Numerically efficient robustness test for nonlinear circuit models

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***Abstract*—We propose an algorithm to test the robustness to parameter variation of complex nonlinear models with many parameters. Our test exploits bifurcation analysis and numerical continuation to accurately follow an orbit as parameters are changed, and continuous optimization to move towards the closest bifurcation point to the nominal parameters value.**

I. Introduction

Virtually all physical phenomena are nonlinear, but for many practical matters the Hartman Großman theorem allows to simplify the analysis of asymptotic dynamics through linearization about an equilibrium point. New applications in biology, robotics, and electronics however are starting to break this comfortable paradigm. Cell dynamics, animal and bio-inspired locomotion, power networks and converters all share a preference for non-equilibrium configurations, where the relevant dynamics is dominated by limit cycles or transitions between rapidly changing dynamically stable regimes. What is more important, the frontiers of science have moved past the point where a qualitative understanding of the basic phenomena was sufficient. Modern technology allows to design, construct and control gene networks, living-like robotic creatures and complex networks of interacting electronic components, and a precise quantitative analysis of their behaviour is required for such a design and control.

When non-equilibrium states are involved, the task of assessing a model's robustness to a change in parameters is particularly challenging. Robustness, meaning the likelihood of a qualitative change in the system's dynamics as a result of a change in parameters, is a measure of the resilience of the model's behaviour to errors in the estimation of the parameters (this is relevant for example in synthetic biology, where precise parameter estimation is extremely challenging and time consuming), and can be used to validate a model by showing agreement with its physical counterpart throughout a wide range of operating conditions [1]–[4]. Rigorously speaking, robustness is a feature typically attributed to a specific orbit of a system (the concept of orbit is formally introduced in the next section), rather than to its global dynamic structure. This is because qualitative changes in the global dynamics of a large nonlinear system can often affect features that are irrelevant to the model's purpose. Robustness of a nominal orbit can be evaluated by measuring its distance in parameter space from the boundaries of its region of existence. These boundaries are the bifurcation points of the orbit. Bifurcation theory is a very well developed subject in nonlinear dynamics. Efficient numerical tools are available to conduct bifurcation analysis in one and two parameters for nonlinear systems of very large dimension, and their use to assess a model's robustness is well established [5], [6]. Common bifurcation analysis techniques however are only practically useful to study an orbit's dependence on one or two parameters.

To circumvent this limitation different approaches have been attempted. Monte Carlo techniques, which estimate the region of existence of a trajectory by testing a randomized sample of parameter values, have been used for example in [7]. These techniques can mitigate, but not avoid the exponential growth of complexity with the parameter dimension of a model. Moreover, being based on a randomized sampling of parameters, they are susceptible to attractor hopping as different parameter sets are chosen in complex nonlinear systems: these often exhibit multiple coexisting attractors, and the numerical convergence towards two qualitatively similar orbits at different parameter values does not guarantee that these orbits are homotopic, that is, that they transform into one-another as parameters are continuously changed. Structured Singular Value analysis has been used to obtain estimates of the robustness of equilibria or limit cycles to simultaneous variations of multiple parameters [5]. This technique is based on a linearisation of the dynamics, therefore it cannot account for the effect of nonlinearities, and the results are only valid within a sufficiently small neighbourhood of the nominal orbit in parameter space. Bifurcation analysis, coupled with Sequential Quadratic Programming, has been used in [8] to bound the distance in parameter space of an equilibrium from a Hopf bifurcation, deducing robustness of a limit cycle that is generated through the Hopf bifurcation. This technique is numerically efficient and naturally suitable to handle nonlinearities. However, in general the Sequential Quadratic Programming step may suffer from the attractor hopping problem highlighted before (as parameters are changed at discrete steps), while the detection of the Hopf bifurcation does not exclude that the limit cycle disappears earlier due to other bifurcations, or that it persists past the bifurcation due to a more complex bifurcation structure (for instance in the presence of a complex structure of fold bifurcations and coexisting limit cycles). Many of these problems are avoided by using *continuation* techniques, as proposed in [9], which allow to numerically follow an orbit (for example an equilibrium or limit cycle) as parameters are changed. In [9] the authors compute an orthogonal basis in parameter space aligned with the direction of steepest increase of the maximum modulus of the Floquet multipliers. The use of continuation along the directions of this basis' vectors allows to follow the desired orbit in parameter space with high accuracy, making it unlikely to hop between different unrelated orbits at different points in parameter space, while

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the choice of n orthogonal continuation directions in the n-parameter system provides a good overview of the structure of the region of existence of such an orbit. However, especially in high-dimensional parameter space, the axes alignment chosen in [9] may greatly overestimate the closest bifurcation point, due to the nonlinear dependence of the Floquet multipliers on the model's parameters.

In this work we introduce some preliminary results on an improvement of the above cited methods, obtained by taking a continuation-based approach (as in [9]) as a step of a continuous optimization algorithm, to search the closest bifurcation point to a nominal set of parameters. Continuous optimization of nonconvex functions is in general a difficult problem, but the test performed so far suggest that the region of existence of an orbit often has fairly simple geometry, and despite the lack of a formal guarantee the optimization approach appears to frequently find the correct global optimum, thus providing a tight upper bound on the maximum allowable perturbation. Moreover, the use of numerical continuation provides a highly reliable guarantee against attractor hopping in a system with multiple coexisting attractors. Formally stated, the present work sketches an algorithm with the following purpose.

Problem 1: Given a nominal parameters vector p_0 and a nominal orbit $x(p_0)$, determine the maximum relative parameter uncertainty that guarantees persistence of the orbit $x(p_0)$, that is, find the parameters vector p that minimizes $\|(p_0 - p)/p_0\|_\infty$ while $x(p)$ undergoes a bifurcation.

The vector division in the above definition is intended element-wise, assuming that all elements of p_h are nonzero. The maximum relative error is a significant robustness measure in many experimental setups, where parameters correspond to physical quantities such as masses, densities, etc. The approach can be easily extended to other error measures.

In the next section we give a short introduction to numerical continuation. Then, in Section III we sketch the proposed algorithm, and in Section IV we show an example application.

II. Notions of Numerical Continuation and Bifurcation Analysis

A generic nonlinear system is written as

$$\dot{s} = f(s, p), \tag{1}$$

where s is the state vector and p is a vector of parameters. A *trajectory* of the above system is any solution $s(t)$ of the differential equation, while an *orbit* is a set $s(\mathcal{T})$ with $\mathcal{T} \subset \mathbb{R}$. In practice the analysis of a system such as (1) is frequently focussed on the existence and qualitative structure of special orbits, such as equilibria, limit cycles, homoclinic and heteroclinic connections, that characterize the long-term dynamics of the model. An equilibrium of (1) is a state and parameter vector satisfying the equation

$$f(s, p) = 0$$

Similarly, a periodic orbit is a set of states and a parameter vector satisfying the boundary value problem

$$\begin{aligned} s(0) &= s(1) \\ \dot{s} &= T f(s, p) \end{aligned}$$

for some $T \in \mathbb{R}_+$. Both cases above, and most other relevant orbits, can be written after suitable time-discretization in the form

$$F(x, p) = 0, \tag{2}$$

where $x \in \mathbb{R}^n$ is the discretized representation of the orbit and $F : \mathbb{R}^{n+m} \to \mathbb{R}^n$. At a *regular point* of $F(x, p)$ (i.e, where the Jacobian of F has maximum rank), (2) locally defines a smooth m-dimensional manifold in $\mathbb{R}^{n+m}$, each point on the manifold corresponding to the same orbit for a different set of parameters. Numerical continuation is a set of numerical techniques and algorithms suitable to follow an orbit on such a manifold. Though the techniques used to obtain efficient and numerically stable schemes can be rather subtle, the basic approach is as follows. A solution of (2) at a point $(x = x_0, p = p_0)$ is assumed to be known, found analytically or by numerical integration. The parameters p are expressed as a smooth function of a scalar perturbation π in the form

$$p = p_0 + P(\pi), \quad P : \mathbb{R} \to \mathbb{R}^m, \quad P(0) = 0. \tag{3}$$

The most common choice by far is of the form $P(\pi) := [1, 0, 0 \ldots]\pi$, i.e. the perturbation is taken along one of the natural parameters. The function F in (2) becomes $F(x, p_0 + P(\pi)) : \mathbb{R}^{n+1} \to \mathbb{R}^n$, and its zero set at a regular point is a one-dimensional smooth manifold. Starting from $(x = x_0, \pi = 0)$, the manifold is followed by iteratively perturbing the variables (x, π) in a direction (δ_x, δ_π) (an overview of effective techniques to construct the perturbation (δ_x, δ_π) is found e.g. in [10], [11]) and numerically solving the equation

$$F(x + \delta_x, p_0 + P(\pi + \delta_\pi)) = 0. \tag{4}$$

Note that this is a much more effective analysis tool than a simple parameter sweep, since the numerical solution of (4) allows to ensure the homotopy of the orbits at successive iterations, avoiding accidental jumps between coexisting and unrelated orbits, and greatly simplifying the task of following orbits through parameter ranges where they become unstable.

While an orbit is being followed, its bifurcations can be detected by checking the value of suitable *test functions* $H(x, p) : \mathbb{R}^{n+m} \to \mathbb{R}$, functions whose value vanishes at a bifurcation. For instance, assuming we are following an equilibrium of (1), the determinant of the Jacobian $f_s := \partial f(s, p)/\partial s$ is a test function for a fold bifurcation, where one real eigenvalue crosses the imaginary axis, while the determinant of the bialternate product matrix $2f_s \odot I_n$, where I_n is the n-dimensional identity matrix, is a test function for the Hopf bifurcation, where a pair of complex conjugate eigenvalues crosses the imaginary axis.

Near a bifurcation point, where the test function $H(x, p) = 0$, the system

$$\begin{aligned} F(x, p) &= 0 \\ H(x, p) &= 0 \end{aligned} \tag{5}$$

defines a smooth $m - 1$ dimensional manifold of bifurcating orbits (assuming the bifurcation point is regular). The manifold can be followed along a one-dimensional curve in the same way as explained before, by expressing the parameters p as in (3) but with $P(\pi) : \mathbb{R}^2 \to \mathbb{R}^m$ (i.e., with a two-dimensional perturbation π), perturbing the state (x, π) in a direction (δ_x, δ_π), and numerically solving (4).

A typical numerical continuation analysis thus consists in following an orbit in parameters up to a point where a test function vanishes, and then following the bifurcating orbit to construct a bifurcation diagram. The main idea of this work is to choose the function P in (3) proportional to the gradient of a suitable scalar function, and use numerical continuation as a step in a continuous optimization algorithm, to find a point of minimum distance of the bifurcation set from a nominal point in parameter space.

III. Robustness Test

The algorithm sketched in this section attempts to solve Problem 1 by proceeding through two steps: the first one seeks a bifurcation near p_0 attempting to find a good first approximation of the nearest bifurcation point; the second minimizes the distance by following a path of decreasing distance on the bifurcation manifold.

To begin with, let us simplify the notation through a change of parameters. Denote by $\tilde{p}$ the original parameters of the system, so that $\tilde{p}_0$ is the vector of the the nominal parameters. Define $f(x,p) := f(x,\tilde{p}_0(1+p))$, where the product $\tilde{p}_0 p$ is element-wise. In the parameters p, the nominal system has $p=0$, while $p \neq 0$ directly represents the relative difference from the nominal parameters. In this notation, Problem 1 consists in finding the bifurcation point that minimizes the infinity norm of p.

The first task is to find a bifurcation near $p=0$. There is only a finite number of bifurcations an orbit can undergo; for example, excluding bifurcations of codimension more than 1, an equilibrium of a smooth and non-symmetric system can undergo Hopf and fold bifurcations, while a limit cycle can have Neimark-Sacker, fold, and flip bifurcations. The following test must be repeated for each possible bifurcation. Chosen a bifurcation and the corresponding test function H, we first use (2) and the implicit function theorem to express the orbit x as a function of the parameters p, and we compute the gradient $H_p := \partial H(x(p),p)/\partial p$; this gives the direction of maximum increase of the test function H in the parameters. Function P in (3) is set equal to $\pi H_p \mathrm{sgn}(-H(x,p))$, so that increasing the scalar π the orbit locally moves towards $H(x,p)=0$ along the steepest direction. The manifold $F(x,p)=0$ is then followed towards $H(x,p)=0$, by numerical continuation, for a fixed number of steps or until a bifurcation is found. The bifurcation is excluded if $\|p\|_\infty$ grows beyond a given maximum distance. This is summarised in Algorithm 1.

Algorithm 1 Location of a Bifurcation

x_i, p_i are the state and parameter vectors at iteration i
while $H(x_i,p_i) \neq 0$ and $\|p_i\|_\infty <$ maximum distance **do**
  $H_p \leftarrow \frac{\partial H(x(p),p)}{\partial p}|_{x=x_i,p=p_i}$
  $P(\pi) := \pi H_p \mathrm{sgn}(-H(x_i,p_i))$
  continue $F(x, p_i + P(\pi)) = 0$ in the variables (x,π) for N steps or until a bifurcation is detected
  assign to (x_{i+1}, p_{i+1}) the values of the last point of the numerical continuation
end while

The above procedure is simply aimed at finding a good first guess for the nearest bifurcation point. Clearly, this could be accomplished by other means, and further investigation might indeed be useful considering that the gradient method we have chosen will in principle fail if it finds a maximum or minimum of H, where $H_p = 0$. In practice, however, this method has proved to be quite reliable.

Assuming that a bifurcation is found, the second task is to move along the bifurcation manifold (defined by equations (5)) towards the point that minimizes $\|p\|_\infty$. To achieve this, we compute a basis B of the tangent plane at p to the bifurcation manifold in the space of the parameters, that is, we construct B as an $(m-1)\times m$ matrix of maximal rank satisfying

$$\frac{\partial H(x(p),p)}{\partial p} B = 0.$$

As before, $x(p)$ can be constructed using (2) and the implicit function theorem. Then, we compute the parameter vector α in $\mathrm{span}(B)$ that minimizes $\|\alpha\|_\infty$. This vector, which is the solution of a linear approximation of Problem 1, can be shown to be equal to

$$\Big(I - \Big[B|0\Big]\Big[B|\mathrm{sgn}(B(B^TB)^{-1}B^Tp - p)\Big]^{-1}\Big)p,$$

where $[a|b]$ is the matrix obtained by concatenating the columns of a and b, 0 is the zero vector, and $\mathrm{sgn}(a)$ is the vector of signs of a. We define

$$d := \alpha - p$$

and set the function P in (3) equal to $(\pi^1 d - \pi^2 p)$, so as to constrain the continuation of $F(x, p + P(\pi^1,\pi^2)) = 0$ within the plane $\mathrm{span}(d,p)$, which contains α. We then follow (5) by numerical continuation and, calling y a curvilinear coordinate along the continuation curve, we stop when a maximum number of continuation steps N is reached or when $\partial\|p\|_\infty/\partial y = 0$. The procedure is iterated until a stopping condition is verified (typically, until the norm of (π^1,π^2) at the end of a continuation step is smaller than a threshold), as described in Algorithm 2. Since the procedure above is based on a linear approximation of the bifurcation manifold, its speed of convergence is quadratic in a neighbourhood of the optimal solution.

Algorithm 2 Distance Minimization

x_i, p_i are the state and parameter vectors at iteration i
while not StopCondition **do**
  $B \leftarrow$ basis of the tangent space to $\{H(x_i,p_i)=0\}$
  $\alpha \leftarrow \Big(I - \Big[B|0\Big]\Big[B|\mathrm{sgn}(B(B^TB)^{-1}B^Tp_i - p_i)\Big]^{-1}\Big)p_i$
  $d \leftarrow \alpha - p_i$
  $P(\pi_1,\pi_2) := (\pi^1 d - \pi^2 p_i)$
  continue $(F(x, p_i + P(\pi^1,\pi^2)), H(x, p_i + P(\pi^1,\pi^2)))$ in the variables (x,π^1,π^2) for N steps or until $\partial\|p\|_\infty/\partial y = 0$
end while

IV. Application to the Laub-Loomis Model

The algorithms described in the previous section have been implemented as a Python script using Auto07p [12] for the numerical continuation and bifurcation detection. The scripts have been tested on the Laub-Loomis model, which was used as a test in [5], [8], [9]

This is a model of a genetic circuit regulated by the following equations

$$\dot{x} = \begin{pmatrix} p^1 x^7 - p^2 x^1 x^2 \\ p^3 x^5 - p^4 x^2 \\ p^5 x^7 - p^6 x^2 x^3 \\ p^7 - p^8 x^3 x^4 \\ p^9 x^1 - p^{10} x^4 x^5 \\ p^{11} x^1 - p^{12} x^6 \\ p^{13} x^6 - p^{14} x^7. \end{pmatrix}$$

The model has 7 state variables and 14 parameters. At the nominal parameter vector $p = (2, 0.9, 2.5, 1.5, 0.6, 0.8, 1, 1.3, 0.3, 0.8, 0.7, 4.9, 23, 4.5)$ the system has an unstable focus equilibrium, and a stable limit cycle, which is the orbit on which the system is expected to evolve. The authors of [8] found that an error of 0.51% in the parameters would cause a Hopf bifurcation of the equilibrium, concluding that at this parameter value the limit cycle would also disappear, through the same bifurcation.

Running the algorithm described here to test the robustness of the limit cycle detects a Hopf bifurcation for a relative parameter error of 0.5091% (at $p = [$ 1.9898, 0.8954, 2.5127, 1.5076, 0.5969, 0.8041, 1.0051, 1.2934, 0.3015, 0.8041, 0.6964, 4.9249, 22.8829, 4.5229 $]$), which is in accordance with the result of [8], and confirms that no fold, flip, or Neimark Sacker bifurcation of the limit cycle is found within a 50% relative perturbation of the nominal parameters.

Though the numerical result of [8] is not improved (it is, quite likely, a global optimum), the approach presented here is generally more robust in that it guarantees the homotopy of the cycle through the whole optimization procedure, and it allows to follow the limit cycle directly, rather than deducing its region of existence from that of the equilibrium.

V. Conclusion

We have proposed an algorithm to assess the maximum relative parameter error that a nonlinear model can withstand without changing its behaviour. We detect a change in the structure of a relevant orbit by checking its bifurcations. We obtain our result by using numerical continuation coupled with a continuous optimization algorithm. The use of numerical continuation ensures homotopy of the orbit throughout the optimization process, avoiding the risk of erroneously jumping between coexisting orbits, while the continuous optimization algorithm allows to provide a good upper bound to the maximum allowable parameter error. Though without a formal guarantee, in our tests the algorithm appears to find a tight upper bound.

The algorithm sketched in this work can still be improved, in particular by addressing some pathological scenarios (highlighted in the text) that could prevent it from terminating correctly. However, more than the specific implementation we believe that the paradigm we proposed is significant. Our optimization algorithm can be easily implemented as an overlay to existing numerical continuation routines, and as such it can be applied to test robustness of any orbit and model for which numerical continuation software exists. These include smooth ODEs and PDEs [10], [11] as well as piecewise smooth and hybrid dynamical systems [13]–[15]. Additionally, the set of parameters over which to run the algorithm is a design choice available to the user, thus the analysis of robustness for arbitrary cross sections of the parameter space (e.g., for pairwise or n-wise parameter perturbations) can be conducted simply by changing the set of parameters that constitute the optimization search space.

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