {c_1}^2{c_4}^2c_5 + c_1{c_2}^2{c_5}^2 + c_0{c_3}^2c_4c_5 - 2c_0c_1{c_5}^2c_4 - c_0c_2c_3{c_5}^2 \\ - c_1c_2c_3c_4c_5 - c_0{c_3}^3 + 3c_0c_1c_3c_5 + c_1c_2{c_3}^2 - 2{c_1}^2c_2c_5 - {c_1}^2c_3c_4 + {c_1}^3\end{aligned}$$

vanishes and the product

$$\left({c_3}^2 - c_1c_5 + c_2{c_5}^2 - c_3c_4c_5\right)\left(c_1c_3 + c_0{c_5}^2 - c_1c_4c_5\right) > 0.$$

The singularity condition may be expressed in terms of the companion matrix for r_e through the matrix polynomial

$$r_o\left(\mathcal{C}_{r_e}\right) = \begin{bmatrix} c_1 & -c_0c_5c_0 & c_0(c_4c_5 - c_3) \\ c_3 & c_1 - c_2c_5 & c_5(c_2c_4 - c_0) - c_2c_3 \\ c_5 & c_3 - c_4c_5 & c_5({c_4}^2 - c_2) + c_1 - c_3c_4 \end{bmatrix}.$$

TABLE 1
Resultant equality and subresultant inequality conditions required for Hopf bifurcation for vector fields of dimension two through six.

n	$\mathcal{R}_{\mathcal{S}}$ $\det(\mathcal{S}_0)\cdot\det(\mathcal{S}_1)$
2	c_1
	c_0
3	$c_0 - c_1c_2$
	c_1
4	$c_0c_3^2 - c_1c_2c_3 + c_1^2$
	c_1c_3
5	$(c_2 - c_3c_4)(c_1c_2 - c_0c_3) + c_1c_4(c_1c_4 - 2c_0) + c_0^2$
	$(c_2 - c_3c_4)\cdot(c_0 - c_1c_4)$
6	$c_0c_5^2(c_0c_5 - c_2c_3) + c_1c_5^2(c_2^2 - c_0c_4) + c_1(c_1^2 + c_0c_3c_5)$ $+ c_1c_5(c_0c_3 - 2c_1c_2) + (c_4c_5 - c_3)(c_0c_3^2 - c_0c_1c_5 + c_1^2c_4 - c_1c_2c_3)$
	$(c_1c_3 + c_0c_5^2 - c_1c_4c_5)\cdot(c_3^2 - c_1c_5 + c_2c_5^2 - c_3c_4c_5)$

Finally, the Bezout matrix associated with (r_e, r_o) is given by

$$\mathcal{B} = \begin{bmatrix} [1,0] & [2,0] & [3,0] \\ [2,0] & [3,0]+[2,1] & [3,1] \\ [3,0] & [3,1] & [3,2] \end{bmatrix} = \begin{bmatrix} c_1c_2 - c_0c_3 & c_1c_4 - c_0c_5 & c_1 \\ c_1c_4 - c_0c_5 & c_1 + c_3c_4 - c_2c_5 & c_3 \\ c_1 & c_3 & c_5 \end{bmatrix}$$

and it is easy to verify $\mathcal{R}_{\mathcal{B}} = \det(\mathcal{B}) = \mathcal{R}_{\mathcal{S}}$. The Bezout subresultant condition provided by the expression

$$\det(\mathcal{B}_0)\cdot\det(\mathcal{B}_1) = \det\begin{bmatrix} c_1 + c_3c_4 - c_2c_5 & c_3 \\ c_3 & c_5 \end{bmatrix}\cdot\det\begin{bmatrix} c_1c_4 - c_0c_5 & c_1 \\ c_3 & c_5 \end{bmatrix}$$

is necessarily positive when p has a pair of imaginary conjugate roots.

Table 1 provides a list of the resultant equality and subresultant inequality conditions, as functions of the polynomial coefficients, for vector fields of dimension two through six.

3. Hopf algorithms using symmetric products.

3.1. Algebraic properties of symmetric products. In practical applications, the computation of the characteristic polynomial coefficients is problematic since known algorithms are numerically unstable. For each method (Danilewski, La

Verrier, etc.) otherwise unremarkable example matrices can be constructed for which the technique yields arbitrarily inaccurate polynomial coefficients; for a detailed discussion, see Wilkinson [27]. Despite this fact, computational methods which employ numerically determined matrix characteristic polynomial coefficients are used extensively in engineering linear systems analysis and control theory where *empirical* evidence suggests they are effective. Thus, while it is clear that numerical calculation of the explicit coefficients cannot be recommended as a general technique, the classes of matrices for which these techniques break down and a complete understanding of their failure modes is not well established. For example, Wilkinson observes that Jacobian matrices derived from damped oscillatory systems are frequently associated with well-conditioned characteristic polynomials. In such circumstances, eigenvalue methods based on explicit use of the coefficients appear to be fast and reliable, based on numerical experiments with an early iterative solver, *DEUCE* [28].

To circumvent difficulties in explicitly determining the characteristic polynomial coefficients, we seek a method to determine whether a square matrix has a pair of eigenvalues whose sum is zero directly from the entries in the Jacobian matrix. A simple procedure for doing this involves *Kronecker* or *tensor* products of matrices.

For the finite-dimensional vector spaces V and W, let $T_1 : V \to V$ be a linear operator with $(n\times n)$ matrix representation $\mathbf{A} = (a_{ij})$ in terms of the basis e_i, and let $T_2 : W \to W$ be another linear operator with $(m\times m)$ representation $\mathbf{B} = (b_{kl})$ in terms of the basis f_k. The tensor product $T_1 \otimes T_2 : V \otimes W \to V \otimes W$ is an $(mn\times mn)$ matrix with entries $a_{ij}b_{kl}$ in terms of the basis $e_i \otimes f_k$ for $V \otimes W$. Moreover, eigenvalues behave multiplicatively under tensor products: if λ_i and μ_k are eigenvalues of T_1 and T_2 corresponding to eigenvectors u_i and v_k, then $\lambda_i\mu_k$ is an eigenvalue of $T_1 \otimes T_2$. If, in addition, we assume T_1 and T_2 are nondefective and $\dim(V) = \dim(W)$, then the tensor sum $(T_1 \otimes T_2 + T_2 \otimes T_1)$ has a special action on its eigenspaces. Since

$$\begin{aligned}(T_1 \otimes T_2 + T_2 \otimes T_1)(u_i \otimes v_k) &= (\lambda_i u_i) \otimes (\mu_k v_k) + (\mu_i u_i) \otimes (\lambda_k v_k)\\ &= (\lambda_i\mu_k + \lambda_k\mu_i)(u_i \otimes v_k)\end{aligned}$$

the spectrum of this operator consists of the n^2 pairwise sums $(\lambda_i\mu_k+\lambda_k\mu_i)$ associated with the eigenvectors $u_i \otimes v_k$ for $1\le i, k \le n$.

This tensor sum suggests an obvious candidate for an augmenting function: if $\mathbf{J}$ is the Jacobian, then $\mathbf{J}$ has an eigenpair that sums to zero if and only if

$$g(x, \alpha; \beta) = \det(\mathbf{J} \otimes \mathbf{I}_n + \mathbf{I}_n \otimes \mathbf{J})$$

vanishes where $\mathbf{I}_n$ is the appropriate identity matrix. Notice that since each eigensum of distinct eigenvalues occurs twice, the tensor sum will have corank-2 at a Hopf bifurcation point, which has important numerical disadvantages.

To remove the twofold redundancy in the eigenvalues of the tensor product, one can split $V \otimes V$ into the eigenspaces for ± 1 of the involution $\sigma : V \otimes V \to V \otimes V$ that interchanges factors: $\sigma(v_1 \otimes v_2) = v_2 \otimes v_1$. The restriction to the $\frac{n}{2}(n-1)$-dimensional eigenspace of -1 for σ is an operator whose eigenvalues are $(\lambda_i\mu_k + \lambda_k\mu_i)$ with $i < k$. If $T_1, T_2 : V \to V$, the operator $T_1 \otimes T_2 + T_2 \otimes T_1$ commutes with σ, so it maps the σ eigenspaces to themselves. In what follows we construct the matrix corresponding to the restriction to the (-1) eigenspace of σ. Using a different approach, the matrix representation of this restricted operator was originally constructed directly from the elements of the argument matrices by Stéphanos [25] and later by Fuller [7].

DEFINITION. *Let* $\mathbf{A}$ *and* $\mathbf{B}$ *be* $n\times n$ *matrices with entries* (a_{ij}) *and* (b_{ij})*, respectively,* $1 \le i, j \le n$*. Set* $m = \frac{n}{2}(n-1)$*. Then the* bialternate product *(or biproduct)*

of $\mathbf{A}$ *and* $\mathbf{B}$*, denoted* $\mathbf{A} \odot \mathbf{B}$*, is an* $m \times m$ *matrix whose rows are labeled* pq *for* $(p = 2, 3, \ldots, n; q = 1, 2, \ldots, p-1)$ *and columns labeled* rs *for* $(r = 2, 3, \ldots, n; s = 1, 2, \ldots, r-1)$ *with entries*

$$(\mathbf{A} \odot \mathbf{B})_{\{pq,rs\}} = \frac{1}{2} \left\{ \begin{vmatrix} a_{pr} & a_{ps} \\ b_{qr} & b_{qs} \end{vmatrix} + \begin{vmatrix} b_{pr} & b_{ps} \\ a_{qr} & a_{qs} \end{vmatrix} \right\}.$$

In the case $\mathbf{B} = 2\mathbf{I}_n$ we obtain from this an operator on an $\frac{n}{2}(n-1)$-dimensional space whose eigenvalues are the pairwise sums of the eigenvalues of $\mathbf{A}$ without repetition: $\lambda_i + \lambda_j$ for $i < j$.

THEOREM 3.1. *Let* $\mathbf{A}$ *be an* $(n \times n)$ *matrix with eigenvalues* $(\lambda_1, \ldots, \lambda_n)$*. Then*

(i) $\mathbf{A} \odot \mathbf{A}$ *has eigenvalues* $\lambda_i \cdot \lambda_j$*, and*

(ii) $2\mathbf{A} \odot \mathbf{I}_n$ *has eigenvalues* $\lambda_i + \lambda_j$

where $\mathbf{I}_n$ *is the* n*-square identity matrix and* $1 \le j < i \le n$*.*

Notice that the subscripts used to compute the biproduct entries are indexed by pairs. To avoid confusion, when the lexicographically ordered pair, or *label*, is used to refer to an element of $\mathbf{A} \odot \mathbf{B}$, we shall enclose it in braces, as in the definition above. When the row/column matrix *index* is used, we employ the standard notation. Thus, the index provides information about the position of the entry in the biproduct matrix while the label indicates which elements of the arguments to the product are involved. As an example, consider an arbitrary 3×3 matrix $A = (a_{i,j})$ for $1 \le i, j \le 3$. Then, the conventions require that

$$(\mathbf{A} \odot \mathbf{A})_{2,3} = (\mathbf{A} \odot \mathbf{A})_{\{31,32\}} = a_{1,2}\, a_{3,3} - a_{1,3}\, a_{3,2}.$$

For compactness in the index notation, when there is no possibility of confusion we drop the comma separating the row and column indices. Thus, in the example, the two products of $\mathbf{A}$ are given by

$$\mathbf{A} \odot \mathbf{A} = \begin{bmatrix} \begin{vmatrix} a_{22} & a_{21} \\ a_{12} & a_{11} \end{vmatrix} & \begin{vmatrix} a_{23} & a_{21} \\ a_{13} & a_{11} \end{vmatrix} & \begin{vmatrix} a_{23} & a_{22} \\ a_{13} & a_{12} \end{vmatrix} \\ \begin{vmatrix} a_{32} & a_{31} \\ a_{12} & a_{11} \end{vmatrix} & \begin{vmatrix} a_{33} & a_{31} \\ a_{13} & a_{11} \end{vmatrix} & \begin{vmatrix} a_{33} & a_{32} \\ a_{13} & a_{12} \end{vmatrix} \\ \begin{vmatrix} a_{32} & a_{31} \\ a_{22} & a_{21} \end{vmatrix} & \begin{vmatrix} a_{33} & a_{31} \\ a_{23} & a_{21} \end{vmatrix} & \begin{vmatrix} a_{33} & a_{32} \\ a_{23} & a_{22} \end{vmatrix} \end{bmatrix},$$

$$2\mathbf{A} \odot \mathbf{I}_3 = \begin{bmatrix} a_{11} + a_{22} & a_{23} & -a_{13} \\ a_{32} & a_{11} + a_{33} & a_{12} \\ -a_{31} & a_{21} & a_{22} + a_{33} \end{bmatrix}.$$

Substituting $\mathbf{I}_n$ into the definition of the bialternate product and solving for the elements yields a simple formula for the entries. For the $\frac{n}{2}(n-1)$-square matrix $2\mathbf{A} \odot \mathbf{I}_n$ with rows pq and columns rs, the entries are given by the formula

$$(2\mathbf{A} \odot \mathbf{I}_n)_{\{pq,rs\}} = \begin{cases} -(\mathbf{A})_{ps} & \text{if } r = q, \\ (\mathbf{A})_{pr} & \text{if } r \neq p \text{ and } s = q, \\ (\mathbf{A})_{pp} + (\mathbf{A})_{qq} & \text{if } r = p \text{ and } s = q, \\ (\mathbf{A})_{qs} & \text{if } r = p \text{ and } s \neq q, \\ -(\mathbf{A})_{qr} & \text{if } s = p, \\ 0 & \text{otherwise.} \end{cases} \tag{9}$$

The algebraic properties of the bialternate product transformation confers a certain structure upon the matrix $\mathbf{A}\odot\mathbf{I}_n$ which may be used in the construction of Hopf algorithms. For example, simple manipulation of the row and column labels yields the following lemma.

LEMMA 3.2. *Let* $\mathbf{A}$ *be an* $(n\times n)$ *matrix. If* $\mathbf{A}$ *is lower (upper) triangular, then* $2\mathbf{A}\odot\mathbf{I}_n$ *is lower (upper) triangular. In particular, if* $\mathbf{A}$ *is diagonal so is* $2\mathbf{A}\odot\mathbf{I}_n$.

Proof. Suppose $\mathbf{A}$ is lower triangular and let $(\mathbf{A})_{ij}$ be nonzero. Notice that if $i=j$ then it contributes only to the diagonal elements of $2\mathbf{A}\odot\mathbf{I}_n$. Consider the case for $1\le j<i\le n$. The first assignment in (9) may be written

$$-(\mathbf{A})_{ij}\mapsto(2\mathbf{A}\odot\mathbf{I}_n)_{\{ik,kj\}}$$

for k such that $1\le j<k<i\le n$. By the row and column label convention,

$$ik \;\mapsto\; k+\sum_{l=0}^{i-2}l = j+\left[(k-j)+\sum_{l=k-1}^{i-2}l\;\right]+\sum_{l=0}^{k-2}l > j+\sum_{l=0}^{k-2}l \;\hookleftarrow\; kj$$

shows $(2\mathbf{A}\odot\mathbf{I}_n)_{\{ik,kj\}}$ is below the diagonal. Similar arguments hold for the second and fourth assignments in (9); the fifth does not apply in the lower triangular case. Thus, $2\mathbf{A}\odot\mathbf{I}_n$ is lower triangular. A similar argument holds for $\mathbf{A}$ upper triangular, and the result for diagonal $\mathbf{A}$ follows immediately. ∎

A simple extension of the index counting arguments used above can be used to establish how a nonzero off-diagonal element in the Jacobian is propagated to the product matrix.

LEMMA 3.3. *Suppose* $(\mathbf{A})_{ij}$ *is nonzero,* $i\neq j$. *Then* $(\mathbf{A})_{ij}$ *appears* $n-2$ *times in entries of* $2\mathbf{A}\odot\mathbf{I}_n$. *Moreover, if* $u=\max\{i,j\}$ *and* $l=\min\{i,j\}$, *each of these entries is contained in a band of width*

$$bw=\frac{1}{2}\left(u^2-l^2+3(l-u)\right).$$

Proof. Suppose $j<i$. The three assignments specified in (9) which apply may be written

$$-(\mathbf{A})_{ij}\mapsto(2\mathbf{A}\odot\mathbf{I}_n)_{\{ik,kj\}} \qquad \text{for } k \text{ such that } 1\le j<k<i\le n, \tag{10a}$$

$$(\mathbf{A})_{ij}\mapsto(2\mathbf{A}\odot\mathbf{I}_n)_{\{ik,jk\}} \qquad \text{for } k \text{ such that } 1\le k<j<i\le n, \tag{10b}$$

$$(\mathbf{A})_{ij}\mapsto(2\mathbf{A}\odot\mathbf{I}_n)_{\{ki,kj\}} \qquad \text{for } k \text{ such that } 1\le j<i<k\le n. \tag{10c}$$

The total number of off-diagonal entries in $2\mathbf{A}\odot\mathbf{I}_n$ contributed by $(\mathbf{A})_{ij}$ is given by $(i-j-1)+(j-1)+(n-i)=n-2$.

The nonzero entry $(\mathbf{A})_{ij}$ may contribute elements $(2\mathbf{A}\odot\mathbf{I}_n)_{\{pq,rs\}}$ through each of the three rules (10a–c) above. Let (i^a_{row},i^a_{col}), (i^b_{row},i^b_{col}), and (i^c_{row},i^c_{col}) denote the row and column indices corresponding to the labels pq and rs under the rules (10a), (10b), and (10c), respectively. To find the bandwidth we wish to maximize the differences $i^*_{row}-i^*_{col}$ where the asterisk is replaced by the rule identifier a, b, or c. Simple calculations show

$$i^c_{row}-i^c_{col}\le i-j, \tag{11}$$

$$i^b_{row}-i^b_{col}\le 1+\frac{1}{2}\left(i^2-j^2-3i+j+2\right), \tag{12}$$

$$i^a_{row}-i^a_{col}\le\frac{1}{2}\left(i^2-j^2+3(j-i)\right). \tag{13}$$

Comparing these bounds establishes the result for $(\mathbf{A})_{ij}$ for $j<i$. The case for $i<j$ follows analogously. □

Finally, since the bialternate product was derived as the restriction of a tensor product of matrices to an invariant subspace, it inherits several important properties from tensor calculus. In particular, it is straightforward to verify the following.

LEMMA 3.4. *For α a scalar and $\mathbf{A}$, $\mathbf{B}$ in $\mathcal{M}$ depending on a parameter λ, the following properties hold:*

(i) $\alpha(\mathbf{A}\odot\mathbf{B}) = (\alpha\mathbf{A})\odot\mathbf{B} = \mathbf{A}\odot(\alpha\mathbf{B})$,
(ii) $(\mathbf{A}+\mathbf{B})\odot\mathbf{C} = (\mathbf{A}\odot\mathbf{C}) + (\mathbf{A}\odot\mathbf{C})$,
(iii) $\mathbf{A}\odot\mathbf{B} = \mathbf{B}\odot\mathbf{A}$,
(iv) $(\mathbf{A}\odot\mathbf{B})^t = (\mathbf{A}^t\odot\mathbf{B}^t)$,
(v) $\frac{\partial}{\partial\lambda}(\mathbf{A}\odot\mathbf{B}) = \left[\frac{\partial}{\partial\lambda}\mathbf{A}\right]\odot\mathbf{B} + \mathbf{A}\odot\left[\frac{\partial}{\partial\lambda}\mathbf{B}\right]$ *(provided the partial derivatives exist),*
(vi) $(\mathbf{AB})\odot\mathbf{I}_n = (\mathbf{A}\odot\mathbf{I}_n)(\mathbf{B}\odot\mathbf{I}_n) - (\mathbf{A}\odot\mathbf{B})$.

3.2. Bialternate product algorithms. From the algebraic theory of symmetric matrix products described above we have a simple *necessary* condition for a Hopf point: if the point (x^*,λ^*) is a Hopf bifurcation point for $\dot{x} = f(x,\alpha)$, then the $(n+1)$-dimensional system

$$F(x^*,\alpha^*) = \left\{ \begin{array}{c} f(x^*,\alpha^*), \\ \det\left(D_x f \odot \mathbf{I}_n \big|_{(x^*,\alpha^*)} \right) \end{array} \right\} \tag{14}$$

vanishes. However, we have not found a condition that distinguishes purely imaginary eigenvalues directly from the Jacobian and its bialternate products in analogy to the subresultant criterion described earlier.

One can use bialternate products effectively in continuation method calculations of Hopf bifurcation curves relying on the observation that transitions where eigenvalues depart from the imaginary axis occur at degenerate bifurcations. As before, we propose following curves of Hopf bifurcations in two-parameter families by solving the equations expressing the singularity of the bialternate product of the Jacobian, while ensuring that the imaginary eigenvalues are bounded away from zero and that multiple imaginary eigenpairs do not occur. We begin with the simple proof that (14) is regular on its zero set provided appropriate genericity and transversality conditions hold.

THEOREM 3.5. *Suppose the system*

$$\dot{x} = f(x,\alpha), \qquad x\in\mathbf{R}^n,\ \alpha\in\mathbf{R}$$

has an equilibrium (x^*,α^*) at which the following properties are satisfied:

(E1) *$D_x f(x^*,\alpha^*)$ is nonsingular,*
(E2) *$D_x f(x^*,\alpha^*)$ has a single pair of eigenvalues $\lambda^*_{1,2}$ whose sum is zero; i.e., $(\lambda^*_1+\lambda^*_2)=0$,*
(E3) *$\frac{d}{d\alpha}[\lambda_1(x,\alpha)+\lambda_2(x,\alpha)]|_{(x^*,\alpha^*)} = \Delta\neq 0$.*

Then (x^*,α^*) is an isolated nonsingular solution of

$$F(x,\alpha) = \left(\begin{array}{c} f(x,\alpha), \\ \det\left(D_x f\odot\mathbf{I}_n\right) \end{array} \right) = 0. \tag{15}$$

Proof. Let $y = (x, \alpha)$. It suffices to show that $D_y F(x^*, \alpha^*)$ is nonsingular. By Keller's bordering lemma [17],

$$D_y F(x^*, \alpha^*) \equiv \begin{bmatrix} \mathbf{J}_x(x^*, \alpha^*) & \mathbf{J}_\alpha(x^*, \alpha^*) \\ w(x^*, \alpha^*) & d(x^*, \alpha^*) \end{bmatrix}$$

$$= \left[\begin{array}{c|c} D_x f(x^*, \alpha^*) & D_\alpha f(x^*, \alpha^*) \\ \hline D_x \left[\det\left(D_x f \odot \mathbf{I}_n\right)\right]\Big|_{(x^*,\alpha^*)} & D_\alpha \left[\det\left(D_x f \odot \mathbf{I}_n\right)\right]\Big|_{(x^*,\alpha^*)} \end{array}\right]$$

is nonsingular if $d(x^*, \alpha^*) \neq w(x^*, \alpha^*) \left[\mathbf{J}_x(x^*, \alpha^*)\right]^{-1} \mathbf{J}_\alpha(x^*, \alpha^*)$ since, by assumption (E1), $\mathbf{J}_x(x^*, \alpha^*)$ is invertible. Let $\{\lambda_k(x, \alpha)\}_{k=3}^n$ be the complement of the critical eigenvalues of $\mathbf{J}_x(x^*, \alpha^*)$. The product

$$\theta(x, \alpha) = \prod_{j=3}^{n} (\lambda_1 + \lambda_j)(\lambda_2 + \lambda_j) \left[\prod_{\substack{i=3 \\ i<j}}^{n} (\lambda_i + \lambda_j) \right]$$

defines a smooth function in a neighborhood of the solution, which, by (E2), is nonzero at (x^*, α^*), say $\theta(x^*, \alpha^*) = \delta$. For simplicity of notation, let $\mathbf{J}_x^* \equiv \mathbf{J}_x(x^*, \alpha^*)$ and $\mathbf{J}_\alpha^* \equiv \mathbf{J}_\alpha(x^*, \alpha^*)$. Then, using Theorem 3.1,

$$\begin{aligned} & D_\alpha \left[\det\left(\mathbf{J}_x \odot \mathbf{I}_n\right)\right]\Big|_{(x^*,\alpha^*)} \\ &= \theta(x^*, \alpha^*) \cdot D_\alpha(\lambda_1 + \lambda_2)\Big|_{(x^*,\alpha^*)} + (\lambda_1^* + \lambda_2^*) \cdot \frac{\partial \theta}{\partial \alpha}(x^*, \alpha^*) \\ &= \Delta\delta \end{aligned} \tag{16}$$

since the second term in the sum vanishes. But it is also true that

$$D_\alpha \left[\det\left(\mathbf{J}_x \odot \mathbf{I}_n\right)\right]\Big|_{(x^*,\alpha^*)} = D_x \left[\det\left(\mathbf{J}_x \odot \mathbf{I}_n\right)\right] \cdot \frac{dx}{d\alpha}\Big|_{(x^*,\alpha^*)} . \tag{17}$$

Differentiating the equilibrium condition $f(x, \alpha) = 0$ and evaluating the result at (x^*, α^*), we have

$$\frac{dx}{d\alpha} = -\left[\mathbf{J}_x^*\right]^{-1} \mathbf{J}_\alpha^* . \tag{18}$$

Substituting (18) into (17) we have

$$-D_x \left[\det\left(\mathbf{J}_x \odot \mathbf{I}_n\right)\right]\Big|_{(x^*,\alpha^*)} \left[\mathbf{J}_x^*\right]^{-1} \mathbf{J}_\alpha^* = \Delta\delta$$

as well. Together with (16) this implies

$$d(x^*, \alpha^*) - w(x^*, \alpha^*) \left[\mathbf{J}_x\right]^{-1} \mathbf{J}_\alpha = 2\Delta\delta \neq 0$$

which establishes the result. ∎

To utilize either augmented system defined by the vanishing of a resultant or biproduct in the Euler–Newton continuation framework we must specify how the Jacobian of the extended system is to be computed since, at each corrector step, a linear system of the form

$$y_{k+1} = y_k - [D_y F(y_k;\beta)]^{-1} F(y_k;\beta)$$

must be solved. Here, and in the discussion that follows, we use $y = (x,\alpha)^t$ to denote the augmented column vector of independent variables of F. Referring to Theorem 3.5, we will assume that the components $D_x f(x,\alpha;\beta)$ and $D_\alpha f(x,\alpha;\beta)$ are readily available either analytically, by automatic differentiation (see [13] and references therein), or, in the worst case, by finite-difference estimation. One way of computing the derivatives

$$D_x\left[\det(D_x f \odot \mathbf{I}_n)\right] \qquad \text{and} \qquad D_\alpha\left[\det(D_x f \odot \mathbf{I}_n)\right]$$

is to apply a forward or central difference formula to the scalar-valued function

$$g(y;\beta) = \det(D_y f \odot \mathbf{I}_n)$$

for the $(n+1)$ required partials. An alternative is suggested by an extension of a lemma due to Halanai (published by Davidenko [6]).

LEMMA 3.6. *Let $\mathbf{A}(x) = (a_{ij}(x))$ be a matrix, $1 \le i,j \le m$, whose entries are C^1 real-valued functions $a_{ij} : \Omega \subset \mathbb{R}^k \to \mathbb{R}$. Then for $1 \le l \le k$,*

$$\frac{\partial}{\partial x_l}\det\left(\mathbf{A}(x)\right) = \operatorname{tr}\left(\operatorname{Adj}(\mathbf{A}(x)) \cdot \frac{\partial}{\partial x_l}\mathbf{A}(x)\right)$$

where tr() *denotes the trace function and* Adj() *is the adjoint matrix of* $\mathbf{A}$. *Moreover, if $\mathbf{A}(x)$ is invertible in Ω, then*

$$\frac{\partial}{\partial x_l}\det\left(\mathbf{A}(x)\right) = \det\left(\mathbf{A}(x)\right) \cdot \operatorname{tr}\left(\mathbf{A}^{-1}(x) \cdot \frac{\partial}{\partial x_l}\mathbf{A}(x)\right)$$

for all $x \in \Omega$.

Identifying the matrix $\mathbf{A}$ in the lemma with either $\mathbf{J} \odot \mathbf{I}_n$ or a resultant matrix from section 2 shows that the partial derivatives of the augmented equation may be computed *without* resorting to differencing the determinant function. Moreover, in those cases when second derivatives of f are known, these formulae indicate how they may be used *directly*. The adjoint form is undesirable since the computation of $\operatorname{Adj}(\mathbf{A}(x))$ is $\mathcal{O}(m^4)$; however, since the objective of the corrector step is, essentially, to drive $\mathbf{A}$ to singularity we expect the calculation of $\mathbf{A}^{-1}$ to be increasingly unstable near a solution point. Therefore we require a similar formula valid near a generic solution where we expect the rank of $\mathbf{A}$ to drop by one due to the vanishing of a single eigenvalue. In the case that the singular values $\sigma_{n-1} > \sigma_n > 0$ of $\mathbf{A}$ are well separated, the results of Chan [4] show that we can isolate the vanishing pivot in its LU decomposition using an appropriately chosen permutation matrix $\mathbf{P}$ to form

$$\mathbf{PAQ} = \mathbf{L}_A\mathbf{U}_A = \begin{bmatrix} \mathbf{L} & 0 \\ v^t & 1 \end{bmatrix}\begin{bmatrix} \mathbf{U} & w \\ 0 & \epsilon \end{bmatrix} \tag{19}$$

where ϵ is on the order of the smallest singular value of $\mathbf{A}$. Thus, we expect the conditioning of $\mathbf{L}$ and $\mathbf{U}$ to be much improved compared with that of $\mathbf{A}$ and, using

TABLE 2
Fraction of entries in the bialternate product matrix $2\mathbf{J} \odot \mathbf{I}_n$ which are nonzero as a function of Jacobian dimension n.

n	Fraction Nonzero
5	70 %
10	38 %
15	26 %
25	16 %
50	8 %

block forms for the inverses of $\mathbf{L}_A$ and $\mathbf{U}_A$ together with the relation $\det(\mathbf{A}) = \epsilon \cdot \det(\mathbf{U})$, we obtain the following.

LEMMA 3.7. *Let $\mathbf{A}$ be a matrix defined as in Lemma 3.6 and suppose that $\mathbf{A}$ is invertible in some open set $\Omega \in \mathbb{R}^k$ with singular values $\sigma_1(x) \geq \cdots \geq \sigma_{n-1}(x) > \sigma_n(x) > 0$. Then for $1 \leq l \leq k$ and each $x \in \Omega$ there exist matrices $\mathbf{P}$, $\mathbf{Q}$, $\mathbf{U}$, and $\mathbf{L}$, vectors v and w and $\epsilon > 0$ such that*

$$\frac{\partial}{\partial x_l} \det(\mathbf{A}(x)) = \det(\mathbf{U}) \cdot \operatorname{tr}\left(\mathbf{Z} \cdot \frac{\partial}{\partial x_l}\mathbf{A}(x)\right)$$

where $\mathbf{P}$ is a permutation matrix, $\mathbf{Q}$ is orthogonal, ϵ is either $\mathcal{O}(\sigma_n)$ or $\mathcal{O}(\kappa_\infty^{-1}(\mathbf{A}))$, and

$$\mathbf{Z} = \mathbf{Q}\begin{bmatrix} \epsilon(\mathbf{L}\mathbf{U})^{-1} + \mathbf{U}^{-1}wv^t\mathbf{L}^{-1} & -\mathbf{U}^{-1}w \\ -v^t\mathbf{L}^{-1} & 1 \end{bmatrix}\mathbf{P}.$$

Applying Lemmas 3.4 and 3.7 to the augmented system defined by (14), one obtains for $1 \leq l \leq (n+1)$

$$\frac{\partial}{\partial y_l} \det(\mathbf{J}(y) \odot \mathbf{I}_n) = \det(\mathbf{U}) \cdot \operatorname{tr}\left(\mathbf{Z} \cdot \left(\left[\frac{\partial}{\partial y_l}\mathbf{J}(y)\right] \odot \mathbf{I}_n\right)\right).$$

As this formula shows, each partial of $\det(\mathbf{J} \odot \mathbf{I})$ is composed of weighted sums of entries in the matrix derivatives of $\mathbf{J}$. In particular, $\mathbf{Z}$ is the weight matrix and $\det(\mathbf{U})$ a scale factor, both dependent upon $\mathbf{J}$ but not on l. Thus, to compute the row of entries in D_yF corresponding to the augmented singularity equation,

$$D_yF(y;\beta) = \left[\begin{array}{c|c} * & * \\ \hline D_x\left[\det\left[D_xf \odot \mathbf{I}_n\right]\right]^t & D_\alpha\left[\det\left(D_xf \odot \mathbf{I}_n\right)\right] \end{array}\right],$$

one needs to evaluate these factors only once per corrector step.

We conclude this section with a few remarks concerning the properties of bialternate product matrices germane to the solution of the linear algebra problems which arise in algorithms for Hopf bifurcation. Specifically, we wish to exploit the structure of $\mathbf{J} \odot \mathbf{I}_n$ in such a way as to mitigate the dimension increase of the linear systems from n to $\frac{n}{2}(n-1)$. Foremost among these is the observation that the bialternate product matrix of $\mathbf{J}$ is sparse—*very* sparse—even for n of modest dimension. Table 2 shows the fraction of nonzero entries in $\mathbf{J} \odot \mathbf{I}_n$ for dense $\mathbf{J}$ as a function of n. The sparsity of the bialternate product is a consequence of its relationship to the tensor

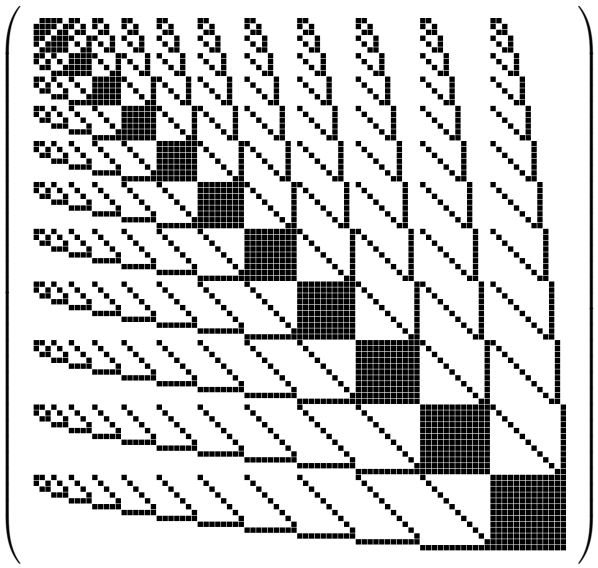
$\mathbf{J} \oplus \mathbf{I}_{14} \; =$ 

FIG. 1. *Sparsity pattern in the bialternate product matrix produced by a dense Jacobian matrix of dimension $n = 14$. Note wedge diagonal structures comprised of subblocks of increasing size.*

sum $\mathbf{J} \otimes \mathbf{I} + \mathbf{I} \otimes \mathbf{J}$ which is composed of a dense block-diagonal band of bandwidth n, and $n^2(n^2-1)$ off-diagonal blocks with (at most) n nonzero entries in each block. A similar internal structure is inherited by the bialternate product matrix, a conclusion which is implied by Lemmas 3.2 and 3.3. For example, consider the fate of the mth lower subdiagonal of $\mathbf{J}$ under the bialternate product transformation; that is, consider the elements of $\mathbf{J}$ for which $i > j$ and $1 \le m = i - j \le (n-1)$. From Lemma 3.2, its image in $\mathbf{J} \odot \mathbf{I}_n$ remains in the lower subtriangle. Inspection of the proof for Lemma 3.3 shows the bound for the difference in row and column indices for elements in the bialternate product matrix originating from $(\mathbf{J})_{ij}$,

$$i_r - i_c \le \frac{1}{2}\left(i^2 - j^2 + 3(j-i)\right) = \frac{m}{2}\left(2i - m - 3\right),$$

is tight and monotonically increasing with i. Thus, the mth subdiagonal of $\mathbf{J}$ generates a wedge or fan-like structure of nonzero entries in $\mathbf{J} \odot \mathbf{I}_n$ which is narrow in the upper-left corner of the bialternate product matrix and achieves its maximum width as a result of the $(n, n-m)$th entry of $\mathbf{J}$. Finally, (9) shows that while the product matrix is not symmetric, in general, its basic sparsity pattern is. To illustrate these observations, Figure 1 shows the sparsity pattern generated by a dense Jacobian matrix of dimension $n = 14$.

The observation that $\mathbf{J} \odot \mathbf{I}_n$ is band structured and sparse may be exploited by Hopf path-following algorithms in a variety of ways. For example, the augmented equation defined above depends upon the singularity of the bialternate product, a property which is preserved under similarity transformation [9]. Thus, (14) may be replaced by

$$\tilde{F}(y;\beta) = \begin{pmatrix} f(x,\alpha), \\ \det\left(\left(\mathbf{M}^{-1}\mathbf{J}\mathbf{M}\right) \odot \mathbf{I}_n\right) \end{pmatrix} \tag{20}$$

where $\mathbf{M} \equiv \mathbf{M}(y;\beta)$ is invertible. Naturally, the most desirable choices for $\mathbf{M}$ will be unitary as well. Reduction of $\mathbf{J}$ to Hessenberg form by choosing $\mathbf{M}$ a product of Householder matrices is numerically stable and yields a bialternate product which has

a block Hessenberg structure with a subdiagonal bandwidth $(n-2)$ and a sparsity structure in the upper triangle as described above. If the Jacobian is reduced to tridiagonal form, $\mathbf{J} \odot \mathbf{I}_n$ is block tridiagonal. Matrix routines designed for these (block) banded structures can then be exploited to achieve a corresponding reduction of computational work.

4. Concluding remarks. The algorithms that we have described for computing Hopf bifurcations are specifically designed to compute points at which there is a simple pair of pure imaginary eigenvalues for the Jacobian of a system [10]. We briefly discuss the extension of the algorithms to ones which seek points of codimension-two bifurcation. There are three cases which arise from codimension-two conditions on the linearization of a vector field at an equilibrium, namely, Takens–Bogdanov bifurcation, double Hopf bifurcation, and simultaneous simple zero and pure imaginary eigenvalues. In each case, we seek minimally inflated systems of $(n+2)$ equations that locate the codimension-two bifurcation points. The case of the Takens–Bogdanov bifurcation is easy. In terms of the characteristic polynomial of the Jacobian, one wants the constant and linear coefficients to vanish. This condition is equivalent to the Jacobian $\mathbf{J}$ having corank-1 and the square of the Jacobian $\mathbf{J}^2$ having corank-2. Alternatively, the Jacobian and the bialternate product of the Jacobian both vanish. These last criteria are also satisfied at a point with a zero eigenvalue and a pair of imaginary eigenvalues. Locating points of double Hopf bifurcation is a bit more complex. One can calculate in terms of polynomial remainder sequences the presence of two pairs of eigenvalues whose sum is zero. At such a parameter value, the two polynomials r_e and r_o constructed from the characteristic polynomial have a common quadratic factor. The coefficients of this polynomial can be computed as subresultants of the Sylvester matrix of r_e and r_o. In order for the two pairs of roots to be imaginary, the common quadratic factor of r_e and r_o should have negative real roots. This is easily expressed as inequalities on the coefficients of the common (monic) factor: it must have positive coefficients and a positive discriminant. Bialternate product methods for computing points of multiple Hopf bifurcation are discussed in a forthcoming paper of Govaerts, Guckenheimer, and Khibnik [11].

In a companion paper [15], we examine the issues relating to implementing Hopf continuation using the resultant and biproduct formulations and study their performance on a suite of example problems of current research interest in neurobiology. Several algorithms, including the ones based on the Bezout resultant and the bialternate product, are applied to compute curves of Hopf bifurcations in a two-dimensional parameter space for the following six-dimensional vector field:

$$
\begin{aligned}
\dot{x}_1 &= -g_{Na}\varphi_2^3(x_1)\,x_4\,(x_1 - v_{na}) - 2g_{Ca}x_5\frac{(x_1 - v_{ca})}{(1+2x_2)} - g_K x_3^4\,(x_1 - v_k) \\
&\quad - 2g_{KCa}x_2\frac{(x_1 - v_k)}{(1+2x_2)} - g_A\psi_2^3(x_1)\,x_6\,(x_1 - v_k) - g_l\,(x_1 - v_l), \\
\dot{x}_2 &= -0.003\left[x_2 - k_{ca}x_5\frac{(x_1 - v_{ca})}{(1+2x_2)}\right], \\
\dot{x}_3 &= 0.8\left[(1-x_3)\,\varphi_3(x_1) - x_3\psi_3(x_1)\right], \\
\dot{x}_4 &= 0.8\left[(1-x_4)\,\varphi_4(x_1) - x_4\psi_4(x_1)\right], \\
\dot{x}_5 &= -.042553\left[x_1 - \phi_+(x_1;\alpha_5,\beta_5)\right], \\
\dot{x}_6 &= \phi_+(x_1;\gamma_5,\delta_5) - x_6
\end{aligned}
$$

where

$$\begin{aligned}
\varphi_1(x_1) &= -(\alpha_1+\beta_1 x_1)\,\phi_-(x_1;\alpha_1,\beta_1), & \psi_1(x_1) &= 4e^{\gamma_1+\delta_1 x_1},\\
\varphi_2(x_1) &= \frac{\varphi_1(x_1)}{\big(\varphi_1(x_1)+\psi_1(x_1)\big)}, & \psi_2(x_1) &= \phi_+(x_1;\gamma_2,\delta_2),\\
\varphi_3(x_1) &= -0.1\,(\alpha_3+\beta_3 x_1)\,\phi_-(x_1;\alpha_3,\beta_3), & \psi_3(x_1) &= 0.125e^{\gamma_3+\delta_3 x_1},\\
\varphi_4(x_1) &= 0.07e^{\alpha_4+\beta_4 x_1}, & \psi_4(x_1) &= \phi_+(x_1;\gamma_4,\delta_4).
\end{aligned}$$

We consider the accuracy and convergence of root-finding algorithms as well as the number of operations required to compute the curves of Hopf bifurcations. Summarizing our findings, the number of floating point operations required for continuation of a curve of Hopf bifurcations using an augmentation function based upon the Bezout resultant required slightly fewer operations (664,777 flops) than the use of an algorithm described by Griewank and Reddien [12] based upon a $(2n+2)$-dimensional augmentation function (701,244 flops). However, in a test of the convergence of root finding from "naturally" chosen initial values for parameter values near a point of double Hopf bifurcation, the method based upon use of the Bezout resultant as an augmentation function gave more consistent results. Use of the the determinant of the biproduct as an augmentation function was substantially slower (2,786,163 flops), but these biproduct calculations did not exploit the sparsity of the biproduct matrix in computing its determinant.

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