Bifurcation using AUTO2000 and the Auto2000 Tellurium Plugin

Continue with some bifurcation

1.1 Introduction

The AUTO2000 plugin serves as a front-end for the AUTO2000 library, which is a library for continuation and bifurcation problems in ordinary differential equations ¹.

Current limitations: Multiple continuation parameters are not supported, i.e. only one parameter can be selected for any continuation problem.

Available properties in the auto2000 plugin are documented in the next section.

¹AUTO2000 by Eusebius J. Doedel , Randy C. Paffenroth, Alan R. Champneys, Thomas F. Fairgrieve, Yuri A. Kuznetsov, Bart E. Oldeman, Björn Sandstede and Xianjun Wang. See http://www.dam.brown.edu/people/sandsted/publications/auto2000.pdf.

1.2 Plugin Properties

The AUTO library have numerous properties that has been wrapped and made available to a plugin client. Each property is listed below with its data type, default value and a short description. For the exact usage and a more in detail description please consult the main AUTO2000 manual.

Property Name	Data Type	Default Value	Description
SBML	string	N/A	SBML document as a string. Model to be used by
			AUTO
TempFolder	string	" ."	Folder used by auto and the plugin for saving temporary
			files
KeepTempFiles	bool	false	Boolean indicating if temporary files should be deleted
			after an AUTO session or not
ScanDirection	string	"Positive"	Parameter instructing AUTO how to sweep its principal
			continuation parameter
PrincipalCont-	string	N/A	The principal continuation parameter (PCP) is the first
inuationParameter			parameter that AUTO will sweep. Currently only one
			parameter is supported, which then by default is the
			PCP

BifurcationPoints	vector < int >	N/A	This integer vector holds the exact point number (in
			the sequence of all output data) for an AUTO solution
			point. It can be used together with the labels in the
			bifurcationlabels property to assist in plotting a bifur-
			cation diagram
BifurcationLabels	stringList	N/A	The bifurcation labels string list holds the AUTO desig-
			nated solution type label for a solution point, as found
			in the bifurcation points property. Consult the AUTO
			documentation for possible label types and their mean-
			ing
BifurcationData	telluriumData	N/A	The BifurcationData property holds the bifurcation di-
			agram after a session. First column is the values of the
			selected parameter, and successive columns are selected
			species

The following properties are used internally by the auto library. Depending on the problem at hand, they may need to be tweaked.

fort2	string	N/A	Property containing the content of the AUTO tempo-
			rary file, fort.2. Fort.2 is the input file for AUTO and
			created by the plugin
fort3	string	N/A	Property containing the content of the AUTO tempo-
			rary file, fort.3. The content of fort.3 file is undocu-
			mented in AUTO's documentation
fort6	string	N/A	Property containing the content of the AUTO tempo-
			rary file, fort.6. The content of fort.6 file is a bifurcation
			session summary
fort7	string	N/A	Property containing the content of the AUTO tempo-
			rary file, fort.7. The content of fort.7 file is a bifurcation
			diagram on success
fort8	string	N/A	Property containing the content of the AUTO tempo-
			rary file, fort.8. The content of fort.8 file contain various
			statistics from the session
fort9	string	N/A	Property containing the content of the AUTO tempo-
			rary file, fort.8. Diagnostic messages, convergence his-
			tory, eigenvalues, and Floquet multipliers are written in
			fort.9

NDIM	int	1	The NDIM property correspond to the dimension of the
			system of equations
IPS	int	1	Constant defining the problem type
IRS	int	1	This constant sets the label of the solution where the
			computation is to be restarted.
ILP	int	1	Fold detection; 1=ON, 0=OFF
NICP	vector < int >	N/A	Property denoting the number of free parameters
ICP	int	N/A	Free parameters
NTST	int	15	The number of mesh intervals
NCOL	int	3	The number of collocation points per mesh interval
IAD	int	3	Mesh adaption every IAD steps; 0=OFF
ISP	int	1	Bifurcation detection; $0=OFF$, $1=BP(FP)$,
			3=BP(PO,BVP), 2=all
ISW	int	1	Branch switching: 1=normal, -1=switch branch (BP,
			HB, PD), 2=switch to two-parameter continuation (LP,
			BP, HB, TR) 3=switch to three-parameter continuation
			(BP)

IPLT	int	0	This constant allows redefinition of the principal solu-
			tion measure, which is printed as the second (real) col-
			umn in the fort.7 output-file. See AUTO manual for
			possible settings
NBC	int	0	Number of boundary conditions
NINT	int	0	Number of integral conditions
NMX	double	1000	Maximum number of steps
RL0	double	0.01	The lower bound on the principal continuation parame-
			ter
RL1	double	30	The upper bound on the principal continuation param-
			eter
A0	double	0	The lower bound on the principal solution measure
A1	int	10000	The upper bound on the principal solution measure
NPR	int	50	Save the solution in the solution file every NPR contin-
			uation steps
MXBF	int	-1	Automatic branch switching for the first MXBF bifur-
			cation points if IPS=0, 1
IID	int	0	Control diagnostic output; 0=none, 1=little, 2=normal,
			4=extensive

ITMX	int	8,	Maximum number of iterations for locating special so-
			lutions/points
ITNW	int	5,	Maximum number of correction steps
NWTN	int	3,	Corrector uses full newton for NWTN steps
JAC	double	0,	User defines derivatives; 0=no, 1=yes
EPSL	double	1e-8	Property setting the convergence criterion for parame-
			ters
EPSU	double	1e-8	Property setting the convergence criterion for solution
			components
EPSS	double	1e-6	Property setting the convergence criterion for special
			points
DS	double	0.001	Session start step size
DS DSMIN	double double	0.001 1e-5	
			Session start step size
DSMIN	double	1e-5	Session start step size Minimum continuation step size
DSMIN DSMAX	double double	1e-5 0.1	Session start step size Minimum continuation step size Maximum continuation step size
DSMIN DSMAX IADS	double double int	1e-5 0.1 1	Session start step size Minimum continuation step size Maximum continuation step size Step size adaption every IADS steps; 0=OFF
DSMIN DSMAX IADS NTHL	double double int int	1e-5 0.1 1 0	Session start step size Minimum continuation step size Maximum continuation step size Step size adaption every IADS steps; 0=OFF The number of modified parameter weights (for BVP)
DSMIN DSMAX IADS NTHL THL	double double int int vector <int></int>	1e-5 0.1 1 0 N/A	Session start step size Minimum continuation step size Maximum continuation step size Step size adaption every IADS steps; 0=OFF The number of modified parameter weights (for BVP) List of parameter weights

NUZR	int	0	The number of user output points specified
UZR	vector <int></int>	N/A	List of values for user defined output

Table 1.1: Plugin Properties

1.3 The execute(bool inThread) function

The execute() function will start a bifurcation session. Depending on the problem at hand, the algorithm may run for a long time.

The execute(bool inThread), do support a boolean argument indicating if the execution of the plugin work will be done in a thread, or not. If set to false, i.e. executing execute(false), the function will be a blocking function and will not return until the plugin work is done. If, on the other hand, the client are setting the argument to true, the execute(true) will return immediately and the plugin work will be executed in a thread. A client can use the isPluginDone(plugin) to query the status of the plugin progression.

The inThread argument defaults to false.

1.4 Plugin Events

The auto2000 plugin are using all of a plugins available plugin events, i.e. the *PluginStarted*, *PluginProgress* and the *PluginFinished* events.

The available data variables for each event are internally treated as *pass trough* variables, so any data, for any of the events, assigned prior to the plugins execute function (in the assignOn() family of functions), can be retrieved *unmodified* in the corresponding event function.

Event	Arguments	Purpose and argument types
PluginStarted	void*, void*	Signal to application that the plugin has started. Both parameters are <i>pass trough</i> parameters and are unused internally by the plugin.
PluginProgress	void*, void*	Communicating progress of fitting. Both parameters are <i>pass trough</i> parameters and are unused internally by the plugin.
PluginFinished	void*, void*	Signals to application that execution of the plugin has finished. Both parameters are <i>pass trough</i> parameters and are unused internally by the plugin.

Table 1.2: Plugin Events

1.5 Python example

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The following Python script illustrate how the auto plugin can be invoked, how to set its properties and finally how to plot a bifurcation diagram.

```
from telplugins import *
1
2
3
   try:
       sbmlModel = "BIOMD0000000203.xm1"
4
       auto = Plugin("tel_auto2000")
 5
 6
 7
        #print auto.listOfPropertyNames()
8
9
        #Setup Auto Propertys
       auto.setProperty("SBML", readAllText(sbmlModel))
10
11
12
       #Auto specific properties
        auto.setProperty("ScanDirection", "Positive")
13
14
       auto.setProperty("PrincipalContinuationParameter", "A")
        auto.setProperty("PCPLowerBound", 10)
15
        auto.setProperty("PCPUpperBound", 200)
16
17
18
        #Max number of points
       auto.setProperty("NMX", 5000)
19
20
21
       #Execute the plugin
22
       auto.execute()
23
24
        # Bifurcation summary
       print "Summary: " + auto.BifurcationSummary
25
26
27
       #Plot Bifurcation diagram
28
       pts
                = auto.BifurcationPoints
29
       lbls
                = auto.BifurcationLabels
30
       biData = auto.BifurcationData
31
32
       biData.plotBifurcationDiagram(pts, lbls)
33
34
       print "Done"
35
36
   except Exception as e:
       print "There was a problem: " + 'e'
37
```

Listing 1.1: Bifurcation example using a complex model.

1.5 Python example

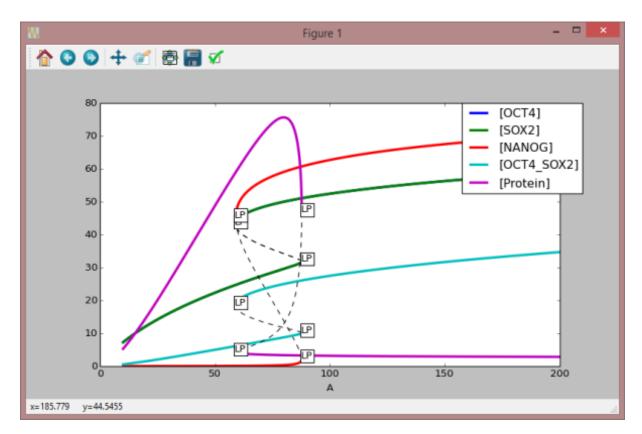


Figure 1.1: Output for the example script above.