To appear in Applied Numerical Mathematics

DETECTION OF GENERIC ONE PARAMETER BIFURCATIONS OF HAMILTONIAN EQUILIBRIA

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Abstract. In this paper several possibilities are considered for constructing test functions which reveal generic one parameter bifurcations of equilibria of Hamiltonian systems. These are alternatives to computing all the eigenvalues of the linearized system. Because of the Hamiltonian structure, most test functions that are used for general systems do not work here. Typically a test function that should change sign at a bifurcation point has a multiple zero and no sign change there for Hamiltonian systems. Methods based on characteristic polynomials and bialternate products of matrices are discussed in detail.

1. Introduction

Consider a Hamiltonian system depending on a real parameter α and defined by a smooth function $h : \mathbb{R}^{2n} \times \mathbb{R} \to \mathbb{R}$

$$\dot{x} = J h_x(x, \alpha) , \qquad \text{where} \qquad J = \left[\begin{smallmatrix} 0 & I \\ -I & 0 \end{smallmatrix}\right] .$$

Let x_α be an equilibrium depending on α

$$h_x(x_\alpha, \alpha) = 0$$

and denote by

$$H(x_\alpha, \alpha) = J h_{xx}(x_\alpha, \alpha)$$

the matrix of the linearized system and by $\sigma(H(x_\alpha, \alpha))$ its spectrum.

A local bifurcation occurs at $\alpha = \alpha_0$ if the structure of the set of trajectories of the system near the equilibrium changes when the parameter crosses the value α_0. Here we study the bifurcations where the linear stability of the equilibrium changes, i.e., the number of the eigenvalues on the imaginary axis changes. Generically, in one parameter families of Hamiltonian systems, there can be two types of such bifurcations (see [1] App. 6, [14],[15]):

1) Hamiltonian saddle–node (fold) bifurcations: $0 \in \sigma(H(x_{\alpha_0}, \alpha_0))$.
2) Hamiltonian Hopf bifurcations: $H(x_{\alpha_0}, \alpha_0)$ has a purely imaginary double eigenvalue $i\omega \neq 0$ (then $-i\omega$ is also a double eigenvalue).

The first can occur for systems with one degree of freedom while the second needs $n \geq 2$. There exist other types of local bifurcations which are caused by resonances. These will be discussed briefly in section 5.

In the Hamiltonian saddle–node bifurcation (see [4],[15]) generically there is a smooth path of equilibria in $\mathbb{R}^{2n} \times \mathbb{R}$, tangent to $\mathbb{R}^{2n} \times \{0\}$ at (x_{α_0}, α_0), such that along this

1991 *Mathematics Subject Classification.* 65L07, 58F05, 58F14.

Key words and phrases. Hamiltonian systems, bifurcation, bialternate product.

This work was carried out while enjoying the hospitality of the School of Mathematics, Georgia Institute of Technology, Atlanta, 1997. Supported by the Academy of Finland under grant No. 26341.

path a pair of purely imaginary eigenvalues changes to two real ones with opposite signs. The eigenvalue zero is defective and the equilibrium disappears for $\alpha > \alpha_0$ (or $\alpha < \alpha_0$).

In the generic Hamiltonian Hopf bifurcation (see [15], [16]) the double eigenvalues are defective. The equilibrium is a smooth function of α and along this path two pairs of purely imaginary eigenvalues collide and change to two complex conjugate pairs with real parts of opposite sign.

In bifurcation analysis the goal is to draw a diagram in parameter space where all the interesting bifurcations occur. That is, to compute the sets of parameter values for which some degeneracy occurs. Usually this is achieved via one dimensional continuation (of e.g. equilibria) in the state and parameter space monitoring sign changes of certain test functions – one for each type of bifurcation (see [5], [10], [11]). When a bifurcation point is found then a branch of such bifurcation points can be computed by adding the equation that the test function being zero and with continuation in a two dimensional set of parameters. This approach needs smooth test functions that, at least generically, change sign at corresponding bifurcation points.

Of course computation of all the eigenvalues at each point reveals the changes in linear stability. The eigenvalues themselves are not smooth functions of parameters, but one can form functions of the eigenvalues which become smooth and serve the purposes of the bifurcation analysis. Here, however, we look for other possibilities.

The aim of the present study is to find test functions to detect situations 1) and 2) above. Many of the techniques here have origin in the works [5],[7], [8], and [10], where test functions for general folds and Hopf bifurcations are considered.

The generic behaviour of standard test functions in the case of Hamiltonian systems is not yet clear. It is shown that the test functions for folds (saddle–node bifurcations) work also for Hamiltonian systems even though the zero eigenvalue is double in these cases. The standard test functions for Hopf bifurcations, however, do not work in the Hamiltonian case.

In Sections 2 and 3 smooth test functions for the detection of Hamiltonian bifurcations of type 1) and 2) are proposed; for generic one parameter families of Hamiltonian systems these functions are shown to change sign at corresponding bifurcation points. A simple example is given in Section 4 and further questions and possible developments are discussed in Section 5. In particular, the present work does not pay much attention to the cost of the numerical computations. In order to gain efficiency many numerical linear algebra issues must be resolved.

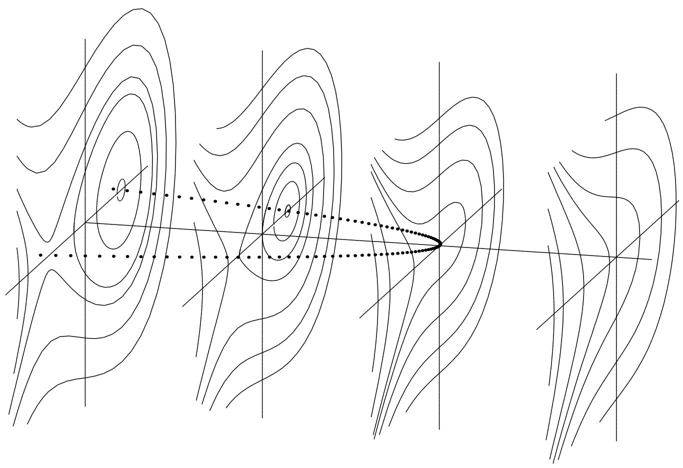
2. Hamiltonian saddle–node bifurcation

Here we consider the case where zero is an eigenvalue of the linearized vector field at the equilibrium. Then it is at least a double eigenvalue[1]. In a one parameter family of Hamiltonian systems it is generically a fold point, the eigenvalue zero is defective and has multiplicity two, and on the path of equilibria a pair of purely imaginary eigenvalues changes to two real ones with opposite signs (see [4],[15] and Thm. 2.1, Rem. 2.1 below).

[1] If $Hv = 0$, then $H^T Jv = 0$ and since $v \perp Jv$ the eigenvalue zero must be at least double.

In the following diagram a typical fold bifurcation is shown. The planes correspond to different parameter values and the dotted curve to the path of equilibria. The solid curves are trajectories of the system. Here

$$h(x,\alpha) = \alpha x_1 + \tfrac{1}{2}\,x_2^2 + \tfrac{1}{3}\,x_1^3\ , \qquad \alpha \in \{-\tfrac{1}{10}, -\tfrac{1}{20}, 0, \tfrac{1}{20}\}\ .$$



We study the numerical detection of fold points. The determinant of the linearized system at the equilibrium is a natural candidate and has been used for fold detection of general systems. For a Hamiltonian system zero is a double eigenvalue of H at the bifurcation point, but nevertheless the determinant will generically cross zero transversally there. This is shown in Theorem 2.1. The determinant, however, is usually badly scaled so that numerically it may be better to use the bordering technique (see [5],[10]). This will also be introduced.

The following theorem shows that, generically, $\eta = \det(H)$ works as a test function to detect folds for Hamiltonian systems.

Theorem 2.1. *For a generic*[2] *one parameter family of Hamiltonian systems the equilibria for which* $\det(H) = 0$ *are fold points. Through each of these fold points there is a smooth curve* $(x(s), \alpha(s))$ *parameterized by arc length and at the fold point*

$$\tfrac{d}{ds}\det\big(H(x(s),\alpha(s))\big)_{|s=0} \neq 0\ .$$

Proof. In the space $\mathcal{J}^2$ of two-jets

$$\mathcal{J}^2 = \big\{\, j^2h(z) = \big(z, h(z), h_z(z), h_{zz}(z)\big) \;\big|\; z = (x,\alpha) \in \mathbb{R}^{2n+1}\ ,\ h \in C^\infty(\mathbb{R}^{2n+1}, \mathbb{R})\,\big\}$$

the equations $h_x = 0$ and $\det(h_{xx}) = 0$ define a Whitney stratified manifold V of codimension $2n{+}1$. Here the stratification is given by pieces of the manifolds V_k corresponding to $\operatorname{rank}(h_{xx}) = 2n-k$, $k = 1,\ldots,2n$ and have codimensions $2n + \frac{k(k+1)}{2}$ (see [2], p. 30). The space $\mathcal{J}^2$ can be identified with $\mathbb{R}^{2n+1} \times \mathbb{R} \times \mathbb{R}^{2n+1} \times \mathbb{R}^{(2n+1)(n+1)}$, where the last

[2]In the Whitney C^∞ topology.

factor corresponds to the space of symmetric $(2n+1)\times(2n+1)$ matrices. Then the manifolds V_k can be written in the corresponding coordinates as

$$V_k = \left\{ \left(u, a, \left[\begin{smallmatrix} 0 \\ b \end{smallmatrix}\right], \left[\begin{smallmatrix} S & v \\ v^T & c \end{smallmatrix}\right]\right) \mid S = S^T,\ \operatorname{rank}(S) = 2n-k \right\} .$$

By the strong transversality theorem of Thom ([2], p. 38, 41), the set $\mathcal{H}_V$ of C^∞ functions h for which the 2-jet j^2h is transversal to V is of the second Baire category.

Let h be in $\mathcal{H}_V$ and let $z_0 = (x_0, \alpha_0)$ be an equilibrium for which $\det(h_{xx}(x_0, \alpha_0)) = 0$, i.e., $j^2h(z_0) \in V$. Assume that $j^2h(z_0) \in V_k$. Then, by transversality,

$$R(D_z j^2 h(z_0)) + T_{j^2h(z_0)} V_k = \mathcal{J}^2 , \tag{2.1}$$

where R denotes the range. Since for any k the tangent space of V_k does not span anything corresponding to the h_x direction, $R(D_z j^2 h(z_0))$ has to span it all. This means that $\operatorname{rank}(\begin{bmatrix} h_{xx} & h_{x\alpha}\end{bmatrix}) = 2n$ at (x_0, α_0). Using the implicit function theorem one easily shows that the local solutions of $h_x(x, \alpha) = 0$ form a smooth curve $(x(s), \alpha(s))$ parameterized by the arc length.

Since $\dim(R(D_z j^2h(z_0))) \le 2n+1$ it is necessary to have $\operatorname{codim}(T_{j^2h(z_0)}V_k) \le 2n+1$ for (2.1) to hold and, since inequality is not possible here, we get $k = 1$ and equalities in both of these. Hence $D_z j^2 h(z_0)$ must be injective and

$$R(D_z j^2 h(z_0)) \cap T_{j^2h(z_0)} V_1 = \{0\} . \tag{2.2}$$

Since $\operatorname{rank}(h_{xx}) = 2n-1$ at z_0, one easily shows that the gradient of the determinant is nonzero at h_{xx}. Now, if

$$\tfrac{d}{ds} \det \left(h_{xx}(x(s), \alpha(s))\right)_{|s=0} = 0 ,$$

then for $(x', \alpha') = \frac{d}{ds}(x(s), \alpha(s))_{|s=0} \neq 0$ we have $h_{xx}x' + h_{x\alpha}\alpha'_{|s=0} = 0$ so that

$$D_z j^2 h(z_0)(x', \alpha') = \left(h_\alpha \alpha', \left[\begin{smallmatrix} 0 \\ h_{\alpha x}x' + h_{\alpha\alpha}\alpha' \end{smallmatrix}\right], \left[\begin{smallmatrix} h_{xxx}x' + h_{xx\alpha}\alpha' & w \\ w^T & r \end{smallmatrix}\right] \right)$$

(for some w, r) is in $T_{j^2h(z_0)}V_1$, which contradicts (2.2). □

Remark 2.1. From the condition $\operatorname{rank}(h_{xx}) = 2n-1$, we see that the double eigenvalue zero of H at the bifurcation point is defective. It follows that, on the local equilibrium path $(x(s), \alpha(s))$, we have $\alpha'(0) = 0$ and the spectrum of H is of the form

$$\sigma\big(H(x(s), \alpha(s))\big) = \{\pm c\sqrt{s} + O(|s|), \dots\} .$$

Modification: the bordering technique. In the continuation process for computing e.g. curves of fold points for the bifurcation diagram, smooth test functions are needed for the Newton method to converge as usual. Of course the determinant is smooth but, in practice, it is often badly scaled so that very small continuation steps may be required for the convergence of Newton's method at the next step. For this reason the determinant is often replaced by another test function as follows (see [5], [10]).

Assume that u and v are vectors such that the matrix $\begin{bmatrix} h_{xx} & u \\ v^T & 0 \end{bmatrix}$ is nonsingular even through fold points. This means that $\operatorname{rank}(h_{xx}) \ge 2n-1$ and if $\det(h_{xx}) = 0$ then

$u \notin R(h_{xx})$ and $v \notin R(h_{xx}^T)$. Then, by Cramer's rule, the η–part of the solution of the system

$$\begin{bmatrix} h_{xx} & u \\ v^T & 0 \end{bmatrix} \begin{bmatrix} \xi \\ \eta \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{2.3}$$

is given by

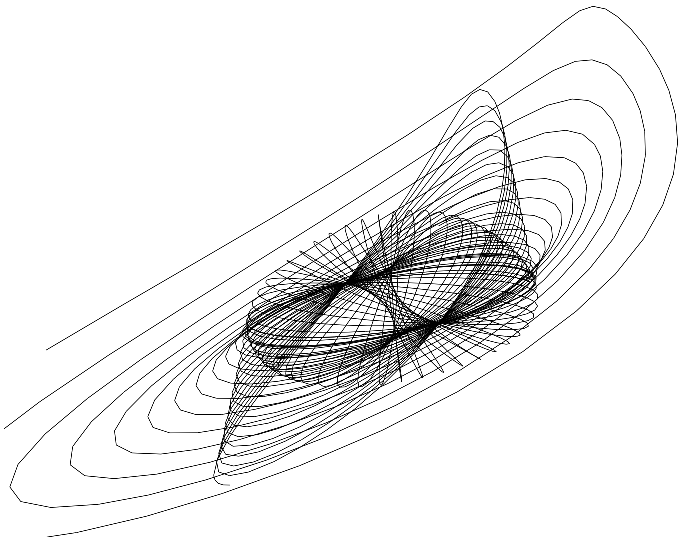
$$\eta = \frac{\det(h_{xx})}{\det\left(\left[\begin{smallmatrix} h_{xx} & u \\ v^T & 0 \end{smallmatrix}\right]\right)} .$$

Hence this function η also generically changes sign at a fold point. The bordering technique is to solve equation (2.3) and use η as a test function. Since, generically, $\operatorname{rank}(\begin{bmatrix} h_{xx} & h_{x\alpha} \end{bmatrix}) = 2n$, a natural choice in this Hamiltonian case is to take $u = v = h_{x\alpha}$. Experiments show that this choice often allows larger continuation steps than the determinant in computing the curve of folds by arclength continuation (in two parameters) on the system

$$\begin{cases} h_x(x, \alpha, \beta) = 0 \\ \eta(h_x(x, \alpha, \beta)) = 0 \end{cases} .$$

3. Hamiltonian Hopf bifurcation

In a Hamiltonian Hopf bifurcation both the double eigenvalues are generically defective. The equilibrium persists through the bifurcation point, is a smooth function of α, and generically along this path two pairs of purely imaginary eigenvalues collide and change to two complex conjugate pairs with real parts of opposite sign (see [1] App. 6, [15] [16], also Theorem 3.1 below).



The diagram above illustrates three dimensional projections of trajectories of the four dimensional system:

$$h(x, \alpha) = \alpha\, x_3^2 + 0.5\, x_2 x_3^2 + x_1 x_4 - x_2 x_3 - 0.02\,(x_1^2 + x_2^2) .$$

The trajectory on the torus describes the situation before the bifurcation ($\alpha = -0.01$, distinct purely imaginary eigenvalues), the trajectory on the middle surface is at the bifurcation point ($\alpha = 0$, polynomially unstable, defective double imaginary eigenvalues), and the outer trajectory is after the bifurcation ($\alpha = 0.01$, eigenvalues have nonzero real parts). All trajectories start at $x(0) = (0.2, 0, 0, 0)$ and the first three coordinates are plotted.

We consider two approaches for detecting this bifurcation. The first is based on computing the characteristic polynomial of the Hamiltonian matrix H and the resultant for determining common zeros of two polynomials. The second is based on the bialternate product of H with the identity matrix. This is a linear map whose eigenvalues are the sums of the eigenvalues of H .

If all the eigenvalues of H are computed then, locally, one can monitor pairs of complex conjugate eigenvalues

$$\mu_1 \pm i\omega_1 \ , \qquad \mu_2 \pm i\omega_2$$

($\omega_1, \omega_2 > 0$) which are close to each other and have small real parts. Then since $\sigma(H) = -\sigma(H)$ (see below) we have $\mu := \mu_1 = -\mu_2$ and if $\mu \neq 0$ then $\omega_1 = \omega_2$. The function

$$b = \mu^2 - (\omega_1 - \omega_2)^2$$

is then smooth and generically changes sign at the bifurcation point. The approaches of Subsections 3.1 and 3.2 that are based on detection of *double eigenvalues* give alternatives to this test function.

3.1. **Detection using characteristic polynomials.** The first new approach is based on computing the characteristic polynomial of the Hamiltonian matrix and the resultant for determining common zeros of two polynomials. A related technique for detecting Hopf bifurcations of general systems $\dot{x} = f(x, \alpha)$ is based on finding two zeros of the characteristic polynomial that are symmetric w.r.t. the origin: $\lambda, -\lambda \in \sigma(f_x)$ (see [8]). This does not work here, since in Hamiltonian systems we always have n such pairs.

Since $J^{-1}H = h_{xx}$ is symmetric and $J^T = -J = J^{-1}$ we have $H^T = -J^{-1}HJ$, so that H is similar to $-H$. In particular, $\lambda \in \sigma(H) \implies -\lambda \in \sigma(H)$ with the same algebraic and geometric multiplicities. This symmetry of the spectrum implies that the characteristic polynomial has only even powers:

$$\det(\lambda I - H) = p(\lambda^2) \ . \tag{3.1}$$

At a Hopf bifurcation point this can be factorized as

$$p(\lambda^2) = (\lambda^2 + \omega^2)^2 \, \widetilde{p}(\lambda^2) \ ,$$

i.e., the polynomial p has a double zero $-\omega^2$. Hence at such a point the polynomials p and p' (the derivative) have a common zero. To detect this situation consider the *resultant* of p and p' . For two polynomials

$$p(t) = a_n t^n + a_{n-1} t^{n-1} + \cdots + a_1 t + a_0$$
$$q(t) = b_m t^m + b_{m-1} t^{m-1} + \cdots + b_1 t + b_0$$

the resultant is defined to be the determinant of size $n+m$:

$$\operatorname{res}(p,q) = \begin{vmatrix}
a_n & a_{n-1} & a_{n-2} & \cdots & a_1 & a_0 & & & \\
 & a_n & a_{n-1} & a_{n-2} & \cdots & a_1 & a_0 & & \\
 & & \ddots & \ddots & \ddots & & \ddots & \ddots & \\
 & & & a_n & a_{n-1} & a_{n-2} & \cdots & a_1 & a_0 \\
b_m & b_{m-1} & b_{m-2} & \cdots & b_0 & & & & \\
 & b_m & b_{m-1} & b_{m-2} & \cdots & b_0 & & & \\
 & & \ddots & \ddots & \ddots & & \ddots & & \\
 & & & b_m & b_{m-1} & b_{m-2} & \cdots & b_0 & \\
 & & & & b_m & b_{m-1} & b_{m-2} & \cdots & b_0
\end{vmatrix} .$$

Here we have m a–rows and n b–rows. If $r_1, \ldots, r_n$ and $s_1, \ldots, s_m$, respectively, are the roots of p and q then (see e.g.: [3], A IV)

$$\operatorname{res}(p,q) = a_n^m b_m^n \prod_{i,j} (r_i - s_j) \ ,$$

which is zero if and only if p and q have a common zero. To detect a double zero of p we take $q = p'$, i.e., $m = n-1$ and $b_j = (j+1)\, a_{j+1}$. Hence

$$\zeta(H) = \operatorname{res}(p, p')$$

is a candidate test function for Hopf detection. The following result shows that generically it works.

Theorem 3.1. *For a generic one parameter family of Hamiltonian systems near any equilibrium $(x(\alpha_0), \alpha_0)$ for which H has a nonzero double purely imaginary eigenvalue, there exists a smooth curve $(x(\alpha), \alpha)$ of equilibria such that*

$$\tfrac{d}{d\alpha} \zeta\big(H(x(\alpha), \alpha)\big)_{|\alpha=\alpha_0} \neq 0 \ .$$

Proof. Since ζ is an analytic function of h_{xx}, the equations $h_x = 0$ and $\zeta = 0$ with $\det(h_{xx}) \neq 0$ define a semianalytic set W in $\mathcal{J}^2$ and this has a Whitney stratification (see [9]) of codimension $\geq 2n+1$.

Again, by the strong transversality theorem, the set $\mathcal{H}_W \subset C^\infty(\mathbb{R}^{2n+1}, \mathbb{R})$ of functions h, for which $j^2 h$ is transversal to W, is of the second category. Further, using results of Galin (see [1] App. 6) we can assume that at points where we have double eigenvalues they are defective and all other eigenvalues are simple. For such a h let $z_0 = (x_0, \alpha_0)$ be such that $j^2 h(z_0) \in W$. Then, as in Theorem 2.1, by transversality and dimension arguments we have the direct sum

$$R(D_z j^2 h(z_0)) \oplus T_{j^2 h(z_0)} W = \mathcal{J}^2 \ , \tag{3.2}$$

where $D_z j^2 h(z_0)$ is injective. Since $\det(h_{xx}) \neq 0$ at (x_0, α_0) the implicit function theorem implies that there exists a smooth function $x(\alpha)$ such that $h_x(x(\alpha), \alpha) = 0$, in particular $h_{xx} x' + h_{x\alpha}{}_{|\alpha=\alpha_0} = 0$. Since the eigenvalue $i\omega$ is defective we can, by Williamson's theorem (see [1] App. 6), bring H by a real symplectic similarity transformation to the form:

$$SHS^{-1} = \begin{bmatrix} \begin{smallmatrix} 0 & 1 \\ -\omega^2 & 0 \end{smallmatrix} & & \begin{smallmatrix} \omega^{-2} & 0 \\ 0 & 1 \end{smallmatrix} & \\ & \widetilde{A} & & \widetilde{B} \\ \begin{smallmatrix} 0 & 0 \\ 0 & 0 \end{smallmatrix} & & \begin{smallmatrix} 0 & \omega^2 \\ -1 & 0 \end{smallmatrix} & \\ & \widetilde{C} & & -\widetilde{A}^T \end{bmatrix}$$

(or with the opposite sign for the $\begin{smallmatrix} \omega^{-2} & 0 \\ 0 & 1 \end{smallmatrix}$ part), where the eigenvalues of $\widetilde{H} = \left[\begin{smallmatrix} \widetilde{A} & \widetilde{B} \\ \widetilde{C} & -\widetilde{A}^T \end{smallmatrix}\right]$ are simple and distinct from $\pm i\omega$.

Let $\widehat{H}$ be a Hamiltonian matrix such that $S\widehat{H}S^{-1}$ has $\begin{smallmatrix} \omega^2 & 0 \\ 0 & 1 \end{smallmatrix}$ in the place of $\begin{smallmatrix} 0 & 0 \\ 0 & 0 \end{smallmatrix}$ in SHS^{-1} and zeros elsewhere. Then

$$p_\varepsilon(\lambda^2) := \det(\lambda I - H - \varepsilon\widehat{H}) = r_\varepsilon(\lambda^2)\,\widetilde{p}(\lambda^2) \ ,$$

where

$$r_\varepsilon(\lambda^2) = \lambda^4 + 2(\omega^2 - \varepsilon)\,\lambda^2 + (\omega^2 + \varepsilon)^2$$

and

$$\widetilde{p}(\lambda^2) = \det(\lambda I - \widetilde{H}) \ .$$

Using the properties of the resultant (see [3], section A IV 6, formulas (29,35,36)) we get

$$\begin{aligned} \operatorname{res}(p_\varepsilon, p_\varepsilon') &= \operatorname{res}(r_\varepsilon\,\widetilde{p}\,,\, r_\varepsilon'\,\widetilde{p} + r_\varepsilon\,\widetilde{p}') \\ &= \operatorname{res}(r_\varepsilon\,,\, r_\varepsilon'\,\widetilde{p} + r_\varepsilon\,\widetilde{p}')\ \operatorname{res}(\widetilde{p}\,,\, r_\varepsilon'\,\widetilde{p} + r_\varepsilon\,\widetilde{p}') \\ &= \operatorname{res}(r_\varepsilon\,,\, r_\varepsilon')\ \operatorname{res}(r_\varepsilon\,,\, \widetilde{p})\ \operatorname{res}(\widetilde{p}\,,\, r_\varepsilon)\ \operatorname{res}(\widetilde{p}\,,\, \widetilde{p}') \ , \end{aligned}$$

where

$$\operatorname{res}(r_\varepsilon\,,\, r_\varepsilon') = \begin{vmatrix} 1 & 2(\omega^2 - \varepsilon) & (\omega^2 + \varepsilon)^2 \\ 2 & 2(\omega^2 - \varepsilon) & 0 \\ 0 & 2 & 2(\omega^2 - \varepsilon) \end{vmatrix} = 16\omega^2\,\varepsilon$$

and

$$C = \operatorname{res}(r_0\,,\, \widetilde{p})\ \operatorname{res}(\widetilde{p}\,,\, r_0)\ \operatorname{res}(\widetilde{p}\,,\, \widetilde{p}') \neq 0 \ .$$

Hence

$$\tfrac{d}{d\varepsilon} \operatorname{res}(p_\varepsilon, p_\varepsilon')_{|\varepsilon=0} = 16C\omega^2 \neq 0 \ ;$$

in particular, the gradient of ζ is not zero at $H(z_0)$.

Then, as in the proof of Theorem 2.1, $\frac{d}{d\alpha}\zeta\big(H(x(\alpha),\alpha)\big)_{|\alpha=\alpha_0} = 0$ implies

$$D_z j^2 h(z_0)\,(x'(\alpha_0), 1) \in T_{j^2 h(z_0)} W$$

leading to a contradiction with (3.2). □

Remark 3.1. One can further show that, generically, the spectrum of H near the bifurcation point α_0 is of the form

$$\sigma\big(H(x(\alpha),\alpha)\big) = \{\pm i\omega \pm c\sqrt{\alpha - \alpha_0} + O(|\alpha - \alpha_0|), \dots\} \ .$$

Remark 3.2. Of course $\zeta = 0$ also at other points with double, e.g., real, eigenvalues. The strategy is first to find the zeros of ζ and then, using, for example, the Euclidean algorithm, to determine the common factor of p and p'. If it has a negative root, then it probably is a Hopf point (see the next remark), otherwise not.

Remark 3.3. The condition that $i\omega$ is a double eigenvalue does not guarantee that it is a Hopf point, nor could be perturbed to such. If the eigenvalue is definite, i.e., if the quadratic form $v^*iJ\ v$ is (positive or negative) definite in the corresponding subspace then the strong stability theorem of Krein (see [17]) says that the nearby eigenvalues of nearby Hamiltonian matrices stay on the imaginary axis. Hence the eigenvalue must be indefinite at a Hopf point. However, this is the generic situation in one parameter families (see [1] App. 6).

Remark 3.4. The issue of computing the characteristic polynomial of H will not be studied here. Effective methods, especially for the case of a sparse H will be a subject of a further study. Here we just recall one possibility. Van Loan (see [13]) squares the Hamiltonian matrix:

$$H = \begin{bmatrix} A & B \\ C & -A^T \end{bmatrix} , \quad H^2 = \begin{bmatrix} A^2 + BC & AB - BA^T \\ CA - A^TC & CB + (A^T)^2 \end{bmatrix} .$$

Then, using suitable Givens' rotations, one can orthogonally block triangularize

$$Q^T H^2 Q = \begin{bmatrix} R & S \\ 0 & R^T \end{bmatrix} .$$

Since $\sigma(H) = -\sigma(H)$ this gives

$$\det(\lambda I - R)^2 = \det(\lambda I - H^2) = (\lambda - \lambda_1^2)^2 \ldots (\lambda - \lambda_n^2)^2$$

and we obtain

$$p(\lambda^2) = \det(\lambda I - H) = (\lambda - \lambda_1)(\lambda + \lambda_1) \ldots (\lambda - \lambda_n)(\lambda + \lambda_n) = \det(\lambda^2 I - R) .$$

So, the problem reduces to computing the characteristic polynomial of a matrix of half the dimension. It would be interesting to know whether one could achieve this without actually squaring H.

3.2. **Detection using bialternate products.** Here we study the possibility of using the bialternate product $H \odot I$ for detecting the Hamiltonian Hopf bifurcation. The product is a linear operator whose eigenvalues are the sums of the eigenvalues of H. For general systems $\dot{x} = f(x, \alpha)$ the standard test function for Hopf bifurcation is $\det(f_x \odot I)$, which is zero if f_x has a pair of eigenvalues whose sum is zero (see [8],[12]) Here this does not work since $\det(H \odot I) = 0$ for every Hamiltonian matrix H. For similar reasons the technique for detecting $1:1$ resonant double Hopf bifurcations of general systems of [7] does not work here either. Here we show how to construct a smooth test function from $H \odot I$ which seems to work in test examples, though it will not be proven that generically it will change sign at the Hamiltonian Hopf bifurcation points.

The usual definition of the bialternate product $A \odot B$ for $A, B \in \mathbb{R}^{n \times n}$ (see [8], [12]) is somewhat abstract[3]. Here we just mention that for a Hamiltonian matrix H, $2H \odot I$

[3] Let T be the linear operator in $\mathbb{R}^{n^2}$ which for vectors of the form $u \otimes v$ is given by $T(u \otimes v) = v \otimes u$, where $\otimes$ denotes the Kronecker product. Then T has eigenvalues ± 1. Let E_- be the $n(n-1)/2$ – dimensional subspace correspoding to -1. Then E_- is $A \otimes B + B \otimes A$–invariant and $A \odot B$ is defined to be half of this sum restricted to E_-, in a suitable basis.

is equivalent to ad_H – the linear map that takes an anti-Hamiltonian matrix F (i.e., $F^T = -JFJ$) to

$$\mathrm{ad}_H(F) = [H, F] = HF - FH$$

– another anti-Hamiltonian matrix. This is a linear operator in a $n(2n-1)$ –dimensional space. If $Hx = \lambda x$ and $Hy = \mu y$ then $x^T JH = -\lambda x^T J$, $y^T JH = -\mu y^T J$, $F = xy^T J - yx^T J$ is anti-Hamiltonian and

$$HF - FH = \lambda xy^T J - \mu yx^T J + \mu xy^T J - \lambda yx^T J = (\lambda + \mu) F .$$

Hence the eigenvalues of ad_H are of the form $\lambda_i + \lambda_j$, $1 \le i < j \le 2n$, where $\{\lambda_1, \ldots, \lambda_{2n}\} = \sigma(H)$.

By the symmetry of $\sigma(H)$ the kernel of ad_H is usually n-dimensional and, by lower semincontinuity of the rank, it stays at least n-dimensional at bifurcation points. If H has a double eigenvalue, then 0 is an eigenvalue with multiplicity $n+2$ and the kernel of ad_H^2 must have dimension at least $n+1$.

Consider the basis $F_{i,j} = J[e_i e_j^T - e_j e_i^T]$, $1 \le i < j \le 2n$, where the e_i's are the standard basis vectors of $\mathbb{R}^{2n}$. It is orthogonal with respect to the inner product $\langle F, G\rangle = \mathrm{tr}(F^T G)$. Let B_H be the matrix of ad_H in this basis. For $1 \le i < j \le 2n$, $1 \le k < l \le 2n$ we have

$$\begin{aligned}\big(B_H\big)_{(i,j),(k,l)} &= \tfrac{1}{2}\ \langle F_{i,j}, \mathrm{ad}_H(F_{k,l})\rangle \\ &= \tfrac{1}{2}\ \mathrm{tr}\,\big([e_j e_i^T - e_i e_j^T]J^T[HJ(e_k e_l^T - e_l e_k^T) - J(e_k e_l^T - e_l e_k^T)H]\big) \\ &= \delta_{i,l} H_{k,j} - \delta_{i,k} H_{l,j} + \delta_{j,k} H_{l,i} - \delta_{j,l} H_{k,i} .\end{aligned} \tag{3.3}$$

Clearly, the elements $\big(B_H\big)_{(i,i+n),(k,k+n)}$, $i, k \le n$, are zero if $i \ne k$, and for $i = k$ they are $-H_{k+n,k+n} - H_{k,k}$ which is also zero. Hence, ordering the basis such that the vectors $F_{1,1+n}, F_{2,2+n}, \ldots, F_{n,2n}$ come last, we get

$$B_H = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & 0_{n\times n}\end{bmatrix} .$$

From (3.3) we also obtain

$$\big((B_H)^T\big)_{(i,j),(k,l)} = \big(B_H\big)_{(k,l),(i,j)} = \delta_{k,j} H_{i,l} - \delta_{k,i} H_{j,l} + \delta_{l,i} H_{j,k} - \delta_{l,j} H_{i,k} .$$

In particular, $(B_H)^T = B_{H^T}$. Further, from

$$\mathrm{ad}_{H^T}(F) = JHJF - FJHJ = -J\big(H(JFJ^T) - (JFJ^T)H\big)J^T ,$$

we see that

$$(B_H)^T = -\widehat{P}\, B_H\, \widehat{P} \tag{3.4}$$

where $\widehat{P}$ is the matrix of the map $\widehat{J}(F) = JFJ^T$. It is easy to check that

$$\widehat{J}(F_{i,j}) = (e_i e_j^T - e_j e_i^T)J = \begin{cases} F_{i+n,j+n} & \text{for } i < j \le n , \\ F_{j-n,i+n} & \text{for } i \le n < j , \\ F_{i-n,j-n} & \text{for } n \le i < j .\end{cases}$$

Hence $\widehat{P} = \begin{bmatrix} P & \\ & I \end{bmatrix}$ is a permutation matrix, where $P^T = P = P^{-1}$ (since $\widehat{J}^2 = I$). So from (3.4) we get

$$\begin{bmatrix} B_{11}^T & B_{21}^T \\ B_{12}^T & 0 \end{bmatrix} = -\begin{bmatrix} P & \\ & I \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & 0 \end{bmatrix} \begin{bmatrix} P & \\ & I \end{bmatrix} = -\begin{bmatrix} PB_{11}P & PB_{12} \\ B_{21}P & 0 \end{bmatrix} . \tag{3.5}$$

At a bifurcation point $\dim(\ker(B_H^2)) \geq n+1$ so that $\operatorname{rank}(B_H^2) < n(2n-1)-n$. Hence

$$\det(B_{11}^2 + B_{12}B_{21}) = 0 . \tag{3.6}$$

If B_{11} is invertible, then (3.6) is equivalent to

$$\det(I_{n\times n} + B_{21}B_{11}^{-2}B_{12}) = 0 . \tag{3.7}$$

Further, if $X = B_{11}^{-1}B_{12}$, then (3.5) gives

$$B_{11}^{-T}B_{21}^T = (-PB_{11}P)^{-1}(-PB_{12}) = PB_{11}^{-1}B_{12} = PX .$$

Hence, at a bifurcation point, we have $\det(I + X^TPX) = 0$. This suggests

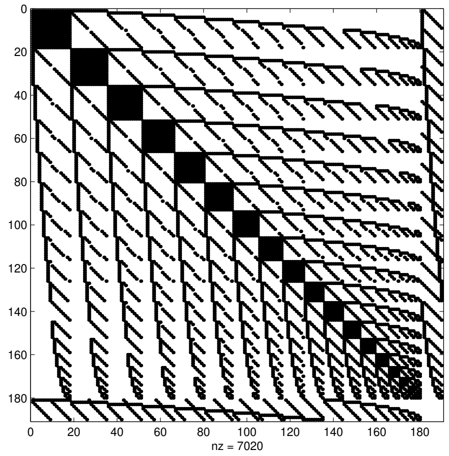
$$\zeta(H) = \det(I + X^TPX) \tag{3.8}$$

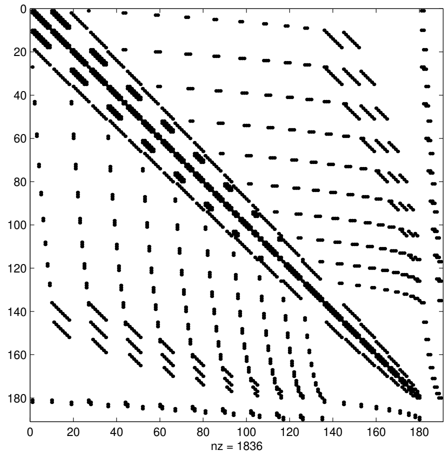
as another candidate for Hamiltonian Hopf detection. It works fine in simple test examples (see the next section). A theorem similar to Thm. 3.1, however, is still needed and this question requires further study. One can also use the bordering technique to obtain a modified version of ζ as in Section 2. Still another test function would be simply to use (3.6), i.e. $\zeta(H) = \det(B_{11}^2 + B_{12}B_{21})$. This, however, is a determinant of a much larger matrix and (rather limited) numerical experience has suggested (3.8) gives a better behaved function.

The use of (3.8) requires the solution of the system

$$B_{11}X = B_{12} . \tag{3.9}$$

Effectiveness of this approach depends on how economically (3.9) can be solved. This is a subject for a numerical linear algebra study to be made in the future. Especially we are interested in (iterative) approximate solution of (3.9) in cases where H is sparse and, consequently, B_H is very sparse. Below on the left the structure of B_H is shown in a case where H is full ($n = 10$) and on the right in a case where $H = \left[\begin{smallmatrix} A & B \\ C & -A^T \end{smallmatrix}\right]$ has A, B, C tridiagonal.





Remark 3.5. Here are two observations that may be useful in the numerical solution of (3.9). First, it is easy to show that $B_{12}\begin{bmatrix}1\\ \vdots\\ 1\end{bmatrix} = 0$. This reduces the right hand side of the equation. Second, it has been (numerically) observed that the singular values of B_{11} are all double. This suggests that some kind of use of the conjugate gradients for the normal equation

$$B_{11}^T B_{11} X = B_{11}^T B_{12}$$

may be effective even though this increases the condition number. This is because, then the conjugate gradient method works essentially in a space of half the dimension.

4. Example

Here we describe briefly how the test functions are used. Consider the Hamiltonian

$$h = \alpha x_3^2 + \beta(x_1x_4 - x_2x_3) + \gamma(x_1^2 + x_2^2) + \delta x_2 x_4^2 + \varepsilon(x_1 - x_2/2 + x_3/3 - x_4^2/2)\ .$$

Fix $\gamma = -0.03$, $\delta = 0.5$, $\varepsilon = -0.02$. Start from the point $\alpha = -0.2$, $\beta = 0.5$. Keeping β fixed let α increase and perform arclength continuation on system

$$h(x,\alpha) = 0$$

from the initial guess $x = 0$, $\alpha = -0.2$. This produces the horizontal line of dots. During this continuation the test functions $\eta(H)$ and $\zeta(H)$ of (2.3) and (3.8) are monitored. At the point "+" a sign change of ζ is observed. Similarly, keeping $\alpha = -0.2$ fixed and letting β decrease we find the vertical line of dots and a sign change of η at "∘".

Starting from the initial guess "+" (and the corresponding equilibrium) we can now find a curve of Hopf bifurcation points (the dashed curve) in the (x,α,β)–space by continuation with the system

$$\begin{cases} h(x,\alpha,\beta) = 0 \\ \zeta(H(x,\alpha,\beta)) = 0 \end{cases} .$$

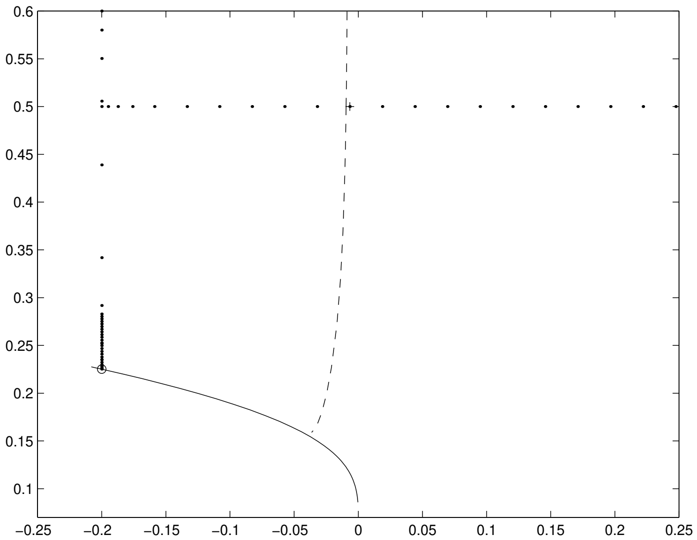
Similarly, starting from "∘" we can find a curve of fold points (the solid curve) by continuation with the system

$$\begin{cases} h(x,\alpha,\beta) = 0 \\ \eta(H(x,\alpha,\beta)) = 0 \end{cases} .$$

These two curves seem to meet at a point. (There, the step length for the continuation of the Hopf curve falls below the prescribed limit.) This is a bifurcation point of higher codimension. It can be found by solving the system

$$\begin{cases} h(x,\alpha,\beta) = 0 \\ \eta(H(x,\alpha,\beta)) = 0 \\ \zeta(H(x,\alpha,\beta)) = 0 \end{cases} .$$

There, zero is an eigenvalue with a four dimensional Jordan block.



5. Further questions

In addition to the theoretical question and numerical linear algebra issues that were left open in Sections 3.1 and 3.2, we outline here a couple of other interesting topics for further study.

Symmetry. Many Hamiltonian systems possess symmetries inherited from the physical origins of the model. It will be an interesting topic to study how the present test functions generically behave in the class of systems having a certain type of symmetry (see [6]) and further, what kind of modifications it requires or whether it simplifies the test functions.

Resonances. Another source of local bifurcations near equilibria is the possible occurence of resonances. This means there are purely imaginary eigenvalues $i\omega_1$, $i\omega_2$ such that $m_1\omega_1 = m_2\omega_2$ for some integers $m_1, m_2 \geq 1$. One possibility for detecting these comes from the characteristic polynomial approach of Section 3.1. Let p be the polynomial given by (3.1). Define $p_m(z) = p(m^2 z)$. Then the system has $m_1 : m_2$ resonance only if the resultant $\xi_{m_1,m_2} := \mathrm{res}(p_{m_1}, p_{m_2})$ vanishes.

References

[1] V. I. Arnold. *Mathematical methods of classical mechanics.* Springer-Verlag, New York, 1989.

[2] V. I. Arnold, S. M. Gusein-Zade, and A. N. Varchenko. *Singularities of differentiable maps I.* Birkhäuser, Boston, 1985.

[3] N. Bourbaki. *Elements of mathematics; Algebra II.* Springer–Verlag, Berlin, 1990.

[4] H. W. Broer, S.-N. Chow, Y. Kim, and G. Vegter. A normally elliptic Hamiltonian bifurcation. *Z. angew. Math. Phys*, 44:389–432, 1993.

[5] E. Doedel, X. Wang, and T. Fairgrieve. Auto94: Software for continuation and bifurcation problems in odes. *California Institute of Technology, Applied Mathematics Technical Report*, 1994.

[6] M. Golubitsky, I. Stewart, and J. Marsden. Generic bifurcation of Hamiltonian systems with symmetry. *Physica D*, 24:391–405, 1987.

[7] W. Govaerts, J. Guckenheimer, and A. Khibnik. Defining functions for multiple Hopf bifurcations. *SIAM J. Num. Anal.*, 34:1269–1288, 1997.

[8] J. Guckenheimer, M. Myers, and B. Sturmfels. Computing Hopf bifurcations I. *SIAM J. Numer. Anal*, 34:1–21, 1997.

[9] R. M. Hardt. Topological properties of subanalytic sets. *Trans. AMS*, 211:57–70, 1975.

[10] H. Keller. *Numerical Methods in Bifurcation Problems.* Springer Verlag, Bombay, 1987. Tata Institute of Fundamental Research.

[11] A. I. Khibnik, Yu. A. Kuznetsov, V. V. Levitin, and E. V. Nikolaev. Continuation techniques and interactive software for bifurcation analysis of ODEs and iterated maps. *Physica D*, 62:360–371, 1993.

[12] Y. A. Kuznetsov. *Elements of applied bifurcation theory.* Springer-Verlag, New York, 1995.

[13] C. Van Loan. A symplectic method for approximating all the eigenvalues of a Hamiltonian matrix. *Linear Alg. Appl.*, 61:233–251, 1984.

[14] J. E. Marsden. *Lectures on mechanics.* Cambridge Univ. Press, Cambridge, 1992.

[15] K. R. Meyer. Generic bifurcations in Hamiltonian systems. *Springer, LN in Math.*, 468:62–70, 1975.

[16] J. C. van der Meer. *The Hamiltonian Hopf bifurcation.* Springer-Verlag, New York, 1985. LN Math. 1160.

[17] V.A. Yakubovich and V.M. Starzhinskii. *Linear differential equations with periodic coefficients I.* John Wiley & Sons, New York, 1975.

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