

On Bifurcations of the Zero Dynamics - Connecting Steady-State Optimality to Process Dynamics

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Abstract: It is well known that certain properties of the process dynamics can be deduced from steady-state information about a process only. In this paper we consider the dual problem, that of determining steady-state properties from process dynamics. In particular, we are concerned with the problem of determining extremum points in the steady-state input-output map from dynamic response data. This is a highly relevant problem in cases where the aim is to determine steady-state optimal operating conditions using real time process measurements. For this purpose, we first consider the connection between bifurcations of the zero dynamics and the steady-state input-output map. Based on these results, we show that steady-state optimal conditions can be determined from the process dynamics through consideration of local phase-lag properties of the process only. We demonstrate the usefulness of this result by showing that the optimum of a chemical reactor can be located, without any prior knowledge, using sinusoidal perturbations and a phase-lock loop.

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1. INTRODUCTION

Bifurcation theory provides a link between the stability of a dynamical system and the branching behavior of its stationary solutions; solution branches meet where eigenvalues of the linearized dynamics cross the imaginary axis [Guckenheimer and Holmes, 2002]. For the case of static bifurcations, it implies that certain dynamic properties can be predicted from steady-state information about the system only, e.g., a singularity in the steady-state input-output map implies that an eigenvalue crosses the imaginary axis at that point and at least one of the steady-state branches emerging from the singularity will be unstable. For the specific case of feedback structures, Morari [1985] derive a number of conditions from which stability properties of the closed-loop system can be deduced based on steady-state information about the process only. He also remarks on the close relationship between these results and those of bifurcation theory.

In this paper we are concerned with what can be viewed as the dual problem; that of deducing steady-state properties of a process from information about its dynamics only. This is in particular relevant when considering real-time optimization problems where the aim is to locate a steady-state optimum based on response data from the process only. A steady-state optimum corresponds to a singularity in the steady-state output-input map, and one would therefore expect it to be related to a static bifurcation in the corresponding zero dynamics. Indeed, as pointed out in Jacobsen and Skogestad [1991], such a singularity should imply that a real zero of the linearized system transfer-function crosses the imaginary axis. Some sketches to

proofs for this is presented in Jacobsen [1994] and Sistu and Bequette [1995]. Here we turn the problem around and consider the implications of local bifurcations in the zero dynamics for the stationary solution branches of a process. In particular, we consider fold, or saddle-node, bifurcations and Hopf bifurcations of the zero dynamics and show that they give rise to different types of input multiplicity. Somewhat surprisingly, very few results exist on the implications of bifurcations of the zero dynamics. One notable exception is Byrnes and Isidori [2002] who use bifurcation analysis of the zero dynamics to study the attractors of high-gain feedback systems in a small neighbourhood of the origin. In the second part of the paper we utilize the information obtained from considering bifurcations of the zero dynamics to predict steady-state extremum points from dynamic response data. In particular, we show how a phase-lock loop can be used to drive a system to its steady-state optimum. All results are demonstrated by application to simple CSTR models.

2. BIFURCATIONS OF THE ZERO DYNAMICS

We consider single-input single-output nonlinear dynamical systems described by a set of ordinary differential and algebraic equations on the input-affine form

$$\begin{aligned}\dot{x} &= f(x) + g(x)u, \quad x \in \mathbb{R}^n, \quad u \in \mathbb{R} \\ y &= h(x), \quad y \in \mathbb{R}\end{aligned}\tag{1}$$

Note that the main results derived below apply also to systems that can not be written on input-affine form, but the derivations are in that case more involved and therefore not included here. The zero dynamics of system

(1) correspond to the state dynamics when the output y is forced to be zero or, more generally, constant. To determine the zero dynamics of the system (1), introduce a state transformation $z = \phi(x)$ to obtain

$$\dot{z}_i = z_{i+1}, \quad i = 1, r - 1 \quad (2)$$

$$\dot{z}_r = b(\xi, \eta) + a(\xi, \eta)u \quad (3)$$

$$\dot{\eta} = q(\xi, \eta) \quad (4)$$

$$y = z_1 \quad (5)$$

where $\xi = z_i, i = 1, r$ and $\eta = z_i, i = r + 1, n$ and r is the relative degree of the system. The zero dynamics are then given by the dynamics of the $n - r$ states η when the first r states ξ are forced to be zero by means of the control input u , i.e.,

$$\dot{\eta} = q(0, \eta) \quad (6)$$

We are here interested in the consequences of bifurcations of the zero dynamics, i.e., when eigenvalues of $q(0, \eta)$ linearised about an equilibrium point cross the imaginary axis. The linear approximation of the zero dynamics at an equilibrium point equals the zero dynamics of the linearized system at the same equilibrium [Isidori, 1989]. That is, eigenvalues of the linearized zero dynamics coincide with the zeros of the linearized dynamics of the open-loop system (1) and bifurcations can hence be determined from consideration of the transmission zeros of

$$\begin{aligned} \dot{x} &= Ax(t) + Bu(t) \\ y(t) &= Cx(t) \end{aligned} \quad (7)$$

where (A, B, C) is the linear approximation of (1) around a given steady-state.

The transmission zeros of the linearized system (7) can be determined from the rank of the matrix

$$M = \begin{pmatrix} A - zI & B \\ C & 0 \end{pmatrix} \quad (8)$$

The transmission zeros are the values of z such that the rank of M is less than the normal rank $n + 1$. A bifurcation of the zero dynamics (6) corresponds to at least one zero z having zero real part. Using Schur's identity we get

$$\det(M) = \det(A - zI)C(A - zI)^{-1}B = 0 \quad (9)$$

from which we get that z is a zero if $\det C(A - zI)^{-1}B = 0$ and z is not an eigenvalue of A . The latter condition rules out pole-zero cancellations. Considering first the case with $z = 0$, corresponding to a static fold or saddle-node bifurcation of the zero dynamics, we get the condition $CA^{-1}B = 0$ which as expected corresponds to a zero steady-state gain $G(0) = 0$ from input to output. To be a bifurcation point, a transversality condition also needs to be fulfilled, i.e., the zero must also move through the origin as the input (and output) is varied. For this purpose, consider the MacLaurin series of $G(s) = C(sI - A)^{-1}B$

$$G(s) = \sum_{i=0}^{\infty} c_i s^i \quad (10)$$

where $c_i = CA^{-1-i}B$. For small non-zero s we can neglect higher order terms and then find that the zero close to $s = 0$ is given by

$$z = -\frac{c_0}{c_1} = -\frac{CA^{-1}B}{CA^{-2}B}$$

Since $CA^{-2}B$ must be non-zero (otherwise there is a double zero at $s = 0$), we find that $CA^{-1}B = G(0)$ changes

sign as the zero changes sign. Thus, a static bifurcation of the zero dynamics, corresponding to a real zero crossing the imaginary axis, implies a change in the sign of the local steady-state gain. This again corresponds to an extremum point in the input-output map.

It is of interest to consider whether the converse of the above result is also true, i.e., that an extremum point in the steady-state input-output map implies a static bifurcation in the zero dynamics. At an extremum point we have $CA^{-1}B = 0$ and we note from the MacLaurin series above that then $z = 0$ is a transmission zero of $G(s)$ unless also all $CA^{-i}B, i > 1$ are also all identically zero. The latter case corresponds to having $G(s) \equiv 0$ at the extremum point, and this is indeed possible if the zero gain is due to a static nonlinearity, as in Wiener and Hammerstein models. However, if the nonlinearity causing the extremum point is inherent in the state dynamics then the system will display a transient response also at the extremum point and $G(s) \neq 0$ for which $G(0) = 0$ implies a zero at $z = 0$ and a change in the sign of $G(0)$ implies a static bifurcation in the zero dynamics at the extremum point.

Before turning to an example, we remark that the above result does not imply that at least one solution has unstable zero dynamics in the case of input multiplicity, as is often claimed e.g., Sistu and Bequette [1995]. The main reason for this is that transmission zeros may move between the complex LHP and RHP through infinity as well, and this does not correspond to a bifurcation and does not affect the steady-state gain. Thus, all we can conclude is that a static bifurcation of the zero dynamics implies an extremum point in the steady-state input-output map. This is also the fact that we will utilize to determine steady-state optima from dynamic data in the second part of the paper.

Example 1: isothermal CSTR. Consider an isothermal perfectly mixed tank reactor with two consecutive reactions $A \rightarrow B, 2B \rightarrow C$, with standard mass action kinetics

$$V\dot{c}_A = F(c_{Af} - c_A) - V k_1 c_A \quad (11)$$

$$V\dot{c}_B = -F c_B + V k_1 c_A - V k_2 c_B^2 \quad (12)$$

where c_A and c_B are concentrations of A and B , respectively. With $V = 1.0, c_{Af} = 1.0, k_1 = 2.0, k_2 = 0.1$ we get from linearization of the model that a static bifurcation of the zero dynamics occurs for

$$c_A^* = \frac{F}{F + 2}; \quad c_B^* = \frac{4}{(F + 2)^2}$$

corresponding to $c_B^* = 0.71$ for $F^* = 0.375$. As expected this is also the maximum value of c_B^* which can be seen from Figure 1. From the figure it can also be seen that the real zero in the RHP for low values of the flow F moves towards the imaginary axis as F is increased from $F = 0$ and crosses into the LHP for $F = 0.375$. The fact that a zero crosses the imaginary axis at the extremum point implies that the process dynamics change significantly around this point. In particular, there will be a large change in the phase lag also for non-zero frequencies and this is what we will utilize below to locate the vicinity of the optimum using dynamic response data.

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