# CL\_MATCONTL: a continuation toolbox for large equilibrium problems in MATLAB.

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#### Abstract

CL\_MATCONT and its GUI version MATCONT are MATLAB packages for the study of dynamical systems and their bifurcations for small and moderate size problems. CL\_MATCONTL is an extension of the functionality of CL\_MATCONT to large-scale computations of equilibria bifurcations, via subspace reduction. It allows to compute curves of equilibria, limit points, Hopf points, and Bogdanov-Takens points and supports branch switching. CL\_MATCONTL can also monitor user - defined functions and locate their roots along computed curves. It can compute all necessary derivatives by finite differences or from file.

In this tutorial we consider two examples. The first example is a finite difference discretization of the 1D Brusselator, a well known model system for autocatalytic chemical reactions with diffusion. The second example is a 1D transport model of a fusion plasma. Most of the capabilities of CL\_MATCONTL are illustrated.

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## 1 Introduction

## 1.1 Overview of Capabilities

Consider a parametrized dynamical system defined as a set of ODEs of the form

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

where  $\alpha$  denotes one or more free parameters. The aim of CL\_MATCONTL is to provide a continuation environment in MATLAB for branches of large stationary problems

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

which is compatible with the standard MATLAB ODE representation. A typical example comes from a spatial discretization of elliptic partial differential equations, in which case  $f_u$  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.

CL\_MATCONT [11] and its GUI version MATCONT [10] are MATLAB packages for the study of dynamical systems and their bifurcations for small and moderate size problems.

The CIS algorithm is an algorithm for computing a smooth orthonormal basis for an invariant subspace  $\mathcal{R}(s)$  of a parameter-dependent matrix A(s) [9, 12, 16, 3], [4], [5]. This allows for computation and continuation of a much smaller restriction  $C(s) := A(s)|_{\mathcal{R}(s)}$  of A(s) onto  $\mathcal{R}(s)$ . To study bifurcations of equilibria we apply the CIS algorithm to  $A(x(s)) = f_u(x(s))$  with  $\mathcal{R}(s)$  the subspace corresponding to the left most eigenvalues of A(x(s)).

We have incorporated the CIS algorithm into CL\_MATCONT to extend its functionality to large-scale computations of equilibria bifurcations, via subspace reduction, see [3], [6], [17], [5], [18], [20], for some initial results. This has resulted in a MATLAB bifurcation package CL\_MATCONTL [8]. The complete description of the algorithms and examples are given in [7]. This toolbox is developed with the following targets in mind:

- detection of singularities via test functions;
- singularity-specific location code;
- processing of regular and singular points;
- support of derivatives from file;
- support for sparse matrices.

The following actions are supported by the present version of CL\_MATCONTL:

- continuation of equilibria with respect to a control parameter;
- detection of fold, Hopf and branching points on curves of equilibria;

- computation of normal form coefficients for fold and Hopf equilibrium bifurcations;
- continuation of fold and Hopf equilibrium bifurcations in two control parameters:
- detection of all codim 2 equilibrium bifurcations (cusp, Bogdanov-Takens, generalized Hopf, zero-Hopf, and double Hopf) on fold and Hopf curves;
- computation of the critical normal form coefficients for codim 2 equilibrium bifurcations, which include multi-linear forms of order up to 5;
- continuation of Bogdanov-Takens bifurcations in three control parameters;
- detection of all codim 3 degeneracies along the Bogdanov-Takens curve (double and triple equilibrium, triple zero and Bogdanov-Takens/Hopf);
- computation of the critical normal form coefficients for the double and triple equilibrium (see [22]);
- branch switching at branch points of equilibria using 3 methods.

The following notation is used for singular points on curves CL\_MATCONTL:

- **H** a Hopf point on a curve of equilibria
- **BP** a branch point on a curve of equilibria
- LP a limit point on a curve of equilibria
- BT a Bogdanov-Takens point on a curve of limit points or Hopf points
- **ZH** a zero-Hopf point on a curve of limit points or Hopf points
- **CP** a cusp point on a curve of limit points
- **BP** a branch point on a curve of limit points
- DH a double-Hopf point on a curve of Hopf points
- **GH** a generalized Hopf, or Bautin point on a curve of Hopf points
- BTa2 a triple equilibrium degeneracy on a curve of Bogdanov-Takens bifurcations
- ${\bf BTb2}$  a double equilibrium degeneracy on a curve of Bogdanov-Takens bifurcations
- BT3 a triple zero degeneracy on a curve of Bogdanov-Takens bifurcations
- **BTH** a Bogdanov-Takens/Hopf degeneracy on a curve of Bogdanov-Takens bifurcations
- **00** the first point on the curve

#### **99** the last point on the curve

We assume that the reader is familiar with dynamical systems theory and knows about equilibria and codimension-1 and 2 bifurcations, see [19], [21]. We also assume an elementary knowledge of MATLAB but do not assume familiarity with numerical methods.

The continuation of the curve of Bogdanov-Takens bifurcations allows to detect codimension-3 degeneracies. These degeneracies provide additional insight in the dynamics on the center manifold of the system (1), see [2], [14], [22], [15], [13]. This can provide more insight in the arrangement of codimension-1 and 2 bifurcations nearby.

## 1.2 Installation and Initialization

The current version of the package is freely available for download at:

http://uah.edu/faculty/pekker

CL\_MATCONTL requires MATLAB 7.\* ?? to be installed on your computer. When using a 64-bit version of MATLAB, you should also make sure that you have a C-compiler installed.

Downloading and unzipping the CL\_MATCONTL package (for example in the MATLAB 'work' directory) creates a directory 'CL\_MATCONTL' on the computer. It contains init.m and ReadMe.txt files, as well as a number of subdirectories.

We start CL\_MATCONTL by changing to the 'CL\_MATCONTL' directory and typing 'init' on the MATLAB command line. The init.m file registers the directories with MATLAB and compiles any .mex files if necessary. If mex files have never been compiled on your machine, MATLAB may prompt you to select a compiler for .mex files. You must run init.m each time you open MATLAB when you wish to use CL\_MATCONTL.

## 1.3 User supplied Files.

The user must prepare the following two m-files.

The problem definition m-file (see Section 3.1) contains functions that define a particular problem, including the function f in equation (2), the symbolic Jacobian matrix, etc.

The run script (see Section 3.2) contains the initial parameters for the problem, the options to be used, and the code that executes continuation.

We advise to create for every problem a new folder in the /User/ directory.

## 2 Tutorials

## 2.1 The 1D Brusselator

The 1D Brusselator is a well known model system, intended to model the Belusov - Zhabotinsky reaction, for autocatalytic chemical reactions with diffusion:

$$\begin{array}{ll} \frac{d_1}{l^2}u'' - (b+1)u + u^2v + a = \dot{u}, & \frac{d_2}{l^2}v'' + bu - u^2v = \dot{v}, & \text{in } \Omega = (0,1), \\ u(0) = u(1) = a, & v(0) = v(1) = \frac{b}{a}. \end{array} \tag{3}$$

This problem exhibits a rich bifurcation scenario and has been used in the literature as a standard model for bifurcation analysis. We utilize the second order central difference discretization

$$f'' \approx \frac{1}{h^2}(f_{i-1} - 2f_i + f_{i+1}), \quad h = (N+1)^{-1},$$

with uniform grid of N grid points. Since there are two unknowns per grid point, the resulting discrete problem, which has dimension n=2N, can be written in the form (2). This discretization of the Brusselator is used in a CL\_MATCONT example [11]. To avoid spurious solutions (solutions that are induced by the discretization but do not actually correspond to solutions of the continuous problem), one can vary the parameter N. If the same solution is found for several discretizations, then we can assume that they correspond to solutions of the continuous problem. The Jacobian matrix is a sparse 5-band matrix. In the problem definition file Tutorial/bruss\_1d/bruss\_1d.m, the Jacobian matrix is introduced as a sparse matrix.

Except for Section 2.1.5, we we use an approximate nonconstant initial equilibrium solution:

$$\begin{cases} u(x) &= a + 2\sin(\pi x), \\ v(x) &= \frac{b}{a} - \frac{1}{2}\sin(\pi x). \end{cases}$$
 (4)

This solution (4) is not an equilibrium, but CL\_MATCONTL will find an equilibrium close to this initial solution. The initial values of the parameters are:  $a=1,\ b=17.1,\ d_1=0.0016,\ d_2=0.08,\ \text{and}\ l=0.06.$  In this demo we use N=500, hence the size of the system (2) is n=1000.

The files for this problem are located in /Tutorial/bruss\_1d. You should make this folder your 'current directory' in MATLAB for this tutorial. Also, make sure you have runned init.m before starting the tutorial (see Section 1.2).

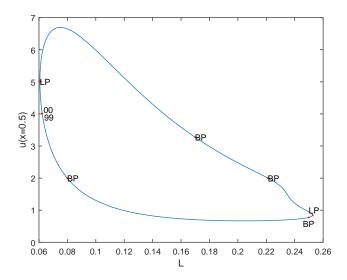


Figure 1: testbruss\_BPO, continuation of an equilibrium branch.

## 2.1.1 testbruss\_BP0: Continuation of an equilibrium

We perform continuation of the equilibrium solution curve with the parameter l free, by typing testbruss\_BPO in MATLAB command line. This produces the following output in the MATLAB command window:

```
>> testbruss_BP0
S ID PT:
                           ||u||
                                          ||f||
           +6.228439e-02
                           8.675355e+01
                                         7.934112e-10
 1 1 00:
       BP:
            +7.984536e-02
                           6.815405e+01
                                         2.548914e-08
                                         3.947069e-10
 62
    3
       BP:
            +2.499571e-01
                           7.523826e+01
 67
    4
       LP:
            +2.526672e-01
                           7.453336e+01
                                         7.217252e-10
85
    5
       BP:
            +2.211210e-01
                           6.815424e+01
                                         6.556548e-08
    6
       BP:
95
            +1.698320e-01 7.775931e+01
                                         2.000414e-08
    7
       LP:
            +6.063973e-02 9.901921e+01
                                         2.870064e-09
    8
            +6.228439e-02 8.675355e+01 7.934112e-10
       99:
Elapsed time = 9.1 secs
Number of Points = 167
```

The computed curve is also visualized by the graph in Figure 1, which is also created when running testbruss\_BPO. From these outputs we see that four branching points (BP) and two Limit Points (LP) are located along the curve. Also note that the continuation is stopped when the starting point is reached again at step 167.

Furthermore, /Data/ and /Logs/ directories have been created inside the /testbruss\_1d/ directory containing the data of the computed curves. See Section 3.2.4 for more information.

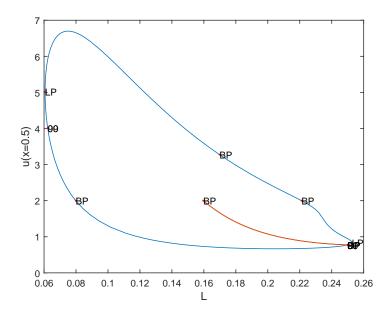


Figure 2: testbruss\_BPO and testbruss\_BP1, branch switching.

## 2.1.2 testbruss\_BP1: Branch switching

When a branch point is located, CL\_MATCONTL attempts to compute a tangent vector to the second branch. If successful, this tangent vector is saved in the .mat file. By using init\_BP\_EP\_L, this tangent vector is used to continue the second branch.

We restart at BP computed at Step 62 with ID=3 of the testbruss\_BP0 run from Section 2.1.1. We switch to the second branch, and perform its continuation by running the test file testbruss\_BP1. This produces the output:

```
>> testbruss_BP1
                                          ||f||
S ID PT: p(2)
                           ||u||
 1 1 00:
           +2.498387e-01 7.522087e+01
       BP:
            +1.596876e-01
                           6.815424e+01
                                         2.532307e-07
    3
                                         2.822453e-08
101
       BP:
            +2.499571e-01 7.523826e+01
    4
       99:
            +2.498387e-01
                           7.522087e+01
Elapsed time = 6.1 secs
Number of Points = 104
```

Note that the run stops at step 104 because the starting point is reached again. Also Figure 2 is produced by the combination of the testbruss\_BP0 and testbruss\_BP1 runs.

Remark 1. The tangent vector to the second branch can be obtained in one of three ways:

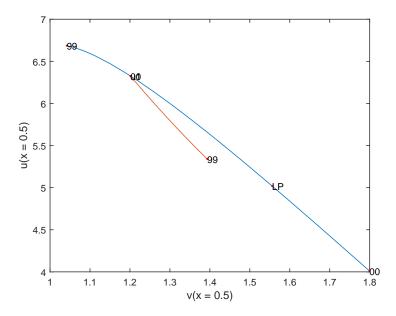


Figure 3: testbruss\_U0 and testbruss\_U1, restarting from a user point.

- 1. Calculating the normal form coefficients and then finding a tangent vector to the second branch by using the algebraic branching equation (ABE).
- 2. Finding an orthogonal vector to the tangent vector to the first branch, in the Null space of the Jacobian matrix at the branch point, and using it as an initial guess for a tangent vector to the second branch.
- 3. A bisection-like procedure, which is an improved version of 2.

testbruss\_BPO uses the third method.

## 2.1.3 testbruss\_U1: Restarting at a user point

A user point is defined by a user function in a problem definition m-file. Once a user point is located and saved, it can be used as the starting point for continuation of another curve. This is illustrated by the files testbruss\_U0 and testbruss\_U1.

We perform continuation of the equilibrium solution curve (u, l), where l is a free parameter, by typing testbruss\_U0 in the MATLAB command window. This produces the following output:

Here the located root of the user function is labeled u1. Running testbruss\_U0 produces the blue curve in Figure 3.

We start continuation from the user point in the parameter *a* by typing testbruss\_U1 in the MATLAB command window. This produces the following output:

```
>> testbruss_U1
S ID PT: p(3) ||u|| ||f||
1 1 00: +2.000000e+00 5.932165e+01 1.869982e-07
15 2 99: +2.069486e+00 5.223176e+01 1.542012e-07

Elapsed time = 0.4 secs
Number of Points = 15
```

The orange curve in Figure 3 is computed.

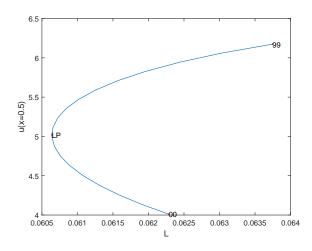


Figure 4: testbruss\_LPO, continuation of an equilibrium branch.

## 2.1.4 testbruss\_LP1: Continuation of limit points

Along the equilibrium curve computed from testbruss\_BP0 in Section 2.1.1, a Limit Point (LP) is located at Step 161 for l=0.060640. We reduce the number of steps needed to find this LP by changing by changing the continuation direction. This results in testbruss\_LP0.m. Running testbruss\_LP0.m produces the following output,

```
>> testbruss_LP0
S ID PT: p(2) ||u|| ||f||
1 1 00: +6.228439e-02 8.675355e+01 7.934112e-10
10 2 LP: +6.063973e-02 9.901921e+01 2.752822e-09
20 3 99: +6.374478e-02 1.147716e+02 3.237868e-07

Elapsed time = 1.1 secs
Number of Points = 20
```

See Figure 4 for the bifurcation diagram.

We restart at the LP computed at Step 13 with ID=2 of the testbruss\_LP0 run, and compute a curve of Limit Points in two free parameters (l, a). The continuation is performed by running testbruss\_LP1. This produces the output:

```
>> testbruss_LP1
S ID PT: p(2)
                          p(3)
                                          ||u||
                                                        ||f||
 1 1 00: +6.063973e-02
                          +2.000000e+00 9.901921e+01
                                                      2.075936e-10
 14
    2 CP: +1.102634e-01 +2.549658e+00
                                        6.982917e+01
                                                      1.259553e-07
105
      CP:
            +3.671906e-01
                          +1.581701e+00 9.729630e+01
                                                      5.947861e-08
    4 BT: +5.466570e-01 +1.045001e+00 1.499048e+02 6.896744e-12
143
           +6.172540e-01 +9.195194e-01 1.698827e+02 1.703222e-07
Elapsed time = 30.0 secs
Number of Points = 150
```

The resulting bifurcation diagram is shown in Figure 5. Along the computed curve two Cusp (CP) bifurcations and one Bogdanov-Takens (BT) bifurcation are located. The second CP bifurcation located at step 105 shows the characteristic 'wedge' shape in the two parameter plot, which can be seen in the detailed view in Figure 6.

Remark 2. This 'wedge' cannot be observed at the first CP bifurcation located at step 14. Inspection of the cubic coefficient in the Log-file testbruss\_LP1.txt shows that  $c = -5.723835 \cdot 10^{-4}$ . This indicates that the first CP bifurcation is (nearly) degenerate, which explains why the 'wedge' is not observed at this CP bifurcation.

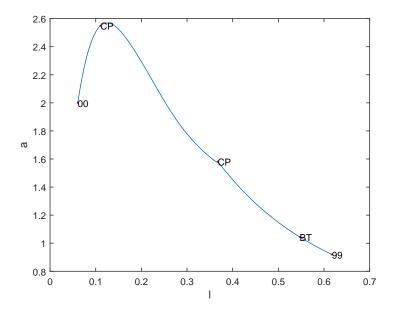


Figure 5:  $testbruss\_LP1$ , continuation Limit Points.

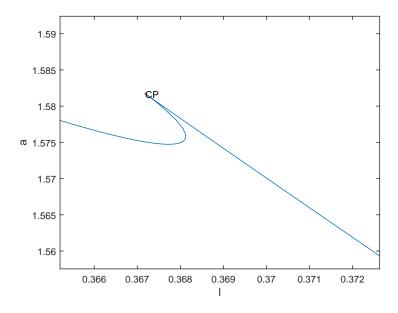


Figure 6: testbruss\_LP1, detailed view near the second CP point.

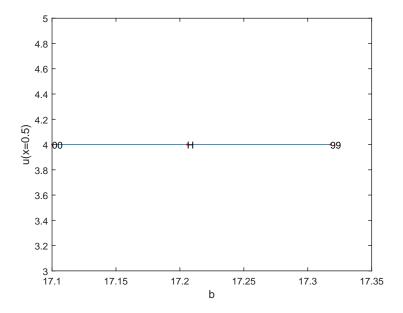


Figure 7: testbruss\_HPO, continuation of equilibria.

## 2.1.5 testbruss\_HP1: Continuation of Hopf points

In this section, we start from a constant equilibrium solution:

$$\begin{cases} u(x) = a, \\ v(x) = \frac{b}{a}. \end{cases}$$
 (5)

The initial values of the parameters are:  $a=4,\,b=17.1,\,d_1=1,\,d_2=2$  and, l=12.

We perform continuation of the equilibrium solution curve (u, b), where b is a free parameter, using testbruss\_HPO. This produces the following output:

```
>> testbruss_HP0
S ID PT: p(4)
                           ||u||
                                         ||f||
 1 1 00: +1.710000e+01
                          8.279568e+01
                                        0.000000e+00
 5
   2
       H :
           +1.720561e+01
                          8.306873e+01
                                        6.022000e-12
            +1.731773e+01
       99:
                          8.335945e+01
                                        9.000568e-11
Elapsed time = 0.7 secs
Number of Points = 10
```

A Hopf point H is located at Step 5 with ID=2. Also Figure 7 is produced.

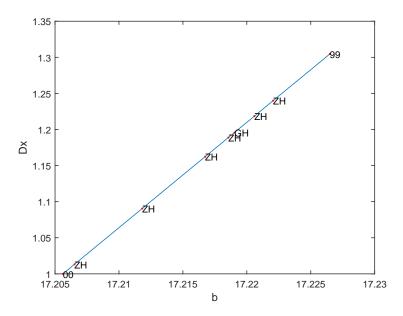


Figure 8: testbruss\_HP1, continuation of Hopf Points.

We then restart at H and compute a curve of Hopf points in two control parameters  $(b, d_1)$  using testbruss\_HP1. This produces the output:

```
>> testbruss_HP1
 S ID PT: p(4)
                            p(5)
                                            ||u||
                                                           ||f||
                            +1.000000e+00
    1
       00:
            +1.720561e+01
                                           8.306873e+01
                                                         1.445879e-07
        ZH:
            +1.720652e+01
                            +1.013273e+00
                                           8.307108e+01
                                                         1.445869e-07
 16
    3
        ZH:
            +1.721182e+01 +1.090524e+00 8.308479e+01
                                                         1.445912e-07
 28
    4
            +1.721674e+01 +1.162332e+00
        ZH:
                                          8.309754e+01
                                                         1.445913e-07
 37
    5
        ZH:
             +1.721856e+01
                            +1.188899e+00
                                           8.310225e+01
                                                         1.445921e-07
 49
    6
        GH:
                                                         1.445918e-07
             +1.721903e+01
                            +1.195760e+00
                                           8.310347e+01
             +1.722059e+01
        ZH:
                            +1.218499e+00
                                          8.310751e+01
                                                         1.445935e-07
 60
    8
       ZH:
            +1.722206e+01
                           +1.240007e+00 8.311133e+01
                                                         1.445590e-07
    9
        99:
            +1.722648e+01
                            +1.304493e+00 8.312278e+01
                                                         1.445570e-07
Elapsed time = 10.4 secs
```

Number of Points = 70

Along the curve six Zero-Hopf (ZH) bifurcations and one Generalized Hopf (GH) or Bautin bifurcation are located. The curve is shown in Figure 8.

Remark 3. Inspection of Log-file shows that there are six eigenvalues with positive real part at the starting point. At each ZH bifurcation one of these eigenvalues moves through the imaginary axis. At the endpoint there are no eigenvalues with positive real part.

#### 2.2A 1D transport model of a fusion plasma

In this section, we consider a finite difference discretization of a one dimensional transport model of a fusion plasma in TOKAMAK reactor. The model was originally proposed in [26]. The transport model consists of three coupled PDEs describing the particle density n, the plasma temperature T and the radial electric field or poloidal rotation Z:

$$\frac{\partial n}{\partial t} = -\frac{\partial \Gamma}{\partial x} \qquad \Gamma = -D(Z) \frac{\partial n}{\partial x}, \tag{6}$$

$$\frac{\partial n}{\partial t} = -\frac{\partial \Gamma}{\partial x} \qquad \Gamma = -D(Z) \frac{\partial n}{\partial x}, \qquad (6)$$

$$\frac{\partial U}{\partial t} = -\frac{\partial q}{\partial x} \qquad q = -\chi(Z) n \frac{\partial T}{\partial x} + \frac{\Gamma T}{\gamma - 1}, \qquad (7)$$

$$\varepsilon \frac{\partial Z}{\partial t} = \mu \frac{\partial^2 Z}{\partial x^2} + c_n \frac{T}{n^2} \frac{\partial n}{\partial x} + \frac{c_T}{n} \frac{\partial T}{\partial x} + G(Z), \tag{8}$$

where

$$D(Z) = D_0 + D_1 \tanh(Z), \tag{9}$$

$$\chi(Z) = \frac{1}{(\gamma - 1)\zeta} D(Z), \tag{10}$$

$$G(Z) = a - b(Z - Z_S) - (Z - Z_S)^3.$$
(11)

The internal energy U is related to temperature T and density n by

$$U := \frac{nT}{\gamma - 1}.\tag{12}$$

The following boundary conditions are used for the problem

$$\Gamma|_{x=\infty} = \Gamma_{\infty}, \qquad q|_{x=\infty} = q_{\infty}, \qquad \frac{\partial Z}{\partial x}|_{x=\infty} = 0, \qquad (13)$$

$$\left. \frac{\partial n}{\partial x} \right|_{x=0} = \frac{n}{\lambda_n}, \qquad \left. \frac{\partial T}{\partial x} \right|_{x=0} = \frac{T}{\lambda_T}, \qquad \left. \frac{\partial^2 Z}{\partial x^2} \right|_{x=0} = 0.$$
 (14)

We use a 3-point finite difference discretization on the nonuniform grid

$$\Theta := \{ 0 = x_0 < x_1 < x_2, \dots, < x_N = L \}, \qquad x_i = L (i/N)^3.$$
 (15)

The finite difference formulas can be found in (for example) [19]. This leads to a system of n = 3(N-1) ODEs, which are specified in the fun\_eval function in the file Tutorial/fusion/fusion.m.

The parameter values at the starting point are  $\Gamma_{\infty} = -0.8$ ,  $q_{\infty} = -0.008$ ,  $D_0=1.9,\ D_1=-1.1,\ a=-0.01,\ b=-0.01,\ \zeta=1.1,\ \mu=0.05,\ \varepsilon=0.05,\ Z_S=0,\ \gamma=5/3,\ \lambda_n=1.25,\ \lambda_T=1.5,\ c_n=1.1,\ {\rm and}\ c_T=0.9.$  In this tutorial, we use N = 50 so the size of the system is n = 147.

## 2.2.1 testfusion\_BT2: Continuation of Bogdanov-Takens points

The dynamics of this model have been studied in [24], [23], and [25]. These studies suggested the presence of a degenerate Bogdanov-Takens in the model. In this tutorial we will locate a degenerate Bogdanov-Takens bifurcation in this model by continuation of Bogdanov-Takens bifurcations.

The files for this problem are located in the Tutorial/fusion directory. Make this your 'current directory' in MATLAB. Also make sure that init.m has been runned before starting the tutorial (see Section 1.2).

To find a starting point on the Bogdanov-Takens curve, we first locate a Limit Point and continue this Limit Point to find a Bogdanov-Takens bifurcation. Alternatively, a starting poin could be found by continuation of a Hopf point.

We find the Limit Point by running testfusionBTO. This produces the following output

Note that the located Hopf and Limit Point are close, which is natural near a Bogdanov-Takens bifurcation. Also the graph in Figure 9 is created.

Remark 4. Observe that the handle jacobian in the problem definition file Tutorial/fusion/fusion.m is empty for this problem, so that the jacobian is computed using finite differences. For this problem, this part is most time consuming. In this example we used the MATLAB's Parallel Computing Toolbox to speed up the computation. The use of the Parallel Computing Toolbox can be enables using the option cont\_ParallelComputing, see Section 3.2.5.

To find the Bogdanov-Takens we continue the located Limit Point by running testfusionBT1. This produces the following output:

```
>> testfusion_BT1
S ID PT: p(3) p(8) ||u|| ||f||
1 1 00: -7.413592e-03 -1.000000e-02 1.272351e+01 3.735505e-09
8 2 BT: -4.549683e-03 -5.056140e-02 1.273870e+01 4.061119e-09
10 3 99: -2.993005e-03 -6.474749e-02 1.271994e+01 2.161779e-08

Elapsed time = 155.2 secs
Number of Points = 10
```

Also the graph in Figure 10 is created.

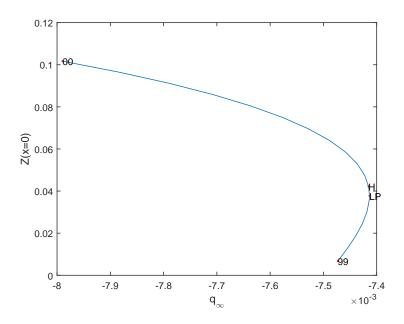


Figure 9:  ${\tt testfusion\_BTO}$ , continuation of equilibria.

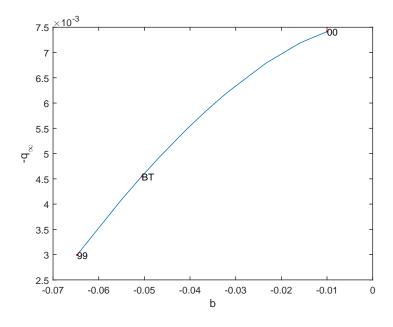


Figure 10: testfusion\_BT1, continuation of Limit Points.

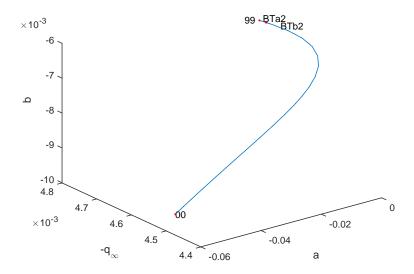


Figure 11: testfusion\_BT2, continuation of Bogdanov-Takens Points.

Now the located Bogdanov-Takens bifurcation is continued in three parameters by running testfusionBT2. This produces the following output:

Also the graph in Figure 11 is created. Observe that the BTa2 and BTb2 bifurcation are very close to each other.

Remark 5. The fact that the BTa2 and BTb2 are very close to eachother seems to indicate that we are in fact close to the (codimension-4) situation where both normal form coefficients  $a_2$  and  $b_2$  vanish simultaneously. The appearance of this codimension-4 situation is nongeneric in a 3-parameter continuation and the reason for its appearance is not completely understood.

## 3 User supplied files

## 3.1 Problem definition m-file

The problem definition m-file describes the particular problem (1). The main function of the problem definition file returns a list of function handles that point to the remaining functions in the file. The main function should have the following structure:

```
function out = PROBDEF
out{1} = @init;
out{2} = @fun_eval
out{3} = @jacobian
out{4} = @jacobian
out{5} = @usernorm
out{6} = @user1
out{7} = @user2
...
```

The handle <code>@fun\_eval</code> is mandatory. All other handles are optional and can be left empty. As an example, consider <code>Tutorial/bruss\_1d/bruss\_1d.m</code>.

The individual functions are described below. Each function has a specific input and output syntax that must be followed for CL\_MATCONTL to be able to use the functions.

## 3.1.1 init (Optional)

```
y0 = init(p_1, ..., p_n)
```

init is the first function handle defined in the primary function. It takes the full list of parameters that are being used for the problem and returns the vector y0, which must be (a good approximation of) an equilbrium solution at the given parameter values.

#### 3.1.2 fun\_eval

```
dxdt = fun_eval(t, x, p_1, ..., p_n)
```

The function fun\_eval takes a scalar t (which should not be used in the problem), the state vector  $\mathbf{x}$ , and the full parameter list used for the problem. It returns the vector  $\mathbf{dxdt}$ . This notation is used to reflect the nature of the non-linear problem  $\dot{x} = f(t, x, p_1, ..., p_n)$ .

The function fun\_eval must be the second function handle returned by the primary function and cannot be left empty.

## 3.1.3 jacobian (Optional)

```
dfdx = jacobian(t, x, p_1, ..., p_n)
```

The jacobian function takes the same inputs as fun\_eval. It returns the Jacobian matrix  $f_u(t, x, p_1, ..., p_n)$ .

If the jacobian function is not defined or not being used, the third function handle returned by the primary function must be empty. When this is the case,  $f_n(t, x, p_1, ..., p_n)$  is computed using finite differences.

## 3.1.4 jacobianp (Optional)

```
dfdp = jacobianp(t, x, p_1, ..., p_n)
```

The jacobian function takes the same inputs as fun\_eval. It returns the Jacobian matrix  $f_p(t, x, p_1, ..., p_n)$ .

If the jacobianp function is not used, the fourth function handle returned by the primary function must be empty. When this is the case,  $f_p(t, x, p_1, ..., p_n)$  is computed using finite differences.

## 3.1.5 Usernorm (Optional)

```
normuser = usernorm(arg)
```

The usernorm function takes a vector arg and returns a real number. The function has all the properties of a norm. usernorm can be used to approximate function norms for ODE and PDE problems.

If the usernorm function is not defined or not being used, the fifth function handle returned by the primary function must be empty. In this case the standard Euclidean norm is used.

## 3.1.6 User Functions (Optional)

```
uf1 = user1(t, x, p_1, ..., p_n)
```

All remaining function handles are assumed to be User Functions. User functions should take the same inputs as fun\_eval and return a real number. Roots of (active) user functions will be located by CL\_MATCONTL.

For every specified userfunction, there must be an element in the cell array UserInfo, containing the following fields

```
UserInfo{i}.name
UserInfo{i}.state
UserInfo{i}.label
```

See Section 3.2.5 for a more detailed discussion of the meaning of the different fields. The structure UserInfo must be set by

```
opt = contset(opt, 'Cont_UserFuncInfo', UserInfo);
```

This allows CL\_MATCONTL to identify and label the user points. An example can be found in Tutorial/bruss\_1d/testbruss\_U0.

## 3.2 Run script

Test run script files contain all of the information required to compute a curve in CL\_MATCONTL. A run script typically consists of the following parts:

**Options** An option structure is created that containing the options that are used during the continuation of the curve using contset.

**Initialization** A starting point and possible tangent vector are found by a call to init\_\*\*\_\*\*\*\_L.

Continuation The curve is computed by a call to contL.

**Processing results** After continuation, the data of the computed curve can be accessed using loadPoint.m.

This structure resembles the structure used in CL\_MATCONT [11]. Below the different parts will be elaborated.

#### 3.2.1 Options

Before specifying options for the specific curve, a new options structure options must be created by a call to

```
options = contset();
```

After that, options can then be set using

```
options = contset(options, optionname, optionvalue);
```

where optionname must be a name of an option supported by CL\_MATCONTL, which is set to the value specified by optionvalue. A list of all options supported by CL\_MATCONTL and their default values can be found in Section 3.2.5.

#### 3.2.2 Initialization

Depending on the curve that will be computed and the available initial point, different initialization functions must be used. Currently, the following initialization functions are available.

```
[x0, v0] = init_EP_EP_L(PROBDEF, u, p, ap)
```

init\_EP\_EP\_L initializes the continuation of a curve of equilibria, starting from the initial equilibrium u at the parameters p. PROBDEF is a handle to the problem definition file, described in Section 3.1. ap is the index of the parameter that is free during the continuation.

When u is empty, the initial point at the parameters p is found by a call to the function init in the problem definition file (see Section 3.1). All other

arguments must be present and cannot be empty. An example of the use of init\_EP\_EP\_L can be found in Tutorial/bruss\_1d/testbruss\_BPO.

init\_EP\_EP\_L can also be used to start continuation from a previously located user point. See Tutorial/bruss\_1d1/testbruss\_U1 for an example.

init\_BP\_EP\_L is used for branch switching at a previously located branching point. Currently, branch switching is only supported when the second tangent vector was found during location of the branching point. data is the data structure that can be found in the structure s from the previously computed equilibrium curve. The active parameter ap must be the same as on the previously computed curve.

PROBDEF and data must always be present. It is recommended to have u, p and ap empty. In this case they are obtained from the data structure and the same as on the previously computed curve. An example of the use of init\_BP\_EP\_L can be found in Tutorial/bruss\_1d/testbruss\_BP1.

init\_LP\_LP\_L initializes the continuation of a curve of Limit Points, either from a Limit Point located on a previously computed equilibrium curve or, from a point on a previously computed Limit Point curve or, from a previously located Bogdanov-Takens point. ap must be a vector of length 2.

When data is present, u, p and ap can be left empty. In this case they are obtained from the data structure and the same as on the previously computed curve. When data is absent, u, p and ap must be present. PROBDEF must always be present. An example of the use of init\_LP\_LP\_L can be found in Tutorial/bruss\_1d/testbruss\_LP1.

init\_H\_H\_L initializes the continuation of a curve of Hopf Points, either from a Hopf located on a previously computed equilibrium curve or, from a point on a previously computed Hopf curve. ap must be vector of length 2.

PROBDEF and data must always be present. u, p and ap can be empty. In this case they are obtained from the data structure and the same as on the previously computed curve. An example of the use of init\_H\_H\_L can be found in Tutorial/bruss\_1d/testbruss\_HP1.

init\_BT\_BT\_L initializes the continuation of a curve of Bogdanov-Takens Points, either from a Bogdanov-Takens point located on a previously computed Limit Point or Hopf curve or a point on a previously computed Bogdanov-Takens curve. ap must be vector of length 3.

When data is present, u, p and ap can be left empty. In this case they are obtained from the data structure and are the same as on the previously

computed curve. When data is not present, u, p and ap cannot be empty. PROBDEF must always be present. An example of the use of init\_BT\_BT\_L can be found in Tutorial/fusion/testfusion\_BT2.

## 3.2.3 contL

```
[s, filename] = contL(CURVEDEF, x0, v0, options);
```

contL continues the curve specified by CURVEDEF. Currently, the following four curves are available in CL\_MATCONTL:

@equilibriumL, curve of equilibria.

@limitpointL, curve of Limit Point bifurcations.

OhopfL, curve of Hopf bifurcations.

ObogdanovtakensL, curve of Bogdanov-Takens bifurcations.

x0 and v0 should be obtained from the properly chosen initialization function, see Section 3.2.2.

options is the options structure discussed in Section 3.2.1.

The function contL returns the signgularity sturcture s and name of the data file filename where the data for that run is stored.

Calling contL also creates a /Data/ folder in the directory TestPath This folder contains the data from the continuation in a .dat and .mat file, named Filename. Also a /Logs/ folder is created in the TestPath directory. This folder contains the log-file. Testpath and Filename can be set using the options structure, see Section 3.2.5. The .dat and .mat file will be discussed in the next section.

#### 3.2.4 Processing results

The data from the computed curve can be loaded from the .dat file in /Data/ folder using

```
[x, v, h, t, u] = loadPoint(filename)
```

Here filename is the name of the .dat from which the data is obtained.

The columns of x contain the state vector and the active parameters at the different points along the curve. The columns of v contain the tangent vectors at the different points along the curve. The vector h provides information about the stepsize. When singularities are located, the columns of t contain the values of the test functions. When userfunctions are active, the columns of u contain the values of the user functions.

The structure **s** contains information about the singular and user points that are located along the curve. **s** is stored in the .mat file and can be loaded using the standard MATLAB-function load. The elements of **s** are structures with the following fields:

- s(i).index the index of the singular point in the .dat file.
- s(i).label the standard CL\_MATCONTL label for the located singularity, see Section 1.1.
- s(i).msg a string describing the singularity
- s(i).data a structure with more information about the singular point. The data structure always contains the fields
  - data.x contains the the state vector and values of the active parameters at the singular point.
  - data.v contains the tangent vector at the singular point
  - data.P0 the value of the parameter vector p at the singular point
  - data.ap indices of the active parameters.

Further, data can contain information about the testfunctions, userfunctions, eigenvalues, normal form coefficients, and the matrices used in the CIS algorithm. Whether this information is available depends on the options used during continuation and the type of singularity that is located.

## 3.2.5 List of options

Here we give a list of the options supported by CL\_MATCONTL. These options should be set using contset, see Section 3.2.1.

- Cont\_LogFile Boolean indicating whether a log file is generated in the /Logs/directory (default: 0)
- Cont\_DiagnosticsLevel Diagnostic level changes the amount of information written to screen and logfile. There are the following possible values
  - -inf: Suppress all output
  - **0: Standard Output** Information about singularities and general information about the curve will be displayed. Level 0 information is always output to the screen when using a log-file.
  - 1: Additional Information Test functions values, step size.
  - **2:** Advanced information Additional information about the convergence of the location of singularities.
  - **3:** Maximal information The dimension of the invariant subspace and unstable subspace (CIS). Eigenvalues near zero.
  - **4: Developer information** Custom messages for development of new code. (Not intended for users)
  - **5: Debugging Information** function markers and other debugging information. (Not intended for users)

( default: 0).

- **Cont\_Direction** Boolean indicating the direction of the continuation (sign of the initial tangent vector)  $v_0$  (default: 0)
- Cont\_InitStepsize The initial stepsize (default: 0.01)
- Cont\_MaxStepsize The maximum stepsize (default: 0.1)
- Cont\_MinStepsize The minimum stepsize (default:  $10^{-5}$ )
- Cont\_SmoothingAngle Maximum allowed angle between tangent vectors at adjacent points (default:  $\frac{\pi}{50}$ ))
- Cont\_Stepsize\_Inc\_fac Factor with which the stepsize is increased after a new point on the curve has been found (default: 1.3)
- Cont\_Stepsize\_Dec\_fac Factor with which the stepsize is decreased when failing to find a new point on the curve (default: 0.5)
- Cont\_MaxNumPoints Maximum number of points on the curve (default: 300)
- **Cont\_CheckClosed** Number of points indicating when to start to check if the curve is closed (0 = do not check) (default: 50)
- Cont\_AdaptSteps Number of points indicating when to adapt the problem while computing the curve (default: 3)
- Cont\_MaxCorrIters Maximum number of correction iterations (default: 10)
- Cont\_MaxNewtonIters Maximum number of Newton-Raphson iterations before switching to Newton-Chords in the corrector iterations (default: 3)
- **Cont\_FunTolerance** Tolerance of function values:  $||F(x)|| \le \text{FunTolerance}$  is the first convergence criterion of the Newton iteration (default:  $10^{-6}$ )
- Cont\_VarTolerance Tolerance of coordinates:  $||\delta x|| \leq \text{VarTolerance}$  is the second convergence criterion of the Newton iteration (default:  $10^{-6}$ )
- **Cont\_Solver** Name of the solver to be used during Newton iteration (default: "Moore-Penrose")
- **Cont\_Eigenvalues** Boolean indicating the computation of the eigenvalues (default: 0)
- **Cont\_IncrFinDiff** The increment to compute the derivatives numerically (default:  $10^{-5}$ )
- Cont\_ParallelComputing Boolean indicating whether the parallel computing toolbox should be used in the computation of the derivatives by finite differences. (default: 0)

- Cont\_Singularities Boolean indicating whether singularities should be detected and located along the curve (default: 0)
- **Cont\_Userfunctions** Boolean indicating whether roots of userfunctions are located (default: 0)
- **Cont\_UserFuncInfo** A cell array with information about the userfunctions. For every user function specified in the Problem definition file, the array must have an element with the following fields:
  - .label short (typically 2 character) label of the userfunction
  - .name name of this particular userfunction
  - .state boolean indicating whether the userfunction is active
- **Loc\_IgnoreSings** vector containing indices of singularities which are to be ignored (default: empty)
- **Loc\_Testf\_MaxIters** Maximum number of iterations to locate a zero of a test-function by bisection (default: 10)
- **Loc\_Testf\_FunTolerance** Tolerance of test functions during bisection to locate a zero of a testfunction (default:  $10^{-5}$ )
- **Loc\_Testf\_VarTolerance** Tolerance for variables during bisection to locate a zero of a testfunction (default:  $10^{-4}$ )
- Loc\_UseLocators Boolean vector indicating whether a Newton based locator should be used (when available) to locate the singularity. (default: empty)
- **Locator\_MaxIters** Maximum number of iterations to locate a singularity by Newton based method (default: 5)
- **Locator\_FunTolerance** Tolerance for function values in the Newton based method used to locate a singularity (default:  $10^{-5}$ )
- **Locator\_VarTolerance** Tolerance for variables in Newton based method used to locate singularity (default:  $10^{-4}$ )
- Loc\_Userf\_MaxIters Maximum number of iterations to locate a zero of a userfunction by bisection (default: 10)
- **Loc\_Userf\_FunTolerance** Tolerance of user functions during bisection to locate a zero of a userfunction (default:  $10^{-5}$ )
- **Loc\_Userf\_VarTolerance** Tolerance for variables during bisection to locate a zero of a userfunction (default:  $10^{-4}$ )
- **EQ\_BranchingMethod** Method used for branch switching with the following possible values (see also Section 2.1.2)
  - 0 Normal Form Method
  - 1 Perpendicular Guess

- 2 Bisection
- (default: 0)
- **EQ\_SingLinSystTol** Tolerance for singular linear system in equilibrium locators (default: 0.1)
- **CIS\_usingCIS** Boolean indicating whether the CIS algorithm is used (default: 1)
- CIS\_AdaptOnOverlap Boolean indicating whether the subspace is adapted on overlap (default: 1)
- ${f CIS\_SparseSolvers}$  Boolean indicating whether sparse solvers are used (default: 0)
- CIS\_InitNUnstable Number of initial unstable eigenvalues. A negative number forces contCIS to compute the number of unstable eigenvalues. (default: -1)
- CIS\_NUnstableGuess Initial guess for the number of unstable eigenvalues. (default: 15)
- CIS\_MaxUnstable Maximum number of the unstable eigenvalues. (default: 40)
- CIS\_InitSubSize Initial Subspace Size (default: 4)
- CIS\_NStableRef The number of stable Reference Eigenvalues for CIS (default: 4)
- CIS\_NExtra The number of extra eigenvalues that are computed to detect overlap. (default: 4)
- **RIC\_Euler** Boolean indicating whether Euler predictor in Ricatti solvers is used (default: 1)
- RIC\_MaxNewtonIters Maximum number of Newton steps in Ricatti solvers (default: 10)
- **RIC\_FunTolerance** Newton residual convergence tolerance in Ricatti solvers (default: 1e-5)
- **RIC\_VarTolerance** Newton step convergence tolerance in Ricatti solvers (default: 1e-5)
- RIC\_Transform Ricatti solver transformation ('none'/'invert'/'cayley') (default: 'none')
- RIC\_Cayley\_Shift Cayley transform shift parameter in Ricatti solvers (default: 1)

- RIC\_Select Method used to select subspace in Ricatti solvers (default: 'ric')
- RIC\_Partial\_Q Keep only Q1 even in dense case in ricatti solvers (default: 0)
- RIC\_schur\_blsz Block size used in the computation of Schur decompsition using the augmented block Householder Arnoldi algorithm (see [1]) (default: 3)
- RIC\_schur\_nbls Number of blocks used in the computation of Schur decompsition using the augmented block Householder Arnoldi algorithm (see [1]) (default: 0)
- RIC\_schur\_maxit Maximum number of iterations for the computation of Schur decompsition using the augmented block Householder Arnoldi algorithm (see [1]) (default: 0)
- **RIC\_schur\_tol** Tolerance used in the computation of Schur decompsition using the augmented block Householder Arnoldi algorithm (see [1]). (default:  $1 \cdot 10^{-6}$ )
- TestPath The full path to the test run file. This is the directory in which the /Logs/ and /Data/ directories are created.

  (default: mfilename('fullpath'))
- **Filename** Name of the data, logs and singularities files in which continuation data of the computed curve is saved. When empty the name of the run script is used (with a time stamp to avoid overwriting previous runs). (default: empty)

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