Bifurcation Analysis of Large Equilibrium Systems in MATLAB

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Abstract. The Continuation of Invariant Subspaces (*CIS*) algorithm produces a smoothly varying basis for an invariant subspace $\mathcal{R}(s)$ of a parameter-dependent matrix $A(s)$. In the case when $A(s)$ is the Jacobian matrix for a system that comes from a spatial discretization of a partial differential equation, it will typically be large and sparse. CL_MATCONT is a user-friendly MATLAB package for the study of dynamical systems and their bifurcations. We incorporate the CIS algorithm into CL_MATCONT to extend its functionality to large scale bifurcation computations via subspace reduction.

1 Introduction

Parameter-dependent Jacobian matrices provide important information about dynamical systems

$$\frac{du}{dt} = f(u,\alpha), \text{ where } u \in \mathbb{R}^n, \ \alpha \in \mathbb{R}, \ f(u,\alpha) \in \mathbb{R}^n. \tag{1}$$

V.S. Sunderam et al. (Eds.): ICCS 2005, LNCS 3514, pp. 50–57, 2005.

For example, to analyze stability at branches $(u(s), \alpha(s))$ of steady states

$$f(u, \alpha) = 0, \tag{2}$$

we look at the linearization $f_u(u(s), \alpha(s))$. For general background on dynamical systems theory we refer to the existing literature, in particular [15]. If the system comes from a spatial discretization of a partial differential equation, then f_u will typically be large and sparse. In this case, an invariant subspace $\mathcal{R}(s)$ corresponding to a few eigenvalues near the imaginary axis provides information about stability and bifurcations. We are interested in continuation and bifurcation analysis of large stationary problems (2).

Numerical continuation for large nonlinear systems of this form is an active area of research, and the idea of subspace projection is common in many methods being developed. The continuation algorithms are typically based on Krylov subspaces, or on recursive projection methods which use a time integrator instead of a Jacobian multiplication as a black box to identify the low-dimensional invariant subspace where interesting dynamics take place; see e.g. [17, 5, 11, 4, 6], and references there.

CL_MATCONT [9] and its GUI version MATCONT [8] are MATLAB packages for the study of dynamical systems and their bifurcations for small and moderate size problems. The MATLAB platform is attractive because it makes them user-friendly, portable to all operating systems, and allows a standard handling of data files, graphical output, etc.

Recently, we developed the Continuation of Invariant Subspaces *(CIS) algorithm* for computing a smooth orthonormal basis for an invariant subspace $\mathcal{R}(s)$ of a parameter-dependent matrix $A(s)$ [7, 10, 12, 3]. The CIS algorithm uses projection methods to deal with large problems. See also [12] for similar results.

In this paper we consider integrating the CIS algorithm into CL_MATCONT. Standard bifurcation analysis algorithms, such as those used in CL_MATCONT, involve computing functions of $A(s)$. We adapt these methods to large problems by computing the same functions of a much smaller restriction $C(s) := A(s)|_{\mathcal{R}(s)}$ of $A(s)$ onto $\mathcal{R}(s)$. Note, that the CIS algorithm ensures that only eigenvalues of $C(s)$ can cross the imaginary axis, so that $C(s)$ provides all the relevant information about bifurcations. In addition, the continued subspace is adapted to track behavior relevant to bifurcations.

2 Bifurcations for Large Systems

Let $x(s) = (u(s), \alpha(s)) \in \mathbb{R}^n \times \mathbb{R}$ be a smooth local parameterization of a solution branch of the system (2). We write the Jacobian matrix along this path as $A(s) := f_u(x(s))$. A solution point $x(s_0)$ is a *bifurcation point* if $\operatorname{Re} \lambda_i(s_0) = 0$ for at least one eigenvalue $\lambda_i(s_0)$ of $A(s_0)$.

A *test function* $\phi(s) := \psi(x(s))$ is a (typically) smooth scalar function that has a regular zero at a bifurcation point. A bifurcation point between consecutive continuation points $x(s_k)$ and $x(s_{k+1})$ is *detected* when

$$\psi\left(x(s_k)\right) \psi\left(x(s_{k+1})\right) < 0. \tag{3}$$

Once a bifurcation point has been detected, it can be *located* by solving the system

$$\begin{cases} f(x) = 0, \\ g(x) = 0, \end{cases} \tag{4}$$

for an appropriate function g.

We consider here the case of a (generic codimension-1 bifurcation) *fold* or *limit point* (LP) and a *branch point* (BP), on a solution branch (2). For both detecting and locating these bifurcations, CL_MATCONT uses the following test functions (see e.g. [15], [13], [9]):

$$\psi_{BP}^{M}\left(x(s)\right) := \det \begin{bmatrix} A & f_\alpha \\ \dot{u}^{\mathrm{T}} & \dot{\alpha} \end{bmatrix}, \tag{5}$$

$$\psi_{LP}^{M}\left(x(s)\right) := \det\left(A(s)\right) = \prod_{i=1}^{n} \lambda_i\left(s\right), \tag{6}$$

where $\dot{x} := dx/ds$. The bifurcations are defined by:

$$\mathrm{BP} : \psi_{BP}^{M} = 0, \qquad \mathrm{LP} : \psi_{LP}^{M} = 0,\ \psi_{BP}^{M} \neq 0. \tag{7}$$

For some $m \ll n$, let

$$\Lambda_1(s) := \left\{\lambda_i(s)\right\}_{i=1}^{m}, \ \mathrm{Re}\,\lambda_m \leq \ldots \leq \mathrm{Re}\,\lambda_{m_u+1} < 0 \leq \mathrm{Re}\,\lambda_{m_u} \leq \ldots \leq \mathrm{Re}\,\lambda_1, \tag{8}$$

be a small set consisting of rightmost eigenvalues of $A(s)$ and let $Q_1(x(s)) \in \mathbb{R}^{n\times m}$ be an orthonormal basis for the invariant subspace $\mathcal{R}(s)$ corresponding to $\Lambda_1(s)$. Then an application of the CIS algorithm to $A(s)$ produces

$$C(x(s)) := Q_1^{\mathrm{T}}(x(s))A(s)Q_1(x(s)) \in \mathbb{R}^{m\times m}, \tag{9}$$

which is the restriction of $A(s)$ onto $\mathcal{R}(s)$. Moreover, the CIS algorithm ensures that the only eigenvalues of $A(s)$ that can cross the imaginary axis come from $\Lambda_1(s)$, and these are exactly the eigenvalues of $C(x(s))$. We use this result to construct new methods for detecting and locating bifurcations. Note, that $\Lambda_1(s)$ is computed automatically whenever $C(x(s))$ is computed.

2.1 Fold

Detecting Fold. We replace $\psi_{BP}^{M}\left(x(s)\right)$ and $\psi_{LP}^{M}\left(x(s)\right)$, respectively, by

$$\psi_{BP}\left(x(s)\right) := \mathrm{sign}\left(\det \begin{bmatrix} A & f_\alpha \\ \dot{u}^{\mathrm{T}} & \dot{\alpha} \end{bmatrix}\right), \tag{10}$$

$$\psi_{LP}\left(x(s)\right) := \prod_{i=1}^{m} \lambda_i\left(s\right). \tag{11}$$

Then LP is detected as:

$$\mathrm{LP} : \psi_{BP}\left(x(s_k)\right)\psi_{BP}\left(x(s_{k+1})\right) > 0 \text{ and } \psi_{LP}\left(x(s_k)\right)\psi_{LP}\left(x(s_{k+1})\right) < 0. \tag{12}$$

Locating Fold. Let $x_0 = x(s_0)$ be a fold point. Then $A(s_0)$ has rank $n-1$. To locate x_0, we use a *minimally augmented system* (see [13], [9]), with A replaced by C, whenever possible. The system consists of $n+1$ scalar equations for $n+1$ components $x = (u, \alpha) \in \mathbb{R}^n \times \mathbb{R}$,

$$\begin{cases} f(x) = 0, \\ g(x) = 0, \end{cases} \tag{13}$$

where $g = g(x)$ is computed as the last component of the solution vector $(v, g) \in \mathbb{R}^m \times \mathbb{R}$ to the $(m+1)$-dimensional *bordered system*:

$$\begin{bmatrix} C(x) & w_{bor} \\ v_{bor}^{\mathrm{T}} & 0 \end{bmatrix} \begin{bmatrix} v \\ g \end{bmatrix} = \begin{bmatrix} 0_{m\times 1} \\ 1 \end{bmatrix}, \tag{14}$$

where $v_{bor} \in \mathbb{R}^m$ is close to a nullvector of $C(x_0)$, and $w_{bor} \in \mathbb{R}^m$ is close to a nullvector of $C^{\mathrm{T}}(x_0)$ (which ensures that the matrix in (14) is nonsingular). For $g = 0$, system (14) implies $Cv = 0$, $v_{bor}^{\mathrm{T}} v = 1$. Thus (13) and (14) hold at $x = x_0$, which is a regular zero of (13).

The system (13) is solved by the Newton method, and its Jacobian matrix is:

$$J := \begin{bmatrix} f_x \\ g_x \end{bmatrix} = \begin{bmatrix} A & f_\alpha \\ g_u & g_\alpha \end{bmatrix} \in \mathbb{R}^{(n+1)\times(n+1)}, \tag{15}$$

where g_x is computed as

$$g_x = -w^{\mathrm{T}} C_x v, \tag{16}$$

with w obtained by solving

$$\begin{bmatrix} C^{\mathrm{T}}(x) & v_{bor} \\ w_{bor}^{\mathrm{T}} & 0 \end{bmatrix} \begin{bmatrix} w \\ g \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{17}$$

Here $C_x v$ is computed as

$$C_x(x)v \approx Q_1^{\mathrm{T}} \frac{f_x(u + \delta\frac{z}{\|z\|}, \alpha) - f_x(u - \delta\frac{z}{\|z\|}, \alpha)}{2\delta} \|z\|, \quad z := Q_1 v \in \mathbb{R}^n. \tag{18}$$

Finally we note that at each Newton step for solving (13), linear systems with the matrix (15) should be solved by the mixed block elimination (see [13] and references there), since the matrix (15) has the form

$$M := \begin{bmatrix} A & b \\ c^{\mathrm{T}} & d \end{bmatrix}, \tag{19}$$

where $A \in \mathbb{R}^{n\times n}$ is large and sparse, $b, c \in \mathbb{R}^n$, $d \in \mathbb{R}$, and A can be ill conditioned.

Once the fold point $x_0 = (u_0, \alpha_0)$ is computed, the corresponding quadratic normal form coefficient

$$a := \frac{1}{2}\widehat{w}^{\mathrm{T}} f_{uu}[\widehat{v}, \widehat{v}]$$

is computed approximately as

$$a \approx \frac{1}{2\delta^2}\widehat{w}^{\mathrm{T}}\left[f(u_0 + \delta\widehat{v}, \alpha_0) + f(u_0 - \delta\widehat{v}, \alpha_0)\right], \ \widehat{v} \approx \frac{Q_1 v}{\|Q_1 v\|}, \ \widehat{w} \approx \frac{Q_1 w}{\widehat{v}^{\mathrm{T}} Q_1 w}. \tag{20}$$

Fold Continuation. We use again the system (13) of $n+1$ scalar equations, but for $n+2$ components $x = (u, \alpha) \in \mathbb{R}^n \times \mathbb{R}^2$, in this case. Again g is obtained by solving (14), where g_x is computed using (16), (17), and (18).

There are four generic codimension-2 bifurcations on the fold curve: *Bogdanov-Takens (or double zero) point* (BT), *Zero - Hopf point* (ZH), *Cusp point* (CP), and a *branch point* (BP). These are detected and located by the corresponding modifications of CL_MATCONT test functions. For example, test function to detect ZH is

$$\psi_{ZH}(x(s)) := \prod_{m \geq i > j} \left(\mathrm{Re}\,\lambda_i(s) + \mathrm{Re}\,\lambda_j(s)\right). \tag{21}$$

2.2 Branch Points

Detecting Branching. The branch point is detected as:

$$\mathrm{BP} : \psi_{BP}(x(s_k))\,\psi_{BP}(x(s_{k+1})) < 0, \tag{22}$$

where ψ_{BP} is defined by (10).

Locating Branching. Let $x_0 = x(s_0)$ be a branch point such that $f_x^0 = f_x(x_0)$ has rank $n-1$ and

$$\mathcal{N}\left(f_x^0\right) = \mathrm{Span}\left\{v_1^0, v_2^0\right\}, \quad \mathcal{N}\left(\left(f_x^0\right)^{\mathrm{T}}\right) = \mathrm{Span}\left\{\psi^0\right\}.$$

We use a minimally augmented system ([14], [2], [1]) of $n+2$ scalar equations for $n+2$ components $(x, \mu) = (u, \alpha, \mu) \in \mathbb{R}^n \times \mathbb{R} \times \mathbb{R}$,

$$\begin{aligned} f(x) + \mu w_{bor} &= 0, \\ g_1(x) &= 0, \\ g_2(x) &= 0, \end{aligned} \tag{23}$$

where μ is an unfolding parameter, $w_{bor} \in \mathbb{R}^n$ is fixed, and $g_1 = g_1(x)$, $g_2 = g_2(x) \in \mathbb{R}$ are computed as the last row of the solution matrix $\begin{bmatrix} v_1 & v_2 \\ g_1 & g_2 \end{bmatrix}$, $v_1, v_2 \in \mathbb{R}^{n+1}$, to the $(n+2)$-dimensional bordered system:

$$\begin{bmatrix} f_x(x) & w_{bor} \\ V_{bor}^{\mathrm{T}} & 0_{2\times 1} \end{bmatrix} \begin{bmatrix} v_1 & v_2 \\ g_1 & g_2 \end{bmatrix} = \begin{bmatrix} 0_{n\times 2} \\ I_2 \end{bmatrix}, \quad V_{bor} = \begin{bmatrix} v_{1,bor} & v_{2,bor} \end{bmatrix}, \tag{24}$$

where $v_{1,bor}, v_{2,bor} \in \mathbb{R}^{n+1}$ are close to an orthonormal basis of $\mathcal{N}\left(f_x^0\right)$, and w_{bor} is close to the nullvector of $\left(f_x^0\right)^{\mathrm{T}}$.

The system (23) is solved by the Newton method [14] with the modifications in [2]. The Newton method is globalized by combining it with the bisection on the solution curve.

3 Examples

All computations are performed on a 3.2 GHz Pentium IV laptop.

Example 1. 1D Brusselator, a well known model system for autocatalytic chemical reactions with diffusion:

$$\begin{array}{ll} \frac{d_1}{l^2}u'' - (b+1)u + u^2v + a = 0, & \frac{d_2}{l^2}v'' + bu - u^2v = 0, \quad \text{in } \Omega = (0,1), \\ u(0) = u(1) = a, & v(0) = v(1) = \frac{b}{a}. \end{array} \tag{25}$$

This problem exhibits many interesting bifurcations and has been used in the literature as a standard model for bifurcation analysis (see e.g. [16]). We discretize the problem with a standard second-order finite difference approximation for the second derivatives at N mesh points. We write the resulting system, which has dimension $n = 2N$, in the form (2). This discretization of the Brusselator is used in a CL_MATCONT example [9]. In Figure 1 a bifurcation diagram in two parameters (l, b) is shown in the case $n = 2560$. We first continue an equilibrium branch with a continuation parameter l (15 steps, 13.5 secs) and locate LP at $l = 0.060640$. We next continue the LP branch in two parameters l, b (200 steps, 400.8 secs) and locate ZH at $(l, b) = (0.213055, 4.114737)$.

Example 2. Deformation of a 2D arch. We consider the snap-through of an elastic arch, shown in Figure 2. The arch is pinned at both ends, and the y displacement of the center of the arch is controlled as a continuation parameter.

Let $\Omega_0 \subset \mathbb{R}^2$ be the interior of the undeformed arch (Figure 2, top left), and let the boundary $\Gamma = \Gamma_D \cup \Gamma_N$, where Γ_D consists of the two points where the arch is pinned, and Γ_N is the remainder of the boundary, which is free. At equilibrium, material points $X \in \Omega_0$ in the deformed arch move to positions $x = X + u$. Except at the control point X_{center} in the center of the arch, this deformation satisfies the equilibrium force-balance equation [18]

$$\sum_{J=1}^{2} \frac{\partial S_{IJ}}{\partial X_J} = 0, \quad X \in \Omega_0, \quad I = 1, 2. \tag{26}$$

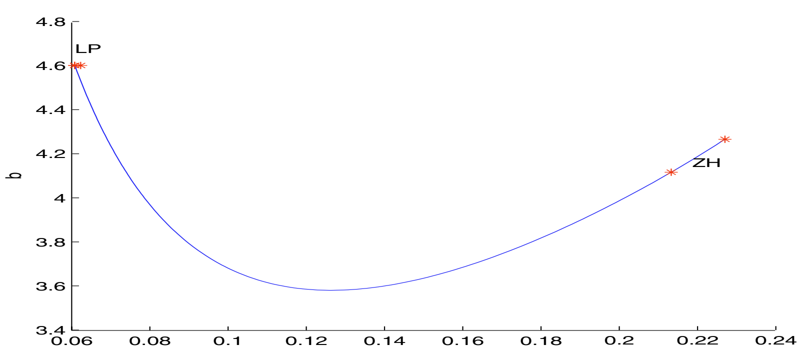

Fig. 1. Bifurcation diagram for a 1D Brusselator

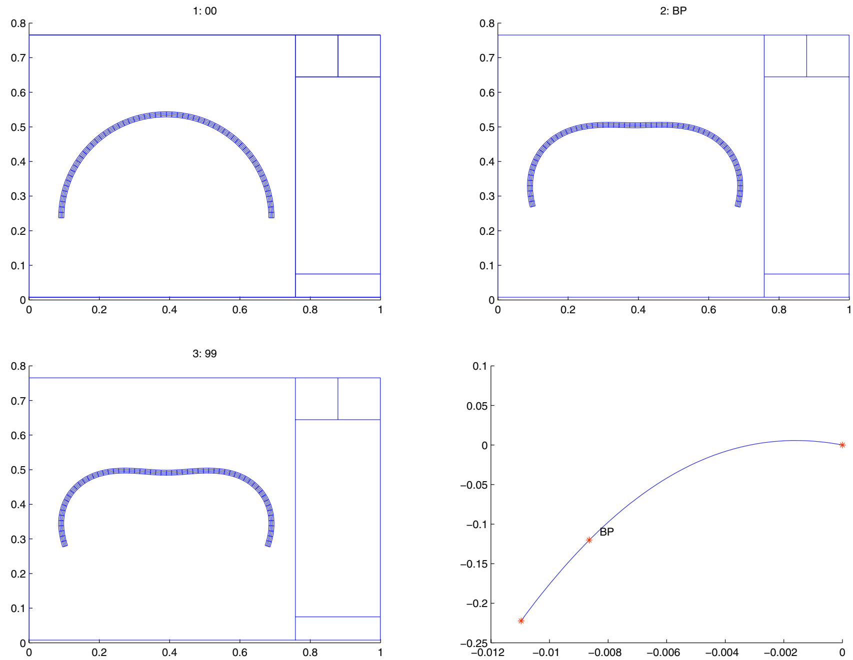

Fig. 2. Top left: the undeformed arch, top right: the arch at the bifurcation point, bottom left: the arch at the end of continuation, bottom right: the bifurcation diagram

where the second Piola-Kirchhoff stress tensor S is a nonlinear function of the Green strain tensor E, where $E := \frac{1}{2}(F^T F - I)$, $F := \frac{\partial u}{\partial X}$. Equation (26) is thus a fully nonlinear second order elliptic system. The boundary and the control point X_{center} are subject to the boundary conditions

$$u = 0 \text{ on } \Gamma_D, \qquad SN = 0 \text{ on } \Gamma_N, \text{ where } N \text{ is an outward unit normal,} \tag{27}$$

$$e_2 \cdot u = \alpha, \qquad e_1 \cdot (FSN) = 0. \tag{28}$$

The first condition at X_{center} says that the vertical displacement is determined; the second condition says that there is zero force in the horizontal direction.

We discretize (26) with biquadratic isoparametric Lagrangian finite elements. Let m be the number of elements through the arch thickness, and n be the number of elements along the length of the arch; then there are $(2m+1)(2n+1)$ nodes, each with two associated degrees of freedom. The Dirichlet boundary conditions are used to eliminate four unknowns, and one of the unknowns is used as a control parameter, so that the total number of unknowns is $N = 2(2m + 1)(2n + 1) - 5$. Figure 2 displays the results in the case when the continuation parameter is y displacement of node in middle of arch; $m = 4$, $n = 60$, $N = 2173$ unknowns; 80 steps took 258.4 secs, one BP was found.

Acknowledgment

Mark Friedman was supported in part under under NSF DMS-0209536.

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