Research Article

Coupling Bifurcation Analysis and Multiobjective Nonlinear Model Predictive Control

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Abstract

Many engineering problems exhibit nonlinearity which manifest in the form of multiple steady- states and oscillatory behavior. The nonlinearity is caused by the presence of singularities which can be classified as limit points, branch points and Hopf bifurcation points. This article demonstrates that the presence of limit and branch points that cause multiple steady-states are advantageous for multiobjective nonlinear model predictive calculations and enable one to obtain the utopia solution. To demonstrate that this is not a coincidence eight different examples are shown. The Matlab program MATCONT is used for the bifurcation analysis and the optimization language PYOMO, is used for performing the multiobjective nonlinear model predictive control. The novelty of this work rests in the integration of bifurcation analysis and optimal control.

Keywords: Bifurcation; Multiobjective; Dynamic optimization

Introduction

The existence of nonlinear phenomena, such as multiple steady-states and oscillatory behavior in chemical processes is often regarded as problematic both from a practical and computational standpoint. Often, the nonlinearity is believed to present obstacles to computationally obtaining the optimal parameters necessary to be able to conduct the process in a beneficial manner avoiding the unnecessary wastage of resources. In this paper, it is shown, that contrary to popular opinion, the singularities that cause multiple steady-states actually are beneficial in obtaining the utopia point, where no compromise is needed. It is seen that In problems where singularities that lead to multiple steady-states (limit point and branch point) are present the utopia solution is easily obtained while performing multiobjective nonlinear model predictive control (MNLMPC) calculations. The main focus of this paper is to demonstrate with several examples that when multiobjective nonlinear model predictive control is performed on problems that exhibit limit and branch points the utopia solution was easily obtained. This paper is organized as follows. First, the bifurcation analysis and the multiobjective nonlinear model predictive control procedures are described. This is followed by an explanation as to why the utopia point is obtained when MNLMPC calculations are performed for these problems. Eight different examples are then presented illustrating this fact. The existence of bifurcations in engineering problems that lead to multiple steady state solutions is well known [1-9]. Bifurcations that lead to multiple steady-state solutions are a) Branch Points and b) limit points. Both these bifurcation points are singularities where the Jacobian matrix of the set of steady-state equations is singular. However, at a branch point there are 2 distinct tangents at the

singular point while at a limit point there is only one tangent at the singular point. Singularities in the Jacobian matrix are often indicative of an optimal solution and this motivates the investigation of how the singular points in the Jacobian matrix, indicated by branch and limit points would affect the multiobjective dynamic optimization and the multiobjective nonlinear model predictive control. One of the most commonly used software to locate these bifurcatons is MATCONT [10-11]. MATCONT uses a continuation procedure implementing the Moore-Penrose matrix pseudo-inverse. A stationary solution of the model under is used to obtain, a set of points that corresponds to the equilibria of the ordinary differential equations. CL_MATCONT detects the singularities and bifurcation points in the solution path and obtains all the branches of the solutions starting from the bifurcation points.

This software detects singular points which are Limit points, branch points and Hopf bifurcation points. Hopf bifurcation points do not cause multiple steady-states and therefore do not result in the formation of a maxima or minima. Limit and Branch points cause the existence of multiple solutions. Consider an ODE system

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

Where $x \in R^n$ Let the tangent plane at any point x be

 $[v_1, v_2, v_3, v_4, ..., v_{n+1}]$. Define matrix A as

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The matrix A can be written in a compact form as

$$A = [B \mid \frac{\partial f}{\partial \beta}] \tag{3}$$

The tangent surface must satisfy the equation

$$Av = 0 \tag{4}$$

For both limit and branch points the matrix B must be singular. For a limit point (LP) the n+1thcomponent of the tangent vector singular [12-14]. $v_{n+1}= 0$ and for a branch point (BP) the matrix $\begin{bmatrix} A \end{bmatrix}$ must be v^T

Multiobjective Nonlinear Model Predictive Algorithm

The multiobjective nonlinear model predictive control strategy (MNLMPC) method was first proposed by Flores Tlacuahuaz [15] and used by Sridhar [16]. This method does not involve the use of weighting functions, nor does it impose additional constraints on the problem unlike the weighted function or the epsilon correction method [17]. For a problem that is posed as

$$\min J(x, u) = (x_1, x_2, x_k)$$
subject to $\frac{dx}{dt} = F(x, u)$

$$h(x, u) \le 0$$

$$x^L \le x \le x^U$$

$$u^L \le u \le u^U$$
(5)

The MNLMPC method first solves dynamic optimization problems independently minimizing/maximizing each any variable p_i individually. The minimization/maximization of p_i will lead to the values p_i . Then the optimization problem that will be solved is

$$\min \{ p_i - p_i^* \}^2$$
subject to $\frac{dx}{dt} = F(x, u)$

$$h(x, u) \le 0$$

$$x^L \le x \le x^U$$

$$u^L \le u \le u^U$$
(6)

This will provide the control values for various times. The first obtained control value is implemented and the remaining discarded. This procedure is repeated until the implemented and the first obtained control value are the same.

The optimization package in Python, Pyomo [18], where the differential equations are automatically converted to a Nonlinear Program (NLP) using the orthogonal collocation method [19]. The Lagrange-Radau quadrature with three collocation points is used and 10 finite elements are chosen to solve the optimal control problems. The resulting nonlinear optimization problem was solved using the solvers IPOPT [20] and confirmed as global solutions with Baron [21] To summarize the steps of the algorithm are as follows

Minimize/maximize p^i subject to the differential and 1. algebraic equations that govern the process using Pyomo with IPOPT and Baron. This will lead to the value p_i^* time intervals t_i . The subscript *i* is the index for each time step.

Minimize $\{p - p^*\}^2$ subject to the differential and 2. algebraic equations that govern the process using Pyomo with IPOPT and Baron. This will provide the control values for various times.

3. Implement the first obtained control values and discard the remaining.

Repeat steps 1 to 4 until there is an insignificant difference between the implemented and the first obtained value of the control variables or if the Utopia point is achieved. The Utopia point is when $p_i = p_i^*$ for all i.

Effect of singularities (Limit Point (LP) and Branch Point (BP)) on MNLMPC

Let the minimization be of the variable p_1 lead to the value M_1 and the minimization of function p_2 lead to the value M_2 . This is equivalent to minimizing $(p_1 - M_1)^2$ and $(p_2 - M_2)^2$. The subsequent multiobjective minimization will be of the function $(p_1 - M_1)^2 + (p_2 - M_2)^2$.

The multiobjective optimal control problem is

$$\min \quad (p_1 - M_1)^2 + (p_2 - M_2)^2$$
subject to $\frac{dx}{dt} = F(x, u)$
(1)

$$\frac{d}{dx_{i}}\left(\left(p_{1}-M_{1}\right)^{2}+\left(p_{2}-M_{2}\right)^{2}\right)=2\left(p_{1}-M_{1}\right)\frac{d}{dx_{i}}\left(p_{1}-M_{1}\right)+2\left(p_{2}-M_{2}\right)\frac{d}{dx_{i}}\left(p_{2}-M_{2}\right)$$
(2)

At the Utopia point both $(p_1 - M_1)$ and $(p_2 - M_2)$ are zero. Hence

$$\frac{d}{dx_i} \left(\left(p_1 - M_1 \right)^2 + \left(p_2 - M_2 \right)^2 \right) = 0$$
(3)

Now let us look at the co-state equation

$$\frac{d}{dt} {}^{(\lambda)}_{i} = -\frac{d}{dx_{i}} ((p_{1} - M_{1})^{2} + (p_{2} - M_{2})^{2}) - g_{x i}^{\lambda}$$
(4)

 $\lambda_i(t_f) = 0$ The first term in this equation is 0 and hence

$$\frac{d}{dt} \begin{pmatrix} \lambda \\ i \end{pmatrix} = -g \lambda \\ \lambda_{i} \begin{pmatrix} \lambda \\ i \end{pmatrix} = 0$$
(5)

If the set of ODE $\frac{dx}{dt} = g(x, u)$ has a limit or a branch point,

 g_X is singular. Hence there are two different vectors-values for $[\lambda_i]$ where $\frac{d}{dt} (\lambda_i)^{>0} = 0$ and $\frac{d}{dt} (\lambda_i)^{<0} = 0$ In between there

is a vector $[\lambda_i]$ where $\frac{d}{dt} (\lambda_i) = 0$. This coupled with the boundary condition $\lambda_i(t_s) = 0$ will lead to $[\lambda_i] = 0$ which will make the problem an unconstrained optimization problem and the one and the onlysolution for the unconstrained problem is the Utopia solution. This is illustrated in eight different examples. presented in the next section.

Results and Discussion

Bifurcation analysis and MNLMPC is performed on eight different problems. In all these cases, limit and branch points are found and the MNLMPC converged to the Utopia solution.

Problem 1

The model of a continuous stirred tank reactor (CSTR) where x is the product concentration [22]

$$\frac{dx}{dt} = \alpha_3 - (1+\lambda)x + \frac{\lambda\alpha_1}{(1+\lambda\alpha_2 \exp(-\frac{\alpha_4 x}{1+x}))}$$
(6)

 $\alpha_1 = 10 - 9$

 $\alpha_2 = -0.9$

where

$$\alpha_1 = 10 - 9\beta + \gamma;$$

$$\alpha_2 = 10 - 9\beta;$$

$$\alpha_3 = -0.9 + 0.4\beta.$$

(7)

$$\lambda, \beta, \gamma, \alpha_4, x$$
 are variables.

 $\lambda, \beta, \gamma, \alpha_4, x$ are variables.

A bifurcation analysis of the ODE describing this process was performed using MATCONT with λ as the bifurcation variable and a limit point of $[\lambda, x] = [0.393180 \ 0.377651]$ was obtained (fig. 2a) The performance of a MNLMPC for the same problem

with λ as the control parameter t_f involved the maximization

of $\sum x(t)$ which produced an answer of 6 and the minimiza-

tion of $t_f \sum \lambda(t)$ which produced an answer of 0. The resulting MNLMPC involved the minimization of

$$(\sum_{0}^{1} x(t) - 6)^{2} + (\sum_{0}^{1} \lambda(t))^{2}$$

this optimization resulted in a value of 0, which is the Utopia point.

All optimization was done subject to the equations representing this process. Figure 2b shows the

(x, λ, t) Pareto surface

Problem 2

The second problem is the Bratu-Gelfand BVP [22]. The equa-

tions governing this problem are

$$\frac{dx}{dt} = y - 2x + ae^{x};$$

$$\frac{dy}{dt} = x - 2y + ae^{y};$$
(8)

The variables are x and y and the bifurcation parameter is a. A bifurcation analysis of the ODE was performed using MAT-CONT with a as the bifurcation variable One limit point whose co-ordinates are [x,y,a]=(1.000001 1.000001 0.367879) is obtained along with a branch point and a Hopf bifurcation point (Figure 3a)

The performance of a MNLMPC for the same probler $\sum x(t)$ a as the control parameter involved the minimization of and the minimization of $\sum y(t)$ each of which produced an answer of 0. The resulting MNLMPC involved the minimization of

 $(\sum_{0} x(t))^{2} + (y(t))^{2}$ which resulted in the utopia point of 0.

Figure 3b shows the [x, y, a] Pareto surface.

Problem 3

In the problem involving a catalytic oscillator [22], the ODE describing the process are

$$\frac{dx}{dt} = 2q_{1}z^{2} - 2q_{5}x^{2} - q_{3}xy$$

$$\frac{dy}{dt} = q_{2}z - q_{6}y - q_{3}xy$$

$$\frac{dz}{dt} = q_{4}z - kq_{5}x$$
(9)

z=1-x-y-s. The parameter values are $q_1 = 2.5; q_3 = 10; q_4 = 0.0675; q_5 = 1; q_6 = 0.1 \ k = 0.4$



Figure 1a: Limit Point is good starting point to obtain Utopia solution



Figure 1b: Branch point is good starting point to obtain Utopia solution











z=1-x-y-s. The parameter values are

 q_2 is the bifurcation variable. Two limit points $[x, y, z, q_2] = (0.024717, 0.450257, 0.375018, 1.042049)$ and (0.054030, 0.302241, 0.459807, 1.052200) along with 2 Hopf bifurcation points (Figure 4a) are obtained.

The MNLMPC involves the maximization $\sum_{0}^{t_{f}} z(t)$ which pro-

duced an answer of 1.4207 and the minimization of

$$\sum_{0}^{l_{f}} (x(t)) + \sum_{0}^{l_{f}} (y(t)) + \sum_{0}^{l_{f}} (s(t))$$

which produced a value of 0.57925. The minimization of the distance from the utopia point which was the minimization of

$$\left(\sum_{0}^{t_{f}}(x(t)) + \sum_{0}^{t_{f}}(y(t)) + \sum_{0}^{t_{f}}(s(t)) - 0.57925\right)^{2} + \left(\sum_{0}^{t_{f}}z(t) - 1, 4207\right)^{2}$$

Resulted in a value of 0 implying that the utopia solution has been obtained. Figure 4b shows the Pareto optimal surface for problem 3.

Problem 4

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For the continuous fermentation problem involving Zymomonas Mobilis [23,24], the dynamic model for the 4 components, substrate (S), microorganism or biomass (X), the key compound (e), and product (P) are given by the following equations.

$$\frac{dC_e}{dt} = \left[k_1 - k_2 C_p + k_3 C_p^2\right] (\underline{C_s C_e}_{K_s + C_s}) + D(C_{e0} - C_e)$$
(10)

$$\frac{dC_x}{dt} = P(\underline{C_sC_e}) + D(C_{x0} - C_x)$$
(11)

$$\frac{dC_s}{dt} = \mathbb{P}\binom{-1}{Y_{sy}} (\underbrace{C_s C_e}_{K_s + C_s}) - \underbrace{m C}_{s_x} + \underbrace{D(C_e - C_e)}_{e}$$
(12)

$$\frac{dC_p}{dt} = P(\frac{1}{Y_{p_X}})(\frac{C_s C_e}{K_s + C_s}) + m C_p + D(C_{p_0} - C_p)$$
(13)

 $\overline{D} = D \tanh(D)$ where D is the dilution rate. The tanh factoris a smoothing factor that was used to avoid the spikes that may occur in the control profile. Table 1 has all the parameter values.

 $C_{S0} = 200$.

When Matcont was used to perform a bifurcation analysis on the set of ODE a limit point was obtained at $[C_e, C_x, C_s, C_p, D]$ = (0.5273520.229513188.9267805.2194200.570281) (Figure 5a).

For the MNLMPC problem, the main product (ethanol) concentration C_P is maximized while the sum of the remaining products, $C_X + C_e + C_s$ is minimized. The maximization of C_P yields a value of 300 while the minimization of products, $C_X + C_e + C_s$ yields a value of 0. Then the function $[C + C + C - 0]^2 + [C - 300]^2$

is minimized subject to the ODE governing this process. The resulting solution was the utopia point 0. The Pareto surface (t,d,Cp) is shown in Figure 5b













Problem 5

This problem involves a two-stage bioreactor [25]. where X and S represent the biomass and the substrate concentrations from the two stages. The ODE governing this process are

$$\frac{dX_1}{dt} = D(X_0 - X_1) + (\frac{X_1}{X_1 + S_1}) - k_D X_1 + \beta \delta D X_2$$
(15)

$$\frac{dS_2}{dt} = D(S_1 - S_2) - \frac{1}{\alpha} (\frac{X_2}{X_2 + S_2})$$
(16)

$$\frac{dX_2}{dt} = D(X_1 - X_2) + (\frac{X_2}{X_2 + S_2}) - k_D X_2 \tag{17}$$

Where α = 0.1019; β = 0.5; γ = 0.1; δ = 0.8; K_{S} = 0.4818; K_{D} = 0.0141; S_{0} =1.05 .

When Matcont was used to perform a bifurcation analysis on the set of ODE led to one branch point

(S1,S2,X1,X2,d) = (1.105257 1.105251 0.000001 0.000002 2.423307) (Figure 6a). For the MNLMPC, the Maximization of

 $\sum X_2$ led to a value of 300 while the minimization of

$$\sum_{0}^{t} S_{2} \text{ led to a value of 0. Then the function} \\ (\sum_{0}^{t} X_{2} - 300)^{2} + (\sum_{0}^{t} X_{2} - 0)^{2}$$

was minimized subject to the ODE governing this process. This minimization led to a value of 0, which is the Utopian point. The [t,d,X2] Pareto curve is shown in fig. 6b

Problem 6

This problem involves the SIR epidemiological model [26]. Here S represents the susceptible population, I the infected and R the recovered population. The ODE representing this model are

$$\frac{dS}{dt} = A - dS - \frac{\beta SI^3}{b + aI + I^2}$$

$$\frac{dI}{dt} = \frac{\beta SI^3}{b + aI + I^2} - (d + \gamma + \varepsilon)I$$

$$\frac{dR}{dt} = \gamma I - dR$$
(18)

and the parameter values are A=2; d=0.1; d=2.4; β = 0.8; ϵ = 0.6; γ = 0.2 . A bifurcation analysis performed in this problem (with a the bifurcation parameter) reveals the existence of a limit point at [S,I,R,a] = (9.559357 1.160071 2.320143 6.628457). Fig 7a shows the bifurcation diagram with LP representing the limit point. For the MNLMPC, the Maximization of

 $\sum_{0}^{t} R$ led to a value of 20 while the minimization of $\sum_{0}^{t} I$ led to a value of 0. Then the function $(\sum_{0}^{t} R - 20)^{2} + (\sum_{0}^{t} I)^{2}$ was minimized subject to the ODE

governing this process. This resulted in the Utopia solution. The t S I surface is shown in fig. 7b

Problem 7

Problem 7 [27] involves a process that consists of a wellstirred, aerobic fermentor in which *Saccharomyces cerevisiae* grows in a medium of sugar cane molasses. Here C_1, C_2 dimensionless concentrations of cell mass, and the substrate conversion, The differential equations governing the process are

$$\frac{dC_{1}}{dt} = -C_{1} + Da(1-C_{2})e^{\frac{\alpha}{\tau}}$$

$$\frac{dC_{2}}{dt} = -C_{2} + Da(\frac{\beta+1}{\beta+1-C_{2}})(1-C_{2})C_{2}e^{\frac{\alpha}{\tau}}$$
(19)







Table 1: Base set of parameters used for the Zymomonas Mobilis fermentation (Garhyan and Elnashaie, 2004).

Parameter	Value
K1	16.0
K2	0.497
К3	0.00383
ms	2.16
mp	1.1
Y _{SX}	0.02444498
Y _{px}	0.0526315
Ks	0.5
Р	0.1283

and the parameter values are $\beta = 0.1; \gamma = 0.4$ A bifurcation analysis with Matcont revealed the existence of two limit points for $[C_1, C_2, Da]$

values of (0.463780 0.293292 0.315235) and (0.516260 0.646558 0.290107) (Figure 8a)

For the MNLMPC, the Maximization of

$$\sum_{0} C_2$$
 led to a value of 3.3366 while the minimization of

 $\sum_{0}^{t} C_{1} \text{ led to a value of 0. Then the function} \\ (\sum_{0}^{t} C_{2} - 3.3366)^{2} + (\sum_{0}^{t} C_{1} - 0)^{2}$

subject to the ODE governing this process. This minimization led to a value of 0, which is the Utopian point. The $[t, C_1, C_2]$ is shown in Figure 8b

Problem 8

This Problem [9] involves adipogenesis were the states of the model are the concentrations of the various species involved.

$$x_{1} = CEBP\beta$$

$$x_{2} = PPAR\gamma$$

$$x_{3} = CEBP\alpha$$

$$x_{4} = pAKT$$

$$x_{5} = IR$$

$$x_{6} = Fat$$

The inputs are the glucocorticoids G and cAMP (cyclic AMP)

$$\frac{d\mathfrak{x}}{dt} = k_1(b_1 + G.cAMP + y_1(\underbrace{x_1^{2^{q_1}}}_{\alpha_1 + x_2^{m_1}}) - d_1x_1$$
(20)
$$\frac{dx_2}{dt} = k_2(b_2 + (\underbrace{(x_1 + x_3)^{n_2}}_{\alpha_2 + (x_1 + x_3)^{m_2}})(\underbrace{x_4}_{\alpha_3 + x_4})) - d_2x_2$$
(21)

$$\frac{dx_3}{dx_3} = k_3(b_3 + y_2(\underline{x_2^{a_3}}) - d_3x_3$$
(22)

$$\frac{dt}{dt} = k \left((b + x) \left(\frac{\alpha_4 + x_2^{-1}}{\alpha_5} \right) \right) - dx$$

$$\frac{dx_4}{dt} = k \left((b + x) \left(\frac{\alpha_5 + G c \, 4MP}{\alpha_5} \right) \right) - dx$$
(23)

$$\frac{dx_5}{dt} = k \underbrace{(b_4 + y_5)}_{5 4} \underbrace{(x_3)}_{3 \alpha_6 + x_3} - dx_5 \underbrace{(24)}_{5 5}$$

$$\frac{dx_6}{dt} = k_6 ((\frac{x_4}{\alpha + x_4})(\frac{x_2}{\alpha + x_2})) - d_{66}$$
(25)

$$\begin{split} k_1 &= 0.378; k_2 = 0.845; k_3 = 3.858; k_4 = 0.091; k_5 = 3.122; k_6 = 0.716\\ b_1 &= 0.124; b_2 = 0.185; b_3 = 0.012; b_4 = 0.005 \end{split}$$

$$d_1 = 0.512; d_2 = 0.647; d_3 = 0.042; d_4 = 0.325; d_5 = 0.066; d_6 = 0.360$$

$$\alpha_1 = 28.02; \alpha_2 = 36; \alpha_3 = 0.2; \alpha_4 = 18.64; \alpha_5 = 1.921; \alpha_6 = 3.6; \alpha_7 = 0.492; \alpha_8 = 1.148$$

$$y_1 = 1; y_2 = 1; y_3 = 1$$

 $n_1 = 2; n_2 = 3; n_3 = 3$

G=0.232

A bifurcation analysis with Matcont revealed the existence of a limit point for $[x_1, x_2, x_3, x_4, x_5, x_6.cAMP]$ Values of (1.223551 0.462982 1.588752 2.297976 14.7203040.470792 6.576315). The bifurcation diagram is shown in Figure 9a The MNLMPC involved the individual minimization of $\sum_{k=1}^{t} x_k$













that led to a value of 0.0474 and \sum_{0} *cAMP* that led to a value of zero.

Then the function $(\sum_{0} x_6 - 0.0474)^2 + (\sum_{0} cAMOP - 0)^2$ was minimized subject to the "

equations governing this process and this led to the Utopia point. Figure 9b shows the $[t, x_6, cAMP]$

In all the examples, limit and branch points for the differential equations that constitute the dynamic constraints are found. The presence of these limit and branch points creates a path to the utopia point which is easily obtained when MN-LMPC is performed.

Conclusions

MATCONT and Pyomo are used to perform the bifurcation analysis and multiobjective nonlinear model predictive control

on several problems governed by differential equations. The presence of limit and branch points that cause multiple steadystates in these differential equations actually are very beneficial because they enable the MNLMPC algorithm to find the Utopia point. Eight different examples have been presented demonstrating that this is not a coincidence the novelty of this work rests in the integration of bifurcation analysis and optimal control.

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