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.

Keywords: Real time optimization, extremum seeking, zero dynamics, phase lock loop, bifurcations, input multiplicity

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 inputoutput 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 steadystate 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 transferfunction 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 steadystate 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

$$\dot{x} = f(x) + g(x)u, \ x \in \mathbb{R}^n, \ u \in \mathbb{R}$$
$$y = h(x), \ y \in \mathbb{R}$$
(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

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

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

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

$$J = z_1 \tag{5}$$

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.,

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

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 openloop system (1) and bifurcations can hence be determined from consideration of the transmission zeros of

$$\dot{x} = Ax(t) + Bu(t)$$
$$y(t) = Cx(t) \tag{7}$$

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

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

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

$$\det(M) = \det(A - zI)C(A - zI)^{-1}B = 0$$
(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 $G(s) = C(sI - A)^{-1}B$

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

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

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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 = 0and 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 inputoutput 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

$$V\dot{c}_A = F(c_{Af} - c_A) - Vk_1c_A \tag{11}$$

$$V\dot{c}_B = -Fc_B + Vk_1c_A - Vk_2c_B^2 \tag{12}$$

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

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

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 = 0and 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.



Fig. 1. Steady-state product concentration c_B^* as a function of the feed flow F in the isothermal CSTR. The lower plot shows the corresponding zero of the transferfunction from F to c_B .

While we in this paper mainly are concerned with the relation between steady-state properties and process dynamics, and hence static bifurcations, it is of interest to also consider the implications of other types of bifurcations of the zero dynamics. Consider the case in which a pair of complex zeros cross the imaginary axis, i.e., $C(i\omega - \omega)$ $(A)^{-1}B = G(i\omega) = 0$ for some $\omega > 0$. This case corresponds to a Hopf bifurcation of the zero dynamics given by (6), and should according to the Hopf Bifurcation Theorem [Guckenheimer and Holmes, 2002] result in a limit cycle in the states η and hence the control input u, when y is kept constant, on one side of the bifurcation point. An interesting consequence of this is that we obtain a new type of input multiplicity in which a constant value of the output can be obtained by both a steady-state input and an oscillating input. We next illustrate this with a simple example below.

Example 2: exothermic CSTR. Consider a CSTR with an exothermic reaction $A \rightarrow B$, Arrhenius kinetics and a cooling jacket

$$\dot{x}_1 = -x_1 + Da(1 - x_1)e^{x_2} \tag{13}$$

$$\dot{x}_2 = -x_2 + BDa(1-x_1)e^{x_2} - \beta(x_2 - x_{2c}) \quad (14)$$

$$\dot{x}_{2c} = \epsilon_{Fc} (x_{fc} - x_{2c}) + \beta (x_2 - x_{2c}) \tag{15}$$

where x_1 is the conversion of A and x_2 and x_{2c} denote dimensionless temperatures in the reactor and cooling jacket, respectively. With $Da = 4.5, \beta = 3, x_{fc} = -5$ we find a purely imaginary pair of zeros between the coolant flow ϵ_{Fc} and the coolant temperature x_{2c} of the linearised

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system for the dimensionless coolant flows $\epsilon_{Fc} = 4.812$ and $\epsilon_{Fc} = 5.824$, respectively. Thus, at these points a branch of oscillations in the zero dynamics, and thereby the input, should appear. Indeed, as can be seen from Figure 2c, in the range between the two Hopf points of the zero dynamics we have a stable limit cycle in ϵ_{Fc} coexisting with the steady-state flow (which has unstable zero dynamics). Thus, we have a new type of input multiplicity in which a given constant output, i.e., x_{2c} , can be achieved with two different stationary inputs; one being steady-state and one being periodic. Note that the zero dynamics are unstable for the first solution and stable for the second, implying that while perfect control of x_{2c} can not be achieved with a constant input this is possible with a periodic coolant flow. We also note that in this case the average coolant flow for the periodic solution exceeds the corresponding steady-state flow for a given x_{2c} , thus in that sense being less optimal. However, in a general system the opposite can obviously be the case and this kind of input multiplicity is therefore of interest to explore also in this respect.

Obviously one can also find cases with further bifurcations of the periodic inputs, resulting e.g., in chaotic inputs producing a constant output, but we do not pursue this here and rather move to the main topic of the paper; that of locating steady-state optima from dynamic response data.

3. USING DYNAMIC RESPONSES TO LOCATE STEADY-STATE OPTIMA

A steady-state optimum, local or global, corresponds to an extremum point in the steady-state input-output map. From the above we conclude that, unless the steady-state optimum is due to a purely static relationship, a real transmission zero is crossing through the imaginary axis at such a point. We here consider the implications of this for the process dynamics and the use of this knowledge for real-time optimization in cases where a process model can not be used to accurately locate the optimum.

The fact that the transfer-function from input to output contains a real zero at the extremum point implies partly that the steady-state gain is zero at that point and partly that the phase-lag is $\pm \pi/2$ rad at steady-state, i.e., for $\omega = 0$. That this real zero crosses the imaginary axis as the operating point moves past the extremum point implies that the steady-state gain remains small close to the extremum point while there is a change in the phaselag of π rad for $\omega = 0$. For higher frequencies, i.e., for the dynamic response, a similar conclusion holds; the gain will be small while there will be a large change in the phase-lag when the operating point is moved past the extremum point. This is illustrated in Figure 3 for some different frequencies in the complex plane. For small nonzero perturbation frequencies we will have a large change in phase lag and some point with a phase-lag $\pm \pi/2$ rad in the close vicinity of the optimum. To see this, consider what happens if we fix the frequency ω and vary the point of linearization locally about the optimum. As we vary u, and thereby y, the transmission zero vary over some interval $[-\epsilon_1, \epsilon_2]$ with $\epsilon_1, \epsilon_2 > 0$. But, then the phase contribution in $G(i\omega)$ from the transmission zero will vary



Fig. 2. Exothermic CSTR: Upper plot shows steady-state values of the coolant temperature x_{2c} as a function of the coolant flow ϵ_{Fc} . The middle figure shows the corresponding root locus of the zeros of the transfer-function from ϵ_{Fc} to x_{2c} . The lower figure shows stationary solutions of ϵ_{Fc} for fixed x_{2c} ; solid (dashed) lines denote (un)stable steady-states while circles denote amplitude of a stable limit cycle.

by $\Delta \varphi$ rad as the transmission zero varies over $[-\epsilon_1, \epsilon_2]$, as illustrated in Figure 3.

From the above discussion, by using a perturbation frequency in the range approximately up to the dominating pole of the open-loop process, one should be able to locate the vicinity of the (local) optimum by moving the process to the operating point where the phase-lag is $\pm \pi/2$ rad at that frequency. Having located the vicinity of the optimum one can then move closer to the optimum by subsequently lowering the frequency. As the frequency is reduced towards zero the system will asymptotically reach the extremum point in the steady-state map. For the purpose of

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Fig. 3. Change in phase contribution of varying real transmission zero z in a linear system on the form $G(s) = (s + z)G_0(s)$. $\Delta \varphi_i$ denotes the change in the phase-lag of the system for the fixed frequencies ω_i as z varies over the interval $(-\epsilon_1, \epsilon_2), \epsilon_1, \epsilon_2 > 0$.

locating the operating point with phase-lag $\pi/2$ rad at a given frequency we here propose to employ a phase-lock loop (PLL). Phase lock loops are frequently employed in communication systems and then for synchronization, i.e., to reproduce the frequency of an input signal [Best, 2007]. Since the difference in frequencies between two signals is reflected in a phase difference, PLLs are generally based on phase estimation combined with feedback of the phase error in which the oscillator frequency is used as the control input. A PLL can be used both for continuous time and sampled systems. Here we employ a continuous PLL to locate an operating point with phase-lag $\pm \pi/2$ rad and use the optimization variable u as the control input. The phase-lock loop we employ is illustrated in Fig. 4. Note that we map all phase angles ϕ into the range $[0,\pi]$ by employing the transformation $\hat{\phi} = a\cos(\cos(\phi))$ in the phase detection unit.



Fig. 4. Phase-locked loop used for steady-state optimization. The reference is set to $\pi/2$ rad.

Note that using a phase-lock loop to drive the process to an operating point with a phase-lag of $\pm \pi/2$ rad does not guarantee that we get close to the optimum. Depending on the choice of frequency, it is of course possible to have a phase-lag of $\pm \pi/2$ rad also at operating points arbitrary far removed from the optimum. This will in particular be the case if the perturbation frequency is chosen well above frequencies corresponding to open-loop poles of the system, and hence the perturbation frequency should be chosen with respect to the dominant time-constant of the process. However, to overcome the potential problem of locking onto non-optimal solutions, while ensuring an asymptotic approach to the true optimum, one can after convergence with the chosen frequency slowly lower the frequency towards lower and lower values. Since the true optimum is a unique stationary solution as the frequency approaches zero, provided the optimization problem is

convex, this will guarantee that one asymptotically approaches the optimum. The reason for not choosing a very low frequency initially is that the initial convergence rate towards even a vicinity of the optimum then becomes impractically slow. Also note that the PLL can be used both for locating the optimum and for maintaining optimal operating conditions in the presence of various disturbances.

Consider again the isothermal reactor in Example 1 above. Figure 5 shows the local phase-lag of the process as a function of the feed flow F for the frequencies $\omega_1 = 0.01$, $\omega_2 = 0.1$ and $\omega_3 = 0.2$, respectively. As can be seen from the figure, for all frequencies there is a large shift in the phase-lag close to the optimal value F = 0.375 and the phase crosses $-\pi/2$ rad close to the optimum. As the frequency is increased, the deviation from the optimum increases somewhat, but for all the considered frequencies we would get close to the steady-state optimum by using a phase-lock loop with setpoint $\pi/2$ rad.



Fig. 5. Isothermal reactor in Example 1: local phase-lag (upper) and gain (lower) of transfer-function from feed flow F to product concentration c_B for different values of F and the three frequencies $\omega_1 = 0.01, \omega_2 = 0.1, \omega_3 = 0.2$. The steady-state optimal value is F = 0.375 and is marked by the dashed vertical line.

Also shown in Figure 5 is the corresponding local gain of the process at the considered frequencies, and as can be seen the gain reaches a minimum close to the steadystate optimum of the process. However, as can also be seen, compared to the large change in phase-lag around the optimum, there is a relatively small change in the gain as we move away from the optimum. Thus, considering noisy and uncertain data it is clearly more advantageous to utilize the distinct shift in phase-lag to locate the optimum. Also, note that using the gain would require finding the minimum gain and hence use of the derivative of the gain which is even more sensitive to noise. With the phase-lock loop one simply needs to estimate the phase lag, for which many robust methods exist, and then set the setpoint to $\pi/2$ rad irrespective of which process is considered.

Figure 6 shows the response in the product concentration c_B when a phase-lock loop is closed around the isothermal CSTR with a setpoint of $\pi/2$ rad and perturbation frequency $\omega = 0.2$. The phase estimator employed here is based on an extended Kalman filter that estimates both amplitude and phase of the process response. As can be seen, the phase-lock loop takes the process close to the steady-state optimal operating point. To achieve a more exact steady-state optimum, one could lower the frequency of the loop when system gets close to steady-state.



Fig. 6. Isothermal CSTR: response in product concentration c_B when using a phase-lock loop with perturbation frequency $\omega = 0.2$ rad/s and set-point $\pi/2$ rad for the phase lag. The dashed line shows the steady-state optimum.

4. SUMMARY AND CONCLUSIONS

We have in this paper considered the connection between the process dynamics and steady-state extrema. In particular, we have shown that static bifurcations of the zero dynamics of a process implies an extremum point in the corresponding input-output map. Since a static bifurcation of the zero dynamics implies that there locally will be a large shift in the phase-lag from the input to the output, it is possible to locate extremum points using dynamic response data. In particular, for a certain frequency band, there will be a phase lag of $\pm \pi/2$ rad in the close vicinity of the optimum. We therefore proposed to use a phase-lock loop with setpoint $\pi/2$ rad to locate the vicinity of the steady-state optimum. The phase-lock loop proposed here is effectively a new type of extremum seeking controller, which traditionally have been based on steady-state gradient estimation and control. The effectiveness of the proposed control loop was demonstrated by application to optimization of the conversion in an isothermal CSTR. To avoid potential problems with the phase-lock loop locking onto non-optimal solutions, and to ensure an asymptotic approach to the true optimum, we proposed to lower the frequency of the phase-lock loop when close to steady-state conditions are obtained.

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