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Eigenvalue optimization-based formulations for nonlinear dynamics and control problems

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Abstract

Eigenvalues play an important role in many fields of applied mathematics to engineering. For some applications it may be desirable to calculate the variables of a model in order to optimize an objective function and/or to verify constraints that involve the eigenvalues of a certain matrix. In general the elements of such a matrix depend nonlinearly on the optimization variables. Despite its potential to address diverse chemical engineering problems, eigenvalue optimization techniques have not been extensively used in the Process Systems Engineering discipline. The objectives of this contribution are to review most relevant topics on eigenvalue optimization and to present formulations and solution strategies to practically address eigenvalue optimization problems in the field of chemical engineering. In order to illustrate the ideas, several small size applications, which have to do with the analysis and control of nonlinear dynamic systems, are developed. Other potential applications and future lines of research are also suggested.

Keywords: Eigenvalue optimization; Nonlinear dynamics and control; Nonlinear programming

1. Introduction

Among the plethora of applications of eigenvalues in mathematics and engineering it can be mentioned numerical analysis, structural design, quantum mechanics and system dynamics of physical, chemical and biological models.

In particular nonlinear dynamics is in a great extent described through eigenvalues. Eigenvalues are important in nonlinear dynamics because they provide information of the behavior of an evolving system governed by a linear operator, namely the Jacobian matrix of the process dynamic system. Information about resonance, instability, and growth or decay rates as time tends to infinity can be obtained through eigenvalue analysis. The reader is referred to [1,2] for comprehensive discussions of eigenvalue analysis in nonlinear dynamics.

In many problems involving eigenvalues the elements of a certain matrix $\mathbf{A}$ may be functions of an amount of variables, $\mathbf{y}$, and the values of such variables are desired to be the solution of some optimization problem involving the eigenvalues of $\mathbf{A}(\mathbf{y})$ as objective functions or constraints.

Within the eigenvalue optimization field, semi-definite programming has received considerable attention in the last decade [3]. In semi-definite programming real symmetric positive definite matrices are considered. The positive definite constraint on real symmetric matrices whose elements linearly depend on the optimization variables are known as linear matrix inequalities, of relevance in systems and control theory [4].

Few contributions dealing with the general unsymmetric, nonlinear case, which typically arise in chemical engineering systems, have been presented so far. Much of the work in nonlinear eigenvalue optimization, from both theoretical and algorithmic points of view, has been produced in the mechanical (structural) engineering field [5]. For a comprehensive survey on eigenvalue optimization, which also includes a historical account of the development of the field, see [6].

In the chemical engineering research literature, many techniques which make use of eigenvalues for design, analysis and control of dynamic systems have been proposed since the seminal works of on chemical reactors' stability [7] and bifurcation analysis of chemical reactors [8]. However, very few contributions up to [9] and [10] have taken advantage of *eigenvalue*

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optimization as a general approach in Process Systems Engineering.

It is not the aim of this paper to make a complete review of the field of eigenvalue optimization, but to discuss in some extent pertinent developments to the chemical engineering discipline. In particular two main optimization problems are considered.

1.1. Problem 1

A classic eigenvalue optimization problem is to optimize a certain objective subject to the constraint on the real part of the eigenvalues of a general matrix to be negative. Several authors proposed such a formulation in the context of design-for-stability. In [11], the aforementioned approach is suggested for the design of economically optimal, dynamically stable reactor networks. Their optimization strategy makes use of analytical expressions of the bounds of the eigenvalues. Such expressions turn to be simple, convex and allow the handling of arbitrarily large systems. Since these bounds can be very conservative a matrix measure relaxation approach is applied in order to iteratively converge to the desired solution.

Ringertz introduces this formulation in the context of the structural design problem of finding the shape of the column that minimizes the structural weight [5]. Ringertz's solution proposal is to translate the constraint on the real part of the eigenvalues of the real unsymmetric matrix to be negative, into a positive definiteness condition on an auxiliary real symmetric matrix (Lyapunov matrix) making use of the Lyapunov's matrix identity. Ringertz's approach to cope with positive definiteness makes use of the property that it is a sufficient and necessary condition for a real symmetric matrix to be positive definite that its eigenvalues be positive. Applying such a condition and matrix determinant properties, the original problem is reformulated making use of interior-point logarithmic-barrier transformation techniques.

In this strategy, Lyapunov matrix positive definiteness has to be ensured along the optimization process in order to avoid lost of feasibility and logarithmic indetermination. For example, its eigenvalues can be evaluated at each iteration and verified to be greater than zero. Alternative, more efficient strategies can be conceived based on Cholesky decomposition techniques. If this condition is violated, backtracking is required in the line search until positive definiteness recovery. Such an approach requires special algorithms since the positive definiteness safeguard has to be implemented as an "additional inner loop" in standard barrier optimization solvers. For a detailed discussion of this issue, see [9].

In [10], the authors proposed an alternative formulation to that of [5] to cope with positive definiteness, which results in a standard NLP formulation. This approach has the important advantage that standard NLP solvers can used. The idea is to apply Sylvester conditions on the Lyapunov matrix. An equation-oriented approach is proposed to solve the resulting problem, which considers the elements of the Lyapunov matrix as optimization variables. The major drawback of the proposed approach is that analytical expressions for the involved determinants are required. Since determinants are highly nonlinear functions, non-convex optimization issues arise, mainly having to do with the provision of adequate bounds and starting points to the optimization variables. Moreover, analytical expressions for determinants are not easily obtained even for small size matrices.

1.2. Problem 2

Another typical eigenvalue optimization problem is to maximize the smallest eigenvalue of a symmetric matrix. In [5], such a formulation is applied in the field of structural engineering to the problem of maximizing the lowest natural vibration frequency of a structure and to linear buckling. The problem is reformulated in terms of an auxiliary variable and also requires a positive definiteness constraint on a certain matrix. The solution strategy implies a logarithmic barrier transformation and specialized numerical optimization algorithms to cope with the positive definiteness condition.

To the best of our knowledge, only [12,10] have proposed chemical engineering pertinent applications of such problem. In [12] the typical control problem of pole placement through state feedback is addressed as the maximization of the minimum eigenvalue of a certain symmetric matrix related to the dynamic system of the process. A required positive definiteness condition is imposed by means of Sylvester criterion. The solution approach also considers an equation-oriented model with the already described implementation drawbacks. In [10] the problem of maximization of the minimum singular value of the process system transfer function matrix, a classic controllability index, is addressed within a multiple objective framework to design-for-operability.

From the above it can be concluded that very few applications of eigenvalue optimization have been proposed so far to address chemical engineering related problems. The focus in this contribution is to illustrate the application of those formulations in the analysis and control of nonlinear dynamic systems of pertinence to the chemical engineering discipline. A common resolution framework for both problems is also suggested.

This article is structured as follows. In the next section, basic eigenvalue optimization theory is introduced, main eigenvalue optimization problems are presented, and novel solution strategies proposed. Next, small-scale chemical engineering applications in the context of nonlinear dynamics and control are posed and solved for the different eigenvalue optimization formulations. A Conclusions and Future work section closes the article.

2. Eigenvalue optimization

As pointed out in [11] there exists the impossibility of obtaining mathematical expressions for the eigenvalues of systems larger than 4×4. This makes it impossible to include eigenvalues within an optimization model in a straightforward manner (as objectives and/or constraints). Furthermore, even in the cases where analytical expressions can be obtained, their usual high complexity and non-convexity make difficult to standard NLP solvers to cope with them.

Besides this issue, a critical difficulty in eigenvalue optimization problems is the potential "coalescence" of eigenvalues [13]. The eigenvalues of a matrix with differentiable elements (smooth in the optimization variables) are themselves non-differentiable (non-smooth) at the points where coalescence occurs. It is also frequent that the optimization objective tends to make the eigenvalues coalesce at the solutions [13]. The following classic example illustrates this point. Consider the following matrix:

$$\mathbf{A}(\mathbf{y}) = \begin{bmatrix} 1+y_1 & y_2 \\ y_2 & 1-y_1 \end{bmatrix}$$

whose eigenvalues are $1 \pm \sqrt{y_1^2 + y_2^2}$.

It can be seen that the maximum eigenvalue is minimized by $y_1 = y_2 = 0$ (Fig. 1). Clearly the maximum eigenvalue is not a smooth function in such a point.

In order to overcome the aforementioned difficulties when eigenvalues are present, it is necessary to develop specialized optimization methods. A couple of classic eigenvalue optimization problems motivate the reminder of this section.

2.1. Optimization with constraints on the real part of the eigenvalues of a real unsymmetric matrix

A classic eigenvalue optimization problem is to optimize a certain objective subject to the constraint on the real part of the eigenvalues of a certain matrix $\mathbf{A}(\mathbf{y})$ to be negative:

$$\min_y \Phi(y)$$
$$\text{s.t.} \quad \begin{aligned} & Re(\lambda_i(\mathbf{A}(\mathbf{y})) < 0, \quad i = 1, \ldots, n \\ & \mathbf{h}(\mathbf{y}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{y}) \leq \mathbf{0}, \\ & \mathbf{y} \in Y = \{y | y^{\mathrm{l}} \leq y \leq y^{\mathrm{u}}\} \end{aligned} \qquad \text{(P1)}$$

$\mathbf{A}(\mathbf{y})$ is a general unsymmetric matrix whose elements depend nonlinearly on $\mathbf{y}$. In the following, the developments in [5,9] are reviewed in some extent to provide adequate theoretical background to address problem (P1).

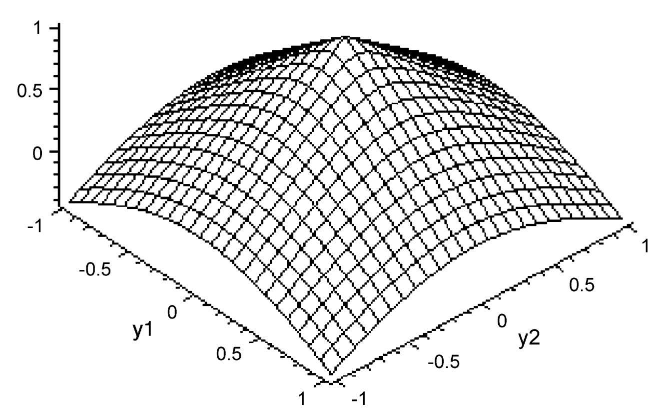

Fig. 1. Non-differentiability of the maximum eigenvalue of Overton's example.

Real symmetric matrices have real eigenvalues. Unsymmetric matrices, on the other hand, have complex eigenvalues in general [14]. It is possible, however, to translate the constraint on the real part of the eigenvalues of a real unsymmetric matrix, $\mathbf{A}(\mathbf{y})$ to be negative, $\mathrm{Re}(\lambda_i(\mathbf{A})) < 0$ ($i = 1, \ldots, n$), into a positive definiteness condition (denoted by symbol $\succ$) on a real symmetric matrix $\mathbf{P}$, $\mathbf{P} \succ 0$, through Lyapunov's matrix identity. [1]: $\mathbf{A}^{\mathrm{T}}\mathbf{P} + \mathbf{P}\mathbf{A} + \mathbf{I} = \mathbf{0}$.

Therefore, problem (P1) can be rewritten as follows

$$\min_y \Phi(y)$$
$$\text{s.t.} \quad \begin{aligned} & \mathbf{A}^{\mathrm{T}}(\mathbf{y})\mathbf{P} + \mathbf{P}\mathbf{A}(\mathbf{y}) + \mathbf{I} = 0 \\ & \mathbf{P} \succ 0 \\ & \mathbf{h}(\mathbf{y}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ & \mathbf{y} \in Y \end{aligned} \qquad \text{(P1}'\text{)}$$

Lyapunov equation forces matrix $\mathbf{P}$ to become unbounded (some element of $\mathbf{P}$ tends to infinite) when the largest eigenvalue of $\mathbf{A}$ in real part approaches zero. This behavior has been reported by [5] and also observed by the authors during their computational experiences. In order to avoid such difficulty, the positive definiteness condition is applied on the inverse of $\mathbf{P}$, which is an equivalent but numerically better-posed constraint [5]:

$$\min_y \Phi(y)$$
$$\text{s.t.} \quad \begin{aligned} & \mathbf{A}^{\mathrm{T}}(\mathbf{y})\mathbf{P} + \mathbf{P}\mathbf{A}(\mathbf{y}) + \mathbf{I} = 0 \\ & \mathbf{P}^{-1} \succ 0 \\ & \mathbf{h}(\mathbf{y}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ & \mathbf{y} \in Y \end{aligned} \qquad \text{(P1}''\text{)}$$

In Ringertz's approach [5] (P1″) is reformulated as an interior-point logarithmic-barrier transformation smooth NLP problem, which requires special algorithms to be addressed. In [9] it was proposed to apply Sylvester conditions on matrix $\mathbf{P}^{-1}$. Sylvester's criterion [14] states that the necessary and sufficient conditions for a symmetric matrix $\mathbf{Q}(n, n)$ to be positive definite, are that the determinants of its successive principal minors $\mathbf{Q}_i$ ($i = 1, \ldots, n$) be positive: $\det[\mathbf{Q}(1, 1)], \det[\mathbf{Q}(2, 2)], \ldots, \det[\mathbf{Q}(n, n)]$. Therefore, (P1″) can be reformulated into a new problem as

$$\min_y \Phi(y)$$
$$\text{s.t.} \quad \begin{aligned} & \mathbf{A}^{\mathrm{T}}(\mathbf{y})\mathbf{P} + \mathbf{P}\mathbf{A}(\mathbf{y}) + \mathbf{I} = 0 \\ & \det(\mathbf{P}_i{}^{-1}) > 0, \quad i = 1, \ldots, n \\ & \mathbf{h}(\mathbf{y}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ & \mathbf{y} \in Y \end{aligned} \qquad \text{(P1N)}$$

This is a standard NLP problem, since the determinants are themselves smooth, and can be addressed with standard gradient-based algorithms. The constraints of greater than zero on the determinants are handled through a small constant ε: $\det(\mathbf{P}_i^{-1}) \geq \varepsilon$, $\varepsilon > 0$. The equation-oriented approach proposed in [9] to address problem (P1N) requires the provision of analytic expressions of the involved determinants, which are highly nonlinear.

In order to avoid the implementation drawbacks of previous approaches (for example in [9]), the following new calculation sequence is presented to evaluate positive definiteness constraints in problem (P1N) as part of the solution procedure with standard NLP solvers:

- Solution procedure for (P1N):
  - *Step 1*: Provide a starting point for $\mathbf{y}$.
  - *Step 2*: Evaluate $\mathbf{A}(\mathbf{y})$ either analytically or numerically.
  - *Step 3*: Evaluate $\mathbf{P}$ by solving Lyapunov equation (resolution of a linear systems of equations).
  - *Step 4*: Evaluate $\mathbf{P}^{-1}$ using standard routines for inverse matrix calculation.
  - *Step 5*: Evaluate $\det(\mathbf{P}_i^{-1})$, $i = 1, \ldots, n$ using standard routines for determinant calculation.

Matrix $\mathbf{P}$ is obtained from $\mathbf{A}(\mathbf{y})$ by solving Lyapunov equation $\mathbf{A}^{\mathrm{T}}(\mathbf{y})\mathbf{P} + \mathbf{P}\mathbf{A}(\mathbf{y}) + \mathbf{I} = \mathbf{0}$ which represents a sparse system of linear equations in $n(n+1)/2$ unknowns. For the problems considered in this work, the Lyapunov equation was reformulated as a linear system of equations and solved for the elements of $\mathbf{P}$ with standard linear systems routines. Alternatively, there exist several efficient iterative techniques to solve large-scale Lyapunov equations that could be used. The ADI method [15], for example generates a sequence of matrices, which converges, often very fast, towards the solution. The ADI method has been implemented in the LYAPACK package, a Matlab toolbox for large Lyapunov and Riccati equations [16].

2.2. *Maximization of the minimum eigenvalue of a symmetric matrix*

Consider now the problem of maximizing the smallest eigenvalue of a real symmetric matrix $\mathbf{A}(\mathbf{y})$:

$$\max_{y} \lambda_{\min}(\mathbf{A}(\mathbf{y})) \quad \text{s.t.} \quad \begin{aligned} &\mathbf{h}(\mathbf{y}) = \mathbf{0} \\ &\mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ &\mathbf{y} \in Y \end{aligned} \tag{P2}$$

Problem (P2) is classically reformulated in terms of an auxiliary variable, z [5]:

$$\max_{y,z} z \quad \text{s.t.} \quad \begin{aligned} &\lambda_i(\mathbf{A}(\mathbf{y})) \geq z, \quad i = 1, \ldots, n \\ &\mathbf{h}(\mathbf{y}) = \mathbf{0} \\ &\mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ &\mathbf{y} \in Y \end{aligned} \tag{P2$'$}$$

From the definition of eigenvalue of $\mathbf{A}$: $\mathbf{Av} = \lambda\mathbf{Iv}$ ($\mathbf{v}$ stands for eigenvector). By subtracting $z\mathbf{Iv}$ to both terms it results: $(\mathbf{A} - z\mathbf{I})\mathbf{v} = (\lambda - z)\mathbf{Iv}$. Then, the condition $\lambda_i > z \Rightarrow \lambda_i - z > 0$ implies that $\mathbf{A} - z\mathbf{I} \succ 0$. Therefore, the above problem can be rewritten as

$$\max_{y,z} z \quad \text{s.t.} \quad \begin{aligned} &\mathbf{A}(\mathbf{y}) - z\mathbf{I} \succ 0 \\ &\mathbf{h}(\mathbf{y}) = \mathbf{0} \\ &\mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ &\mathbf{y} \in Y \end{aligned} \tag{P2$''$}$$

In [5] it is proposed the use of the positive condition on the eigenvalues of a symmetric matrix to ensure positive definiteness of matrix $\mathbf{A}(\mathbf{y}) - z\mathbf{I}$. Such an approach results in a logarithmic barrier transformation problem, which requires specialized algorithms to be addressed.

In order to pose a regular NLP problem which can be tackled with standard NLP solvers, the positive definiteness condition in problem (P2$''$) can be expressed in terms of the determinants of the principal minors of matrix $\mathbf{A}(\mathbf{y}) - z\mathbf{I}$, leading to the new formulation:

$$\max_{y,z} z \quad \text{s.t.} \quad \begin{aligned} &\det\{(\mathbf{A}(\mathbf{y}) - z\mathbf{I})_i\} > 0, \quad i = 1, \ldots, n \\ &\mathbf{h}(\mathbf{y}) = \mathbf{0} \\ &\mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ &\mathbf{y} \in Y \end{aligned} \tag{P2N}$$

The greater than zero constraints on the determinants are handled through a small constant ε: $\det[(\mathbf{A}(\mathbf{y}) - z\mathbf{I})_i] \geq \varepsilon$, $\varepsilon > 0$. The following new calculation sequence is presented to evaluate positive definiteness constraints:

- Solution procedure for (P2N):
  - *Step 1*: Provide a starting point for $\mathbf{y}$ and z.
  - *Step 2*: Evaluate $\mathbf{A}(\mathbf{y})$ either analytically or numerically.
  - *Step 3*: Evaluate $\mathbf{A}(\mathbf{y}) - z\mathbf{I}$.
  - *Step 4*: Evaluate $\det[(\mathbf{A}(\mathbf{y})\text{-}z\mathbf{I})_i]$, $i = 1, \ldots, n$.

3. Applications of eigenvalue optimization to dynamics and control problems

Many problems in analysis, design and control of nonlinear dynamic systems are addressed using simulation-based approaches since dynamic simulation allows the handling of large-scale nonlinear systems in a straightforward manner. Dynamic simulation, however, may be a time consuming and computationally expensive activity and alternative systematic approaches to address such problems are usually desired.

In this section, small-scale examples of classic problems in system dynamics and control are addressed by making use of eigenvalue optimization problems (P1) and (P2). The resulting models are solved according to formulations (P1N) and (P2N) and the proposed positive definiteness calculation sequences, respectively. The case study is a typical non-isothermal CSTR taken from [17], which presents a rich dynamic behavior and challenging control features.

The dimensionless model of the system, which corresponds to a non-isothermal irreversible series first order reaction, A → C → P, is

$$\dot{x}_1 = 1 - x_1 - \mathrm{Da}\, x_1 k_1(x_3) + v \tag{1}$$

$$\dot{x}_2 = -x_2 + \mathrm{Da}\, x_1 k_1(x_3) - \mathrm{Da}\, S x_2 k_2(x_3) \tag{2}$$

$$\dot{x}_3 = -x_3 + B\,\mathrm{Da}\, x_1 k_1(x_3) - B\,\mathrm{Da}\,\alpha S x_2 k_2(x_3) - \beta(x_3 - u) \tag{3}$$

where

$$k_1(x_3) = \exp\left(\frac{x_3}{1 + x_3/\varphi}\right) \tag{4}$$

$$k_2(x_3) = \exp\left(\frac{\gamma x_3}{1 + x_3/\varphi}\right) \tag{5}$$

Here x_1 is the component A dimensionless concentration, x_2 the component C dimensionless concentration and x_3 is the reactor dimensionless temperature. u is the coolant dimensionless temperature and v is considered as a bounded input that changes the value of the inlet concentration of reactant A.

It is assumed that x_3 is the controlled variable and u is manipulated for control purposes. Parameter B is considered as a disturbance and modeled as

$$B = B_n(1 + \delta) \tag{6}$$

where δ is a percentage of disturbance. Model parameters are: $\mathrm{Da} = 0.26$, $\varphi = 100$, $\beta = 7.995$, $\gamma = 1$, $S = 0.5$, $B_n = 75.1$, $\alpha = 0.426$ and $v = 0$.

The system has an open loop ($u = 0$) equilibrium point at ($x_{1\mathrm{ss}}$, $x_{2\mathrm{ss}}$, $x_{3\mathrm{ss}}$) = (0.0361, 0.0671, 4.8582). For $\delta \leq -0.1$ (-10%) the system presents oscillatory behavior (even limit cycles) and chaos for $\delta = -0.23$ (-23%). For $\delta \leq -0.64$ the system recovers asymptotic stability.

In order to stabilize such a complex behavior several feedback schemes are proposed in [17]. The simplest one is an only proportional law:

$$u(t) = k_c(x_{3,\mathrm{set}} - x_3) \tag{7}$$

where $x_{3,\mathrm{set}}$ is the desired set-point for the controlled variable and $k_c > 0$ the controller gain. See [17] for a detailed analysis of the open loop and closed loop behavior of the system under study.

In the following, three dynamic and control problems of the described CSTR are addressed as eigenvalue optimization problems (P1) and (P2). All the NLPs were solved according to the proposed strategies making use of the FFSQP feasible path SQP solver [18]. In all cases matrix **A** was numerically evaluated and parameter ε was set equal or lower than 1.0E−3 in the different problems.

3.1. Identification of bifurcations

Critical values of parameters in which steady state equilibrium solutions bifurcate are of major importance in the analysis of dynamic systems. At bifurcation points, multiple equilibriums (pitchfork bifurcations) or limit cycles (Hopf bifurcations) appear. At bifurcation points, the eigenvalues of the Jacobian matrix of the dynamic system cross the imaginary axis (annulment of the real part of the eigenvalues). For a basic introduction to bifurcations see [2].

The reactor under study presents an open loop ($k_c = 0$) bifurcation point for a certain value of parameter δ, as shown by simulation in [17]. In the following we pose the problem of finding the critical value of parameter δ at which the bifurcation occurs. We seek to minimize δ between its bounds, such that the spectrum of the Jacobian matrix of the dynamic system, **A**, critically belongs to the stable half of the complex space. The problem turns to be a type (P1) formulation:

$$\begin{aligned} &\min_{\delta, x_{1\mathrm{ss}}, x_{2\mathrm{ss}}, x_{3\mathrm{ss}}} \quad \delta \\ &\text{s.t.} \quad \begin{aligned} &\mathrm{Re}(\lambda_i(\mathbf{A})) < 0, \quad i = 1, \ldots, 3 \\ &\text{Eqs. } \{(1), \ldots, (3)\} \text{ in stationary fashion } (\dot{x}_i = 0) \\ &\text{Eqs. } \{(4), \ldots, (7)\} \\ &-0.30 \leq \delta \leq 0.10 \end{aligned} \end{aligned} \tag{8}$$

The optimization variables are δ and the steady state of the system ($x_{1\mathrm{ss}}$, $x_{2\mathrm{ss}}$, $x_{3\mathrm{ss}}$). The solution of problem (8) reformulated according to (P1N) is $\delta_c = -0.066$ (-6.6%) and ($x_{1\mathrm{ss}}$, $x_{2\mathrm{ss}}$, $x_{3\mathrm{ss}}$) = (0.0472, 0.0859, 4.550). The asymptotically stable transient response of the system for $\delta < \delta_c$, is shown in Fig. 2(a) for $\delta = -0.050$ (-5.0%) applied at $t = 2$. At $\delta = \delta_c$ the spectrum of the Jacobian matrix is {−1.3064E−6 ± 23.970i; −3.907}. The system has a pair of complex (critically imaginary) eigenvalues, which implies that a Hopf bifurcation occurs at the bifurcation point with limit cycle formation. This behavior is shown by simulation in Fig. 2(b) where sustained oscillations are obtained for a perturbation of $\delta = -0.0745$ at $t = 2$.

The system possesses another bifurcation point at $\delta_c \cong -0.635$. For $\delta \leq \delta_c$ the system recovers asymptotic stability. In order to estimate this other bifurcation point, problem (8) is slightly modified in order to maximize δ between say $-0.90 \leq \delta \leq -0.23$. The solution of the resulting (P1N) formulation is $\delta_c = -0.634$ and ($x_{1\mathrm{ss}}$, $x_{2\mathrm{ss}}$, $x_{3\mathrm{ss}}$) = (0.527, 0.326, 1.252). The corresponding eigenstructure is {−1.355E−2 ± 3.00i; −1.320}. Fig. 2(c) shows the resulting open loop oscillatory transient response.

3.2. Minimum gain for control of chaos

In the following we pose the problem of finding the smallest gain, k_c such that the resulting operating point is Lyapunov stable for $\delta = -0.23$ (-23%) for which the system verifies open loop chaos.

We seek to minimize k_c between its bounds, such that the spectrum of the Jacobian matrix of the dynamic system, **A**,

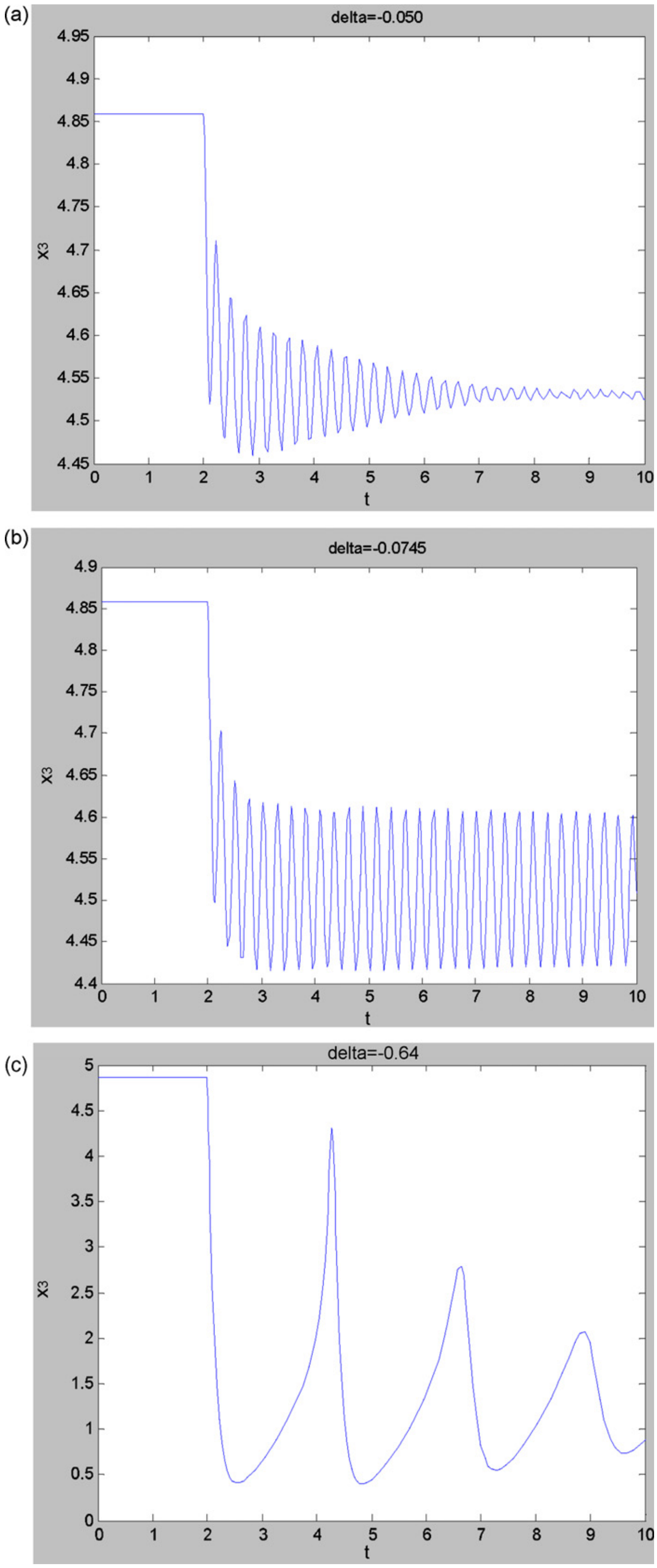

Fig. 2. Open loop transient response: (a) $\delta = -0.050$, (b) $\delta = -0.0754$, and (c) $\delta = -0.64$.

critically belongs to the stable half of the complex space. Again the problem turns to be a type (P1) formulation:

$$\min_{k_c, x_{1ss}, x_{2ss}, x_{3ss}} \quad k_c$$

$$\text{s.t.} \quad \begin{array}{l} \mathrm{Re}(\lambda_i(\mathbf{A})) < 0, \quad i=1, ..., 3 \\ \text{Eqs. } \{(1), \ldots, (3)\} \text{ in stationary fashion } (\dot{x}_i = 0) \\ \text{Eqs. } \{(4), \ldots, (7)\} \\ 0 \leq k_c \leq 5 \end{array} \tag{9}$$

The optimization variables are k_c and the steady state of the system (x_{1ss}, x_{2ss}, x_{3ss}). As result of the solution of problem (9) reformulated according to (P1N), the minimum value of the controller gain to achieve a stable response is $k_c = 0.9670$, which means that the system can be stabilized for any $k_c > 0.9670$. In Fig. 3 it can be appreciated the dynamic response for a control action applied at $t = 2$ for two values of k_c. From Fig. 3(a) it is evident that chaotic behavior is not suppressed with $k_c = 0.1$, while it is effectively controlled with $k_c = 1.0$ (Fig. 3(b)). The steady

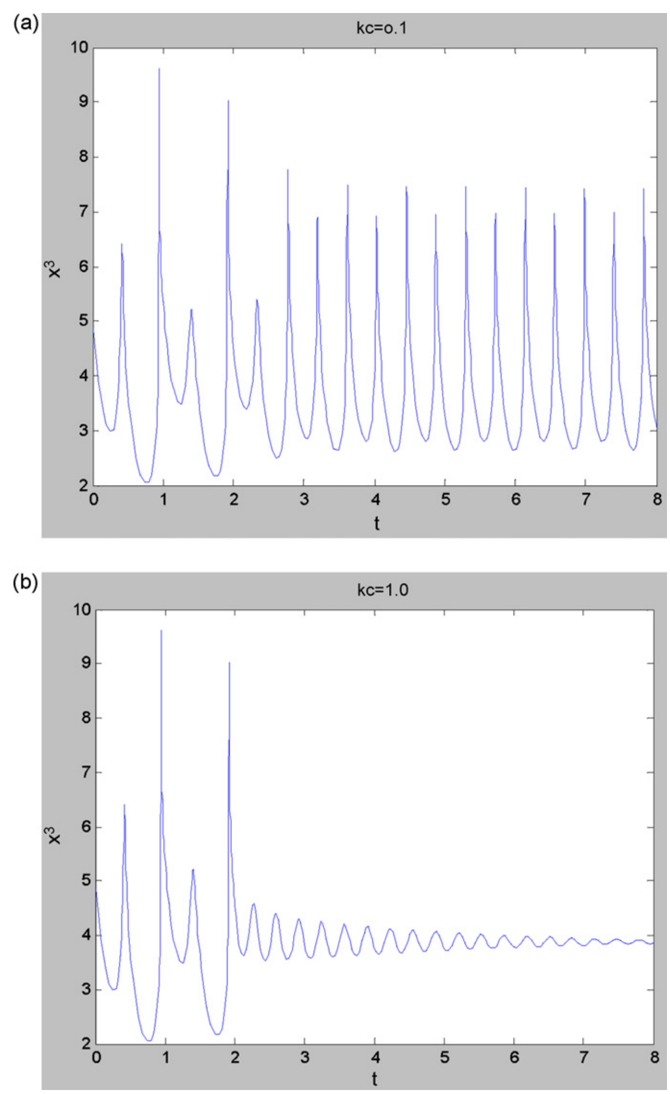

Fig. 3. Closed loop response for: (a) $k_c = 0.1$ and (b) $k_c = 1.0$.

state operating point for $k_c = 0.967$ is $(x_{1ss}, x_{2ss}, x_{3ss}) = (0.0844, 0.1425, 3.876)$. The spectrum of the corresponding Jacobian matrix is $\{-9.208\text{E}{-5} \pm 18.911\text{i}; -3.580\}$. The system has a pair of complex eigenvalues, which are very close to the imaginary axis. This implies that a Hopf bifurcation occurs at $k_c = 0.9670$ for $\delta = -0.23$ (limit cycle formation) and suggests oscillatory transient responses for $k_c > 0.967$. This behavior can be appreciated in Fig. 3(b) for $k_c = 1.0$.

3.3. Optimizing the transient response

Lyapunov's direct method provides a technique to characterize the transient response of a dynamic system [19]. Let $V(\mathbf{x})$ be a Lyapunov function of $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$. Consider parameter η defined as, $\eta = \min_x\{-\mathrm{d}V(\mathbf{x})/\mathrm{d}t/V(\mathbf{x})\}$, which may be loosely regarded as the inverse of the largest time constant of the system in the region of asymptotic stability and may be considered as a dynamic performance index of the system [19]. A large value of η suggests that the system returns rapidly to the origin. In particular, for a Lyapunov function of the form $V(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\mathbf{P}\mathbf{x}$ it stands that $\eta = \lambda_{\min}(\mathbf{P}^{-1})$.

It seems reasonable, then, to pose a design problem in order to maximize the aforementioned index, giving rise to a (P2) type eigenvalue optimization formulation:

$$\max_{k_c, x_{1ss}, x_{2ss}, x_{3ss}} \lambda_{\min}(\mathbf{P}^{-1})$$
$$\text{s.t.} \quad \begin{cases} \mathbf{A}^{\mathrm{T}}\mathbf{P} + \mathbf{P}\mathbf{A} + \mathbf{I} = \mathbf{0} \\ \text{Eqs. } \{(1), \ldots, (3)\} \text{ in stationary fashion } (\dot{x}_i = 0) \\ \text{Eqs. } \{(4), \ldots, (7)\} \\ 0 \le k_c \le k_c^{\mathrm{u}} \end{cases} \qquad (10)$$

There exists a straightforward relationship between $V(\mathbf{x})$ and the Lyapunov equation in (10) (see [1] for details). The optimization variables are z, k_c and the steady state of the system $(x_{1ss}, x_{2ss}, x_{3ss})$. The solution of (10) reformulated as (P2N) is presented In Table 1 for several values of k_c^{u}. According to the results in [17], the larger the gain the quicker the suppression of oscillations. This effect can be observed in Fig. 4(a) and (b) for two different values of k_c and $\delta = -0.23$. In agreement with such results, the upper bound, $k_c = k_c^{\mathrm{u}}$, is the value which optimizes parameter η as a result of solving problem (10). It can also be appreciated from Table 1 that z is effectively a lower bound of the smallest eigenvalue of $\mathbf{P}^{-1}$.

Table 1
Parameter η as a function of k_c

k_c^{u}	k_c	z	$\eta = \lambda_{\min}(\mathbf{P}^{-1})$
1.0	1.0	4.69183E−4	4.69189E−4
2.0	2.0	1.83360450E−2	1.83360457E−2
3.0	3.0	4.3717764E−2	4.3717765E−2
4.0	4.0	7.68382492E−2	7.68382499E−2
5.0	5.0	0.117723585	0.117723587

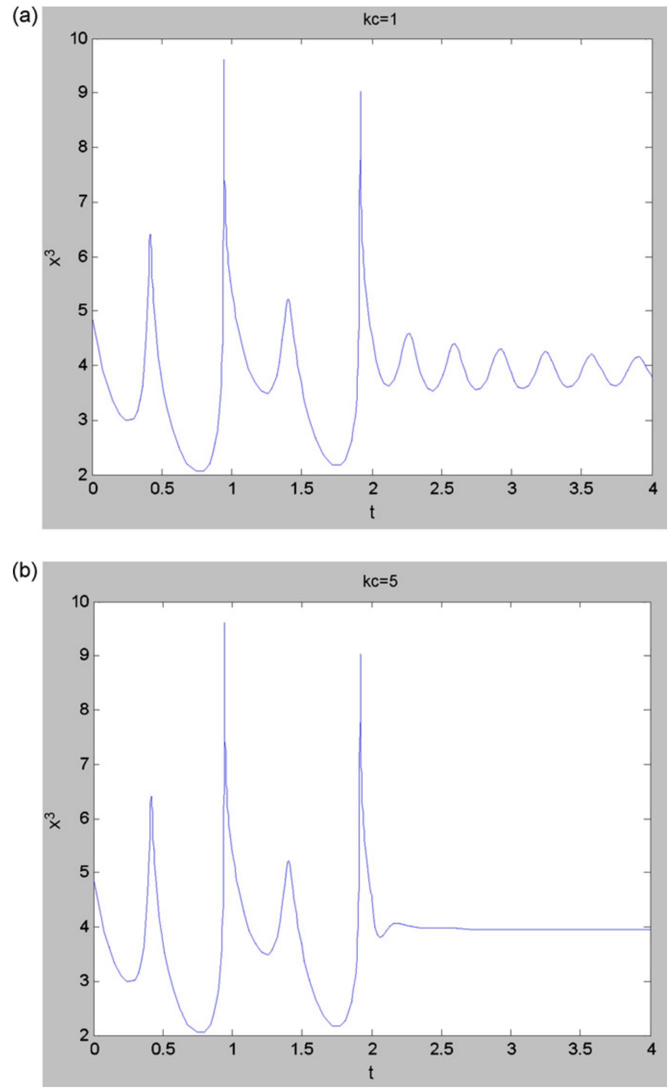

Fig. 4. Closed loop response for: (a) $k_c = 0.1$ and (b) $k_c = 1.0$.

4. Conclusions and future work

In this work, outstanding theoretical aspects on eigenvalue optimization, relevant to chemical engineering applications have been reviewed. Since existing techniques for eigenvalue optimization are numerically hard to implement, novel solution procedures were also introduced. The principal advantage of such solution strategies is that they present regular NLP formulations and can therefore be tackled with standard NLP solvers. The presented formulations were illustrated by means of applications to the dynamic and control problems of a chemical engineering pertinent system: a nonlinear CSTR with a rich dynamic behavior. The appealing feature of the proposed eigenvalue optimization techniques is that they allow a rather systematic "optimization-based" approach to some dynamic problems which have a classic tedious "simulation-based approach".

Future work on the subject will consider larger dynamic models in the state and parameters spaces in order to address more realistic chemical engineering systems. Preliminary results have been obtained in [20] for a medium scale system (matrix **P** of dimension 26) where the redesign-for-stability problem of the Tennessee Eastman Challenge Process, an open loop unstable recycle reactor, was addressed in the context of problem (P1)/(P1N). However, for larger scale problems the calculation of the inverse of **P** might become a limitation and alternative formulations could be required.

It is also considered that eigenvalue optimization techniques might represent a valuable tool in a comprehensive study of bifurcations in the context of problem (P1). In the proposed approach for identification of bifurcation points (Section 3.1), only information about the type of bifurcation, Hopf or pitchfork, can be inferred from the nature of the eigenvalues (real or complex) at the bifurcation point. In order to obtain information about the nature of the bifurcation (sub- or super critical), of relevance in engineering applications, higher order bifurcation conditions should be included in problem (P1).

Moreover, the generalization of flexibility techniques to cope with disturbance and parametric uncertainty in the context of formulation (P1), as those proposed in [21], would represent a meaningful contribution to nonlinear systems analysis. For example systematic techniques to estimate multi-parametric bifurcation surfaces, instead of single parameter bifurcation points, as well as domains of attractions of equilibrium points would be welcome since such studies have up to date a rather "artistic" approach, limited to low dimension state and parameter spaces.

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Appendix A. Nomenclature

$\mathbf{A}$	general matrix
Da, φ, β, γ, S, B_n, α, υ	parameters of the CSTR
$\det(\cdot)$	determinant
$\mathbf{f}(\cdot)$	general dynamic functions vector
$\mathbf{h}(\cdot)$	vector of equality constraints
$\mathbf{g}(\cdot)$	vector of inequality constraints
$\mathbf{I}$	identity matrix
k_c	controller gain of the CSTR
n	dimension of the dynamic system
$\mathbf{P}$	Lyapunov matrix
u	manipulated variable of the CSTR
$\mathbf{v}$	general vector
$V(\cdot)$	general Lyapunov function
$\mathbf{x}$	general state vector
x_1, x_2, x_3	states of the CSTR
$x_{1ss}, x_{2ss}, x_{3ss}$	steady state values of the CSTR
$x_{3,set}$	set point value for state x_3 of the CSTR
$\mathbf{y}$	vector of optimization variables
Y	space of optimization variables
z	auxiliary variable

Greek letters

δ	disturbance variable of the CSTR
ε	small positive constant
$\Phi(\cdot)$	general objective function
η	dynamic performance index
λ_i	eigenvalue
λ_{min}	minimum eigenvalue

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