OPTIMAL CONTROL APPLICATIONS AND METHODS

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Optimal control of nonlinear chemical reactors via an initial-value Hamiltonian problem

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SUMMARY

The problem of designing strategies for optimal feedback control of nonlinear processes, specially for regulation and set-point changing, is attacked in this paper. A novel procedure based on the Hamiltonian equations associated to a bilinear approximation of the dynamics and a quadratic cost is presented. The usual boundary-value situation for the coupled state-costate system is transformed into an initial-value problem through the solution of a generalized algebraic Riccati equation. This allows to integrate the Hamiltonian equations on-line, and to construct the feedback law by using the costate solution trajectory. Results are shown applied to a classical nonlinear chemical reactor model, and compared against suboptimal bilinear-quadratic strategies based on power series expansions. Since state variables calculated from Hamiltonian equations may differ from the values of physical states, the proposed control strategy is suboptimal with respect to the original plant. Copyright © 2005 John Wiley & Sons, Ltd.

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1. Introduction

Chemical reactors are a classical source of problems in the nonlinear control literature, and a number of other nonlinear chemical processes are receiving increasing attention ([6, 7, 14, 1, 18, 4], and their references). Due to this diversity, control techniques still compete on applicability and efficiency for general nonlinear processes. Since nonlinearities and main qualitative features of industrial processes are often detected without having a complete mathematical description of their dynamics, some techniques are being developed to overcome the use of models in designing control laws. Partial Control is one of these novel decentralized strategies conceived for meeting multiple economic objectives by feedback control of a few 'dominant variables' (see [26]). The concept is appealing because, if successful, a few SISO control loops replace the conventional process model for control purposes. Individual loops are in principle simpler to treat, instrument, and tune than multidimensional interconnected situations. But this simplification is not always possible, as the model chosen in this paper for illustration shows.

The steady-states' phase-plots for nonlinear dynamics adopt different patterns, sometimes leading to bifurcations, limit cycles, or strange attractors in high dimensions [23, 6]. These patterns may change, even structurally, when parameters of the dynamics vary (equilibrium control values may be regarded as parameters, specially when each manipulated variable is proportional to some physical variable like temperature or flow rate [2]. Consequently, changing operation from one steady-state to another may imply working near periodic orbits or bifurcation points, where model information is essential.

Disjoint from heuristic methods there exist a range of model-based approaches, Model Predictive Control (MPC) becoming the most widely quoted in recent literature. Still, for nonlinear systems MPC is only recommended in very special situations [11, 19] given the computational complexity of the calculations involved. Most successful industrial applications of MPC reported so far are in refining and petrochemical plants, where (continuous) processes are run near optimal steady-states and model linearizations are reliable approximations. Only one of the available commercial software packages was cautiously suggested for truly nonlinear or batch processes in a recent survey [20].

Some numerical implementations of MPC discretize the whole space $\mathcal{X} \times \mathcal{T}$ from the beginning, which for nonlinear systems have predictable shortcomings ($\mathcal{X}$ denoting the state space and $\mathcal{T}$ the time span where the performance is to be optimized). Trajectory perturbations are increasingly important in the nonlinear case, specially near unstable steady-states. Since states are allowed to take only discrete positions in the calculations, being near unstable equilibria may not be noticed by the algorithms. Contrarily, feedback laws are determined from ODE's parameters that contain all stability information. Also, control values calculated from these laws generally depend on the exact (actual) values of state variables. However sometimes a suboptimal control can be constructed from approximate state values generated numerically on-line, as will be illustrated through numerical examples.

To attain the same degree of accuracy with the MPC approach involves refining the discretization (so increasing the computing time, which makes troublesome to keep on-line work), and guaranteeing convergence of this refining (rarely taken into account). Minimizing computing time in nonlinear MPC is not a trivial problem, as reflected by the variety of unrelated techniques (Hammerstein, Wiener, and ARX polynomials, neural networks, piecewise linear models) used to attack the resulting Nonlinear Programming set-up numerically. Basically MPC requires exploring and calculating the cost of many trajectories at many time instants. Also, some review literature asserts that MPC does not guarantee success in general MIMO systems situations [24].

In this paper, an optimal control technique based on universal approximations of general systems coupled with quadratic-type expressions of the economic objectives is proposed for nonlinear processes. This technique is specially applicable to multivariable situations that are not reducible to single loops. Some positive features of both partial control and MPC approaches are present in this proposal, while avoiding their main limitations and inconveniences. Feedback control laws instead of nonlinear programming are adopted, as in the first class of techniques; but model-based rather than empirical knowledge guides the calculations, in accordance with the second class. Bilinear approximations describe the dynamics. They have shown to be able to approximate fairly general nonlinear systems under bounded control situations and for a prescribed time period [12, 25], a feature that linear systems can not meet in general [17]. Bilinear models were introduced long ago in the chemical engineering literature (see for instance [5]), and since then a number of improvements have been devised to treat different control problems on these systems, like regulation, tracking, and filtering. In particular, the optimal state estimate (in the least-squares sense) for bilinear systems is the solution to the Kalman-Bucy differential equation (with a slightly different time-dependent linear coefficient, see [8] for details). The Kalman-Bucy equation can be integrated on-line, along the lines of the control strategy devised in this paper.

As the case-application a well known nonlinear reactor model is revisited [21]. Equations correspond to the 'series/parallel Van de Vusse reaction', taking place in a perfectly mixed container. There are clearly two variables in the example that need to be controlled, and just one variable (a flow rate) available for manipulation. No I/O pairing is possible since both states must be optimized, however the exact values of the states are not continuously needed to construct the suboptimal control. They are approximated from the solution to the Hamiltonian equations, which are run in parallel.

The graph of equilibrium control values contains closed curves in phase space, situation described as 'system with input multiplicities' in the literature. Therefore, changes in set point not always involve changes in the final equilibrium value of the manipulated variable (a parameter whose value may have been optimized a priori).

Adaptive strategies will not be discussed here for simplicity. The formulas used in the numerical examples were advanced in [8]. Set-point changes are eventually treated as tracking problems (following [9, 10]) for comparison with the typical servo formulation.

In the following sections we describe the control strategy, the system to be controlled, some numerical results and comparisons with other methods applied to the controlled process, and conclusions.

2. The control strategy

Nonlinear control processes under consideration will be those accurately modeled by equations of the form

$$\dot{x} = f(x, u), \tag{1}$$

where the function f is at least continuously differentiable and the admissible control strategies are at least piecewise continuous, uniformly bounded functions of time t, the implicit independent variable taking values in an interval $\mathcal{T}$ of the real numbers. States x are assumed to evolve in some open set $\mathcal{O}$ of the n-dimensional Euclidean space, so $\mathcal{X} = \mathcal{O}$ in what follows, and just for simplicity of notation [15] the control values will be taken as scalars. Special restrictions on the state variables will not be consider here. They usually lead to difficult problems that exceed the scope of this paper, as those requiring the setup of control on manifolds.

Restrictions on control values admit the same treatment given to the linear-quadratic problem in standard texts (see for instance [3], sec. 6-20 and chapter 10). The resulting optimal control in those cases is continuous, and simply sticks to the bound when the 'unbounded solutions' trespasses the limiting set (see figure 10 in this paper). The trade-off between maintaining control constraints and maintaining unbounded optimality is impossible to assess in the quadratic-cost context, sense the (only) parameter r measuring the control effort is independent of u (in other words, imposing a control bound in this context is equivalent to say: 'if the control value exceeds the bound, then the cost will be infinite').

Under these conditions, as announced in the Introduction, nonlinear systems can be universally approximated by bilinear models of the form

$$\dot{x} = Ax + (B + Nx)u, \qquad x(0) = x_0, \tag{2}$$

where the initial state $x_0 \in \mathcal{O} \subset \mathbb{R}^n$, real matrices A, B, and N having the appropriate orders. An equilibrium of the original system is a pair $(\bar{x}, \bar{u})$ that makes $f(\bar{x}, \bar{u}) = 0$. When the system evolves near such an equilibrium a natural bilinearization would be $A = \frac{\partial f}{\partial x}(\bar{x}, \bar{u})$, $B = \frac{\partial f}{\partial u}(\bar{x}, \bar{u})$, $N = \frac{\partial^2 f}{\partial u \partial x}(\bar{x}, \bar{u})$. When the trajectories of the approximate model depart from real trajectories more than accepted, then a Carleman type of technique can be used to construct a higher-order, more accurate, bilinear model [17, 7] from the original nonlinear equations and without lacking physical meaning of the states. It has been shown [5] that the optimal control of the sequence of bilinear approximations (each one suboptimal with respect to the original nonlinear plant) tend to the optimal control for the fully nonlinear-quadratic problem. Then it will be assumed that model mismatch can be mitigated still maintaining the bilinear context. The underlying objective function will be the classical quadratic cost $J_T(x_0, 0, u(\cdot))$ referred to the (x, u) trajectories generated by control functions $u(\cdot)$, starting (when $t = 0$) at the state $x(0) = x_0$, acting during a time span of duration (with horizon) $T \in (0, \infty]$, and evaluated from

$$J_T(x_0, 0, u(\cdot)) = \int_0^T [(x(t) - \bar{x})' Q(x(t) - \bar{x}) + r(u(t) - \bar{u})^2(t)]dt + (x(T) - \bar{x})' S(x(T) - \bar{x}) \quad (3)$$

where Q and S are positive semi-definite matrices ($S = 0$ for $T = \infty$), and r is a positive scalar (the case $r = 0$ is explicitly excluded, sense it implies a 'singular optimal control problem', whose solution, even for the linear-quadratic case, may not exist as an ordinary function but may belong to the class of 'distributions' or 'generalized functions', see for instance [27]).

Therefore, in what follows the optimal control problem would consist on minimizing J_T with respect to all admissible (piecewise continuous) control trajectories $u(\cdot)$. For the regulator problem, $(\bar{x}, \bar{u})$ should be regarded as the original equilibrium (a pair where $\bar{x}$ is a steady-state and $\bar{u}$ the corresponding constant control value), and from which disturbances should be abated. Usually, in regulation problems the variables are defined relative to this equilibrium, and then assuming $(\bar{x}, \bar{u}) = (0, 0) \in \mathcal{O}$ is appropriate. For the servo (or set-point change) problem no relative values for states or controls will be used, since there are more than one equilibrium involved: $(\bar{x}, \bar{u})$ is the pair consisting of the target set-point and its corresponding equilibrium control, which usually should be reached from the original equilibrium (x_0, u_0). It will become clear that in the nonlinear context the servo problem can not be reduced to a relative regulator problem around the target set-point.

The Hamiltonian for the regulator problem can be written then

$$H(x, u, \lambda, t) = H(x, u, \lambda) = x'Qx + ru^2 + \lambda'[Ax + (B + Nx)u]. \tag{4}$$

Here the adjoint variable (or costate) λ is a column vector, associated in optimal control theory to the transpose of the (row) gradient $\frac{\partial V}{\partial x}$ of the value function V defined by

$$V(x, t) \quad \triangleq \quad \inf_{u(\cdot)} \quad J_T(x, t, u(\cdot)). \tag{5}$$

This Hamiltonian is regular [16], and has the unique extremum

$$u^0(x, \lambda) \triangleq -\frac{1}{2r}(B + Nx)'\lambda, \tag{6}$$

which does not depend explicitly on t.

The Hamiltonian expression of this optimal control problem, (or its Hamiltonian equations, see for instance [22]), takes the form of the following two-point boundary-value problem

$$\dot{x} = \left(\frac{\partial \mathcal{H}}{\partial \lambda}\right)'(x, \lambda); \quad x(0) = x_0, \tag{7}$$

$$\dot{\lambda} = -\left(\frac{\partial \mathcal{H}}{\partial x}\right)'(x, \lambda); \quad \lambda(T) = 2Sx(T), \tag{8}$$

where $\mathcal{H}(x,\lambda) \triangleq H(x, u^0(x,\lambda), \lambda)$. For regular Hamiltonians, to solve this boundary-value problem is equivalent to solve the Hamilton-Jacobi-Bellman (HJB) partial differential equation

$$\frac{\partial V}{\partial t} + \mathcal{H}\left(x, \left(\frac{\partial V}{\partial x}\right)'\right) = 0, \tag{9}$$

with the boundary condition

$$V(x,T) = x'Sx \qquad \forall x \in \mathcal{O}. \tag{10}$$

The regulator problem for an infinite horizon ($T = \infty$) has been solved [5] by proposing

$$V(x,t) = V(x); \qquad \lambda = \left(\frac{\partial V}{\partial x}\right)'(x) = 2P(x)x, \tag{11}$$

with $P(x)$ an $n \times n$ symmetric matrix allowing a generalized power series expansion

$$P(x) = P_1 + P_2\frac{x}{2!} + P_3\frac{x^{[2]}}{3!} + P_4\frac{x^{[3]}}{4!} + \cdots \tag{12}$$

where $x^{[i]}$ is the i^{th}-generalized power of the vector x (see [5] for details) and the $P_i, i = 1, 2, \ldots$ are constant matrices of appropriate dimensions. Since there is no time-dependence of the value function, the HJB equation reads in this case

$$\mathcal{H}(x,\lambda) = x'Qx + \lambda' Ax - \frac{1}{4r}\lambda'(B + Nx)(B + Nx)'\lambda = 0 \tag{13}$$

Equations for the series coefficients of $P(x)$ were originally found from the conventional method of replacing the series expression into the HJB equation and collecting terms. The results of this approach have shown some practical inconveniences, since there exists no theoretical indication as to how many coefficients should be evaluated in each problem to obtain the desired accuracy for all state trajectories. The dimensions of the matrix coefficients P_i increase fast with the generalized power i, so it may become cumbersome to calculate, store, and use those coefficients to evaluate the feedback law in real time.

In this paper a novel and simpler procedure is presented. By calling

$$W(x) \triangleq \frac{(B+Nx)(B+Nx)'}{r} \tag{14}$$

then, equation (13) is equivalent to

$$x'[Q + 2P(x)A - P(x)W(x)P(x)]x = 0 \qquad \forall x \in \mathcal{O}. \tag{15}$$

Since $P(x)$ was assumed symmetric, and equation (15) must be verified for all x in an open set that contains the origin, then it will be sufficient to ask that

$$Q + P(x)A + A'P(x) - P(x)W(x)P(x) = 0 \qquad \forall x \in \mathcal{O}. \tag{16}$$

Equation (16) is a Riccati equation for each x, of the same type as the Algebraic Riccati Equation (ARE) appearing in the classical linear-quadratic regulator problem, and therefore (see [22]), under the restrictions imposed on the constant matrices, it is known that there exists a unique symmetric positive definite solution $P(x)$ for each x.

This result allows then to write the optimal feedback law in the form

$$u^*(x) = -\frac{1}{r}(B+Nx)'P(x)x. \tag{17}$$

Now, solving a Riccati equation for each x is not quite appropriate for on-line control in general, but the existence of $P(x)$ is most useful. In fact, it is the basis for the alternative method proposed below, which can be readily implemented in real time.

Actually, if equation (16) is solved just for x_0, then the Hamiltonian equations associated to the optimal-control problem can be posed as an initial-value problem, namely

$$\dot{x} = \left(\frac{\partial \mathcal{H}}{\partial \lambda}\right)' = Ax - \frac{1}{2}W(x)\lambda; \quad x(0) = x_0 \tag{18}$$

$$\dot{\lambda} = -\left(\frac{\partial \mathcal{H}}{\partial x}\right)' = -2Qx - A'\lambda + \frac{1}{2r}N'\lambda(B+Nx)'\lambda; \quad \lambda(0) = 2P(x_0)x_0 \tag{19}$$

Notice that for nonlinear systems, even in the infinite horizon case, the initial value for the costate λ is not known, so this formulation may be considered as an important indirect contribution of using bilinear models as approximations. It is also interesting to check, by making $N = 0$ in these equations, that the bilinear result is reduced to the well-known linear-quadratic steady-state solution, and $P(x) = P$, the solution to the standard ARE equation.

Summarizing, the new strategy for obtaining the optimal control of the bilinear-quadratic regulator problem would consist in: (i) solving equation (16) for $P(x_0)$, and then (ii) integrating the Hamiltonian equations on-line, which allows to evaluate the optimal control in feedback form by using the costate solution $\lambda(\cdot)$ to equations (18-19), i.e.

$$u^*(x,t) = u^0(x,\lambda(t)) = -\frac{1}{2r}(B+Nx)'\lambda(t). \tag{20}$$

The optimal control is constructed from both the state x and the costate λ calculated from equations (18-19). Therefore, as long as the bilinear approximation is accurate, then the physical states need not be continuously measured. This is an important feature when dealing with chemical reactors, for instance, since concentrations are usually not available at all times.

Another advantage of this method, in the regulation context, is its robustness. It is known that the optimal bilinear-quadratic solution generates a closed loop with infinite gain margin (see [13] for details).

For the servo problem, still in the infinite horizon case, the same type of strategy can be derived through the slightly different proposal

$$V(x,t) = V(x); \qquad \lambda = \left(\frac{\partial V}{\partial x}\right)'(x) = 2\tilde{P}(x)(x-\bar{x}), \tag{21}$$

where $\bar{x}$ is the target set-point to which the initial state x_0 (eventually the original set-point) should be driven.

The extremum of the Hamiltonian is found to be attained for

$$u^0(x,\lambda) \triangleq \bar{u} - \frac{1}{2r}(B+Nx)'\lambda, \tag{22}$$

and the corresponding Hamiltonian equations in initial-value form can be written now:

$$\dot{x} = Ax + (B+Nx)\bar{u} - \frac{1}{2}W(x)\lambda; \quad x(0) = x_0 \tag{23}$$

$$\dot{\lambda} = -2Q(x-\bar{x}) - \tilde{A}'\lambda + \frac{1}{2r}N'\lambda(B+Nx)'\lambda; \quad \lambda(0) = 2\tilde{P}(x_0)(x_0-\bar{x}) \tag{24}$$

where $\tilde{A} \triangleq A + \bar{u}N$, and $\tilde{P}(x)$ is the unique symmetric positive definite solution to the Riccati equation

$$Q + \tilde{P}(x)\tilde{A} + \tilde{A}'\tilde{P}(x) - \tilde{P}(x)W(x)\tilde{P}(x) = 0. \tag{25}$$

Formally, the optimal feedback law for the servo problem is then

$$u^*(x) = \bar{u} - \frac{1}{r}(B+Nx)'\tilde{P}(x)(x-\bar{x}), \tag{26}$$

but in practice the on-line-appropriate form is preferred:

$$u^*(x,t) = u^0(x, \tilde{\lambda}(t)) = \bar{u} - \frac{1}{2r}(B + Nx)'\tilde{\lambda}(t), \tag{27}$$

where $\tilde{\lambda}(\cdot)$ is the costate-part of the solution to equations (23-24).

A final observation: the Hamiltonian equations (18-19) for the regulator problem may be recovered from equations (23-24) associated to the servo problem (simply put $(\bar{x}, \bar{u}) = (0, 0)$). But the converse is not true. If deviations from the target equilibrium, namely $x - \bar{x}$, $u - \bar{u}$, and their dynamics are replaced by x, u in the regulator equations (18-19), then the servo equations (23-24) are not obtained as written above unless the system is linear ($N = 0$). This shows that the regulator and servo problems are not equivalent in the nonlinear context, as announced.

3. A classical nonlinear chemical process. The flow structure.

Consider a nonlinear continuous stirred tank reactors (CSTR) in which the exothermic first-order irreversible Van de Vusse reaction is taking place (we follow the notation and order-reduction assumptions of [21]). The dimensionless equations for the mass and heat balances are

$$\begin{aligned} \dot{x}_1 &= -\theta x_1 \exp(\frac{x_2}{1 + x_2/\gamma}) + q(x_{1f} - x_1) \\ \dot{x}_2 &= \beta\theta x_1 \exp(\frac{x_2}{1 + x_2/\gamma}) + q(x_{2f} - x_2) - \delta x_2 \end{aligned} \tag{28}$$

Typical values for the parameters are $\theta = 0.135$, $\gamma = 20.0$, $x_{1f} = 1.0$, $\beta = 11.0$, $x_{2f} = 0.0$, and $\delta = 1.5$, the variable x_1 is the dimensionless extent of reaction and x_2 is the dimensionless reactor temperature. The independent variable is $\tau = t/t_c$, where t is the physical time and t_c a characteristic time of the reactor. For the parameter values used here, t_c is in the order of

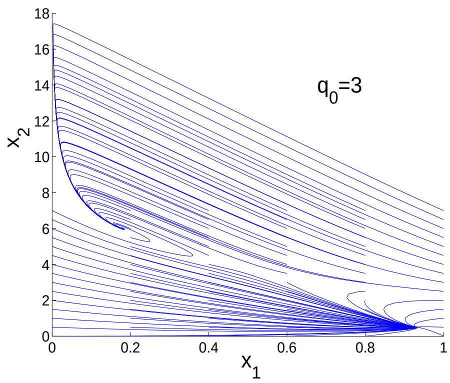

Figure 1. Phase plane for $q_0 = 3$

one minute (see [21] and the references therein). Each numerical simulation has consumed a computer time in the order of one second, which indicates that online calculations can readily be implemented.

The dimensionless feed flow rate q is the only variable that can be manipulated. Usually it is chosen to conduct operation around a fixed value q_0 of the flow-rate, and then an appropriate definition for the control variable would be $u = q - q_0$.

So in what follows the dynamics under consideration will be

$$\dot{x}_1 = -0.135 x_1 \exp\left(\frac{x_2}{1 + x_2/20}\right) + (q_0 + u) - (q_0 + u)x_1 \tag{29}$$

$$\dot{x}_2 = 1.485 x_1 \exp\left(\frac{x_2}{1 + x_2/20}\right) - 1.5 x_2 - (q_0 + u)(x_2) \tag{30}$$

In figure (1) the phase plane plot shows the qualitative behavior corresponding to multiple equilibria for a fixed value of the parameter q_0. Since q_0 is associated with flow rate, an operational problem arises when trying to change the (state) set-point without changing the final value of q (possibly dictated by the steady-state functioning of the rest of the plant) since the state trajectory must navigate through potentially adverse conditions as the structure of the flow changes.

4. Numerical simulations

The two typical feedback control situations are explored for the reactor model of section 3: regulation control near an operational set-point, and optimal changes of set-point (typically from one steady-state of the system to another).

4.1. Regulation

In this case it will be assumed that a perturbation occurs when the reactor is conducted around the (generic) steady-state $x = 0$, and control is required to return the system to rest. The system is bilinearized near the steady-state, rendering the bilinear matrices: A, B, N. The optimization parameters where fixed at the following nominal values: $T = 2$, $Q = I$, $r = 0.33$. These values were adopted in a roughly proportional correspondence with a previous one-dimensional version of the optimal control of the Van de Vusse reactor ([10], figures 7-9), which was compared against the referential Sistu and Bequette strategy [21]. Just to improve resolution the figures in the present paper do not always cover the whole time-horizon. In practice all optimization parameters should be consistent with the subjacent static optimization objectives decided at the designing level.

The goal in this regulation problem is to maintain the system near the steady-state

$$\bar{x} = \begin{pmatrix} 0.932 \\ 0.501 \end{pmatrix}.$$

with the minimum quadratic cost. As a first example the simulated initial states (post perturbation) are set at

$$x_0 = \begin{pmatrix} 1.4 \\ 0.9 \end{pmatrix}.$$

The bilinear approximation calculated near equilibrium through partial derivatives of the original dynamics renders the matrices:

$$A = \begin{pmatrix} -3.22017 & -0.195209 \\ 2.42191 & -2.3527 \end{pmatrix}, B = \begin{pmatrix} 0.068373 \\ -0.501403 \end{pmatrix}, N = \begin{pmatrix} -1.0 & 0.0 \\ 0.0 & -1.0 \end{pmatrix}.$$

The value of $P(\hat{x}_0)$ at the original perturbation $\hat{x}_0 = x_0 - \bar{x}$ results

$$P(\hat{x}_0) = \begin{pmatrix} 0.1923 & 0.0599 \\ 0.0599 & 0.1843 \end{pmatrix},$$

which is easily checked to be symmetric and positive-definite. Then, the initial value of the costate, needed to start integration of the Hamiltonian equations on-line is

$$\lambda(0) = 2P(\hat{x}_0)\hat{x}_0 = \begin{pmatrix} 0.2277 \\ 0.2031 \end{pmatrix}.$$

The states and control trajectories resulting from the feedback law devised in Section 2, corresponding to the optimal bilinear-quadratic problem but applied to the original nonlinear dynamics, are shown in figures 2-3. These are also plotted and compared against the solution to the same problem obtained by using power series expansions, which is less accurate, probably due to truncation errors (coefficients only up to P_2 were kept). Matrices A, B, N were automatically adapted using the software devised in [8], but the dimension of the bilinear model was maintained at $n = 2$.

Note that the states go to zero but not both monotonically, which indicates that the nonlinear behavior is an essential characteristic of this problem (an optimal linear-quadratic problem produces trajectories going monotonically to zero in norm, since the optimal feedback law is also linear).

The simulation also produced the costate trajectories (not depicted), which go to zero as desired; and the value of the Hamiltonian along the combined $(x(\cdot), \lambda(\cdot))$ trajectory, calculated from equation (13), which stays negligibly deviated from zero. This possibility of evaluating the Hamiltonian on-line (actually, of checking the whole HJB equation) may help to decide when to increase the dimension of the bilinear approximation.

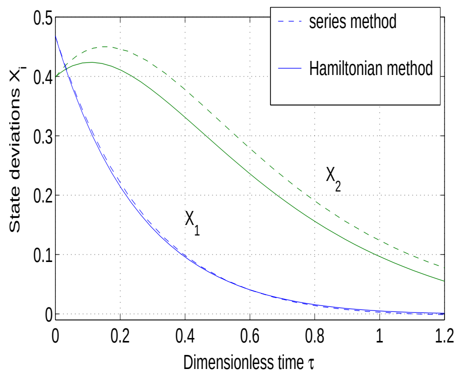

Figure 2. States deviations $X_i = x_i - \bar{x}_i$ vs. time trajectories for the regulation case. Steady-state $\bar{x} = (0.932, 0.501)'$ perturbed to $(1.4, 0.9)'$. Equilibrium control $q = \bar{u} = 3$. The leftmost curves correspond to $(x_1 - \bar{x}_1)$ and the others to $(x_2 - \bar{x}_2)$.

The optimal control law works well in this case, despite the strongness of the simulated perturbation (around half the size of the desired values). This behavior may be inferred from the dynamics: the perturbed initial state lies in a region for which the flow trajectories do not change their qualitative pattern, and the values of q involved have little variation.

Another perturbation around the same $\bar{x}$, much smaller in size but differing in sign for the

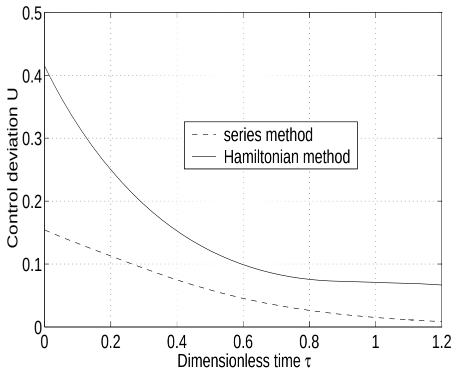

Figure 3. Control deviation $U = u - \bar{u}$ vs. time-trajectory for the regulation case. Steady-state: $(0.932, 0.501)'$ perturbed to $(1.4, 0.9)'$. Equilibrium control $q = \bar{u} = 3$.

two states, is regulated with little effort (a small overshooting appears for one of the states), as shown in figures 4 and 5.

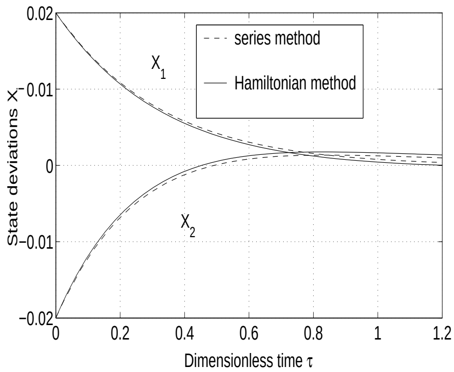

Figure 4. Evolution of regulated state variables. Steady-state: $(0, 0)'$ (relative), perturbed to $(0.02, -0.02)'$. Steady-state (absolute): $\bar{x} = (0.932, 0.501)'$. $X = x - \bar{x}$.

Even when perturbations are small, a linear approximation treated with `Matlab` MPC (see figure 6) results unable to send both states to zero simultaneously with just one manipulated variable, and also its cost is higher than the cost of the nonlinear strategy. The cumulative

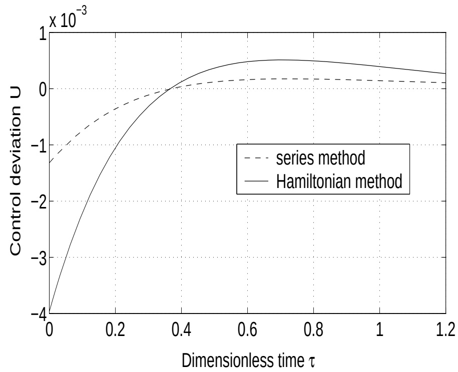

Figure 5. Evolution of regulating control variable. Steady-state: $(0, 0)'$ (relative), perturbed to $(0.02, -0.02)'$. Steady-state (absolute): $\bar{x} = (0.932, 0.501)'$. $\bar{u} = 3$. $U = u - \bar{u}$.

cost for this regulation process is about 0.075. Meanwhile, the correspondent MPC calculated cost (same units of measure) is 0.133.

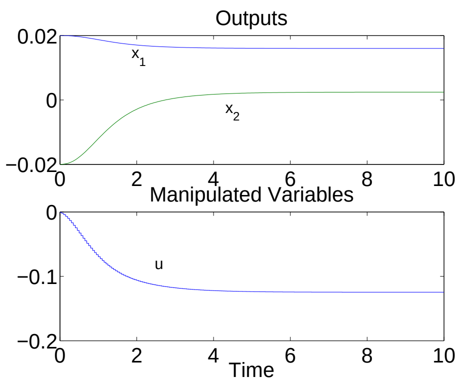

Figure 6. States vs. time trajectories for the regulation case using MPC. Steady-state: $(0, 0)'$ (relative), perturbed to $(0.02, -0.02)'$. The uppermost curve corresponds to x_1 and the lower one to x_2.

4.2. Changes of set-point. The servo problem.

Operational flexibility may induce to change the set-point, which in principle has to be performed in an optimal fashion. Decisions of this kind have been reported in the classical Chemical Engineering literature, even conducting to unstable equilibria, usually obeying to 'new' economical restrictions.

The problem under consideration may be reformulated as one of tracking, with the reference trajectory $x_r(\cdot) \equiv \bar{x} \quad \forall t \in [0, T]$. The tracking objective pursues the control $u(\cdot)$ that leads the initial state (eventually the original set-point) x_0 to the target set-point $\bar{x}$ in an optimal way. This problem has been treated in [10] and the references herein, so only the relevant equations are recalled here.

The solution of the HJB equation for linear dynamics suggests for the bilinear situation a generalization like

$$V(x,t) = \varphi(t) - x'\xi(t) + x'P_1(t)x + x'P_2(t)\frac{x^{[2]}}{3!} + x'P_3(t)\frac{x^{[3]}}{4!} + \dots \tag{31}$$

which can be also written

$$V(x,t) = \varphi(t) - x'\xi(t) + x'P(x,t)x. \tag{32}$$

The partial derivatives will allow for simple expressions

$$V_t(x,t) = \dot{\varphi}(t) - x'\dot{\xi}(t) + x'\dot{P}_1(t)x + \dots \tag{33}$$

$$V_x(x,t) = -\xi(t) + 2P_1(t)x + \dots = -\xi(t) + 2P(x,t)x \tag{34}$$

which replaced into the HJB equation and collecting terms generate the following set of ordinary differential equations

$$\dot{\varphi} \quad = \quad -\bar{x}'Q\bar{x} + \frac{1}{2r}\xi'BB'\xi \tag{35}$$

$$\dot{\xi} = -2Q\bar{x} + A'\xi + \frac{1}{2r}P_1'BB'\xi - \frac{1}{2r}N'\xi\xi'B \tag{36}$$

$$\begin{aligned}\dot{P}_1 &= -Q - A'P_1 + P_1A + \frac{1}{r}P_1'BB'P_1 - \frac{2}{r}(N'\xi B'P_1 + P_1'NB'\xi) \\ &\quad + \frac{1}{r}N'\xi\xi'N + \frac{1}{r}(\xi'\widetilde{BB'}P_2)\end{aligned} \tag{37}$$

$$\begin{aligned}\dot{P}_2 &= -3A'P_2 + \frac{3}{r}P_1'BB'P_2 - \frac{3}{r}B'\xi N'P_2 - \frac{3}{r}N'\xi B'P_2 \\ &\quad + \frac{3}{r}(P_1'B - N'\xi)(N'\widetilde{P_1 + P_1'}N)\end{aligned} \tag{38}$$

where the symbol $\widetilde{\ }$ stands for symmetrization tensor operations needed to express P_i as a matrix of dimension $n\times(i+1)$. One-dimensional expressions for higher order ($i > 2$) $\dot{P}_i$'s appear in [10], where it was found that their contribution to control performance for the simplified Van de Vusse reactor is negligible. The boundary condition adapted to the set-point-change case reads

$$V(x(T), T) = (x(T) - \bar{x})'S(x(T) - \bar{x}) \tag{39}$$

so the final conditions for ODEs (35-38) are

$$\varphi(T) = \bar{x}'S\bar{x}, \tag{40}$$

$$\xi(T) = S\bar{x}, \tag{41}$$

$$P_1(T) = S, \tag{42}$$

$$P_2(T) = P_3(T) = \ldots = 0, \tag{43}$$

Notice that the equations for the linear case correspond exactly to the first three ODEs (35-37), for $N = 0$ and when P_2 is neglected. In that case P_1 plays the role of the gain coming from the solution to the standard Differential Riccati Equation (DRE). Then, increasing accuracy for nonlinear systems requires to keep more P_i's (which can be visualized as high order gains). Correspondingly, it will be necessary to solve 'backwards' an increasing number of simultaneous

ODEs, and to keep all results in memory, since they will be finally used 'forwardly' when constructing the feedback law. In all numerical examples final deviations were penalized with the same weight as deviations along trajectories, i.e. $S = Q = I$.

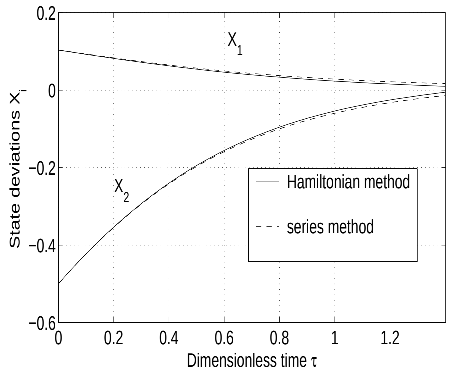

Figure 7. Relative states' trajectories $X_i = x_i - \bar{x}_i$ for the tracking case. Starting steady-state: $x_0 = (0.931877, 0.5)'$ (old set point). New set point: $\bar{x} = (0.828312, 1.0)'$, $\bar{u} = 1.68812$.

4.2.1. Change towards a stable set point. In figure 7 the process of change of set point between two stable set points of the system is illustrated. In this case the tracking goal is to lead the system to the state

$$\bar{x} = \begin{pmatrix} 0.828312 \\ 1.0 \end{pmatrix},$$

where the starting state is

$$x_0 = \begin{pmatrix} 0.931877 \\ 0.5 \end{pmatrix}.$$

The initial bilinear approximation calculated for this case was calculated from partial derivatives of the nonlinear dynamics around x_0:

$$A = \begin{pmatrix} -3.2277 & -0.195027 \\ 2.41867 & -2.36252 \end{pmatrix}, B = \begin{pmatrix} 0.068123 \\ -0.5 \end{pmatrix}, N = \begin{pmatrix} -1.0 & 0.0 \\ 0.0 & -1.0 \end{pmatrix}.$$

The resulting trajectories of the Hamiltonian and the power series approaches to this case are shown in figure 7, where only minor differences appear. Optimal controls calculated by both methods are also very similar (not plotted).

A second example shows the change from an unstable set-point

$$x_0 = \begin{pmatrix} 0.527964 \\ 3.0 \end{pmatrix}$$

towards the same (stable) steady-state $\bar{x}$ used in the previous example.

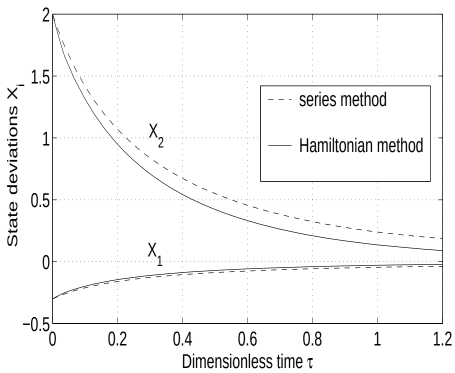

Figure 8. Relative states' trajectories $X_i = x_i - \bar{x}_i$ for the tracking case. Starting steady-state: $x_0 = (0.527964, 3.0)'$ (old set point). New set point: $\bar{x} = (0.828312, 1.0)'$, $\bar{u} = 1.68812$.

The initial bilinearization resulting in this case is

$$A = \begin{pmatrix} -3.8768 & -0.730708 \\ 20.1683 & 4.49446 \end{pmatrix}, B = \begin{pmatrix} 0.472936 \\ -3.0 \end{pmatrix}, N = \begin{pmatrix} -1.0 & 0.0 \\ 0.0 & -1.0 \end{pmatrix}.$$

The evolution of the states is depicted in Fig. 8. Even when the initial set-point x_0 in this example is an unstable steady-state of the system, the Hamiltonian strategy works equally well, as in the stable-to-stable case.

4.2.2. Change towards a saddle (unstable) set point. It is chosen here to illustrate the change from a stable to an unstable set-point, both steady-states corresponding to the same q-value $= q^*$. The value of input flux may be bounded and/or fixed by production rate restrictions or for technical reasons, so the situation of keeping equal the original and final inputs may be desirable. It is also realizable for this particular system, because it presents the so called 'input multiplicity' property [21]. Since q is the manipulated variable, a nontrivial optimal control has to move above and/or below q^*.

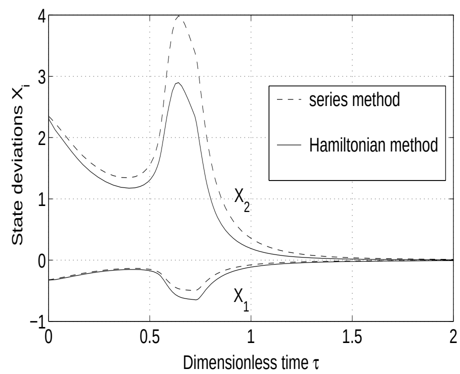

Figure 9. Relative state variables $X_i = x_i - \bar{x}_i$ evolution for changing set points from steady-state: $x_0 = (0.178, 6.031)'$ (old set point) to $\bar{x} = (0.498, 3.682)'$ (new set point), $\bar{u} = q^* = 3$.

In figures 9-10 this process of changing set-points from a stable

$$x_0 = \begin{pmatrix} 0.178 \\ 6.031 \end{pmatrix}$$

towards the unstable steady-state

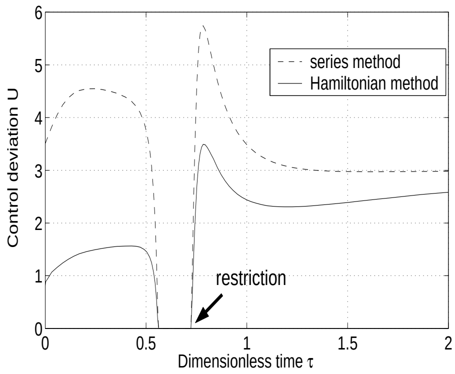

Figure 10. Control variable evolution for changing set points from steady-state: $x_0 = (0.178, 6.031)'$ (old set point) to $\bar{x} = (0.498, 3.682)'$ (new set point), $\bar{u} = q^* = 3$. $U = u - \bar{u}$.

$$\bar{x} = \begin{pmatrix} 0.498 \\ 3.682 \end{pmatrix}$$

is illustrated.

The bilinear approximation calculated for this case results

$$A = \begin{pmatrix} -6.02442 & -1.07421 \\ 33.2686 & 7.31628 \end{pmatrix}, B = \begin{pmatrix} 0.502027 \\ -3.68153 \end{pmatrix}, N = \begin{pmatrix} -1.0 & 0.0 \\ 0.0 & -1.0 \end{pmatrix}.$$

The main feature to remark from this example is the robustness of the optimal control strategy. Since the system has to go through adverse flow conditions to reach an unstable equilibrium, the evolutions of state and control variables are not monotonically smooth. They grow and decrease around the final desired values, reflecting the directions of the flow in the different regions of phase space. In a given moment (see figure 10) a restriction is applied to the control $u = q$, since it can not naturally assume negative values, but this instantaneous absence of control action has no adverse effect. This is an important consequence of working with optimal feedback control laws, since deviations from the optimal original strategy do not imply a need for recalculations or re-tuning.

5. Conclusions

It has been shown in this paper that a centralized control strategy, based on a new treatment of the Hamiltonian equations, is able to efficiently manage some optimal regulation and set-point changes in multidimensional nonlinear processes. The control obtained from the costates, which are integrated on-line, is effective even when manipulated variables are fewer than those to be controlled.

The approach resorts to bilinear approximations of the dynamics, subject to optimization objectives of the quadratic type. A previous solution method to the bilinear-quadratic problem through power series expansions of the value function and its derivatives, still demanded to evaluate the series' coefficients off-line. This inconvenience has been overcome here.

The new optimal control law requires solving an algebraic Riccati-type equation only at the initial time, which allows to integrate the Hamiltonian differential equations as an initial-value problem, and therefore the optimal costates can be calculated and inserted into the optimal control law completely on-line.

Since the states and costates are available at all times, the performance of this strategy can be continuously assessed by testing the Hamilton-Jacobi-Bellman equation associated with the problem. Observability aspects are not significant in this context since states are directly recuperated from the solutions to Hamiltonian equations.

The approach has been illustrated through its application to a classical chemical reaction problem. Simulations successfully compare against the power series version of bilinear-quadratic control and with standard MPC at the regulation level, near enough to the operational steady-state as to approximate the dynamics by linearizations. The available version of MPC seems to be sensitive to the deficiency in the number of control versus state variables, probably due to errors introduced by the overall discretization involved in MPC strategy. Furthermore, implementation in real time of the control law involves much less computational effort than MPC-type approaches (based on extensive trajectories' costs evaluation).

Robustness is guaranteed for the regulator problem, i.e. pure-gain perturbations will not affect the stability of the closed loop. For the servo problem, the stability properties of trajectories between set-points can not be ascertained in general. However the resilient behavior of the Hamiltonian strategy is best appreciated when controlling the test reactor towards an unstable set-point, since the bilinear approximation is adapted without increasing the dimension of the state, despite the fact that the original (stable) set-point is far from the target in phase space.

The examples also show the ability to manage conflicting cost terms inside the objective function. Though in this case only quadratic expressions for the individual costs were used, their number need not be as many as the control (neither the state) variables, eventually required by decentralized control schemes.

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