

Analysis and Control of a Heroin Dynamic Model

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ABSTRACT

Bifurcation analysis and multi-objective nonlinear model predictive control (MNLMP) calculations are performed on a heroin dynamic model. Bifurcation analysis is a powerful mathematical tool used to deal with the nonlinear dynamics of any process. Several factors must be considered, and multiple objectives must be met simultaneously. The MATLAB program MATCONT was used to perform the bifurcation analysis. The MNLMP calculations were performed using the optimization language PYOMO in conjunction with the state-of-the-art global optimization solvers IPOPT and BARON. The bifurcation analysis revealed the existence of a branch point in the model. The branch point (which causes multiple steady-state solutions from a singular point) is very beneficial because it enables the Multiobjective nonlinear model predictive control calculations to converge to the Utopia point (the best possible solution) in the model. It is proven (with computational validation) that the branch points were caused because of the existence of two distinct separable functions in one of the equations in the dynamic model. A theorem was developed to demonstrate this fact for any dynamic model.

Keywords: Bifurcation; Optimization; Control; Heroin

Background

Garten, et al.¹, investigated the rapid transmission of hepatitis C virus among young injecting heroin users in Southern China. White, et al.² discussed the treatment and ODE modelling of heroin epidemics. Samanta³ studied the dynamic behaviour for a nonautonomous heroin epidemic model with time delay. Liu, et al.⁴ investigated the global behaviour of a heroin epidemic model with distributed delays. Wang, et al.⁵ studied the dynamics of a heroin epidemic model. Huang, et al.⁶ studied the global stability for a heroin epidemic model with distributed delay, Wangari, et al.⁷ developed an analysis of a heroin epidemic model with a saturated treatment function. Wang, et al.⁸ provided an analysis

of an age-structured multi-group heroin epidemic model. Khan, et al.⁹ discussed optimal control strategies for a heroin epidemic model with age-dependent susceptibility and recovery-age. Sowndarajan, et al.¹⁰ performed optimal control of a heroin epidemic mathematical model.

This work aims to perform bifurcation analysis and multiobjective nonlinear control (MNLMP) studies on a microbiome dynamic model described in Sowndarajan, et al.¹⁰. The paper is organized as follows. First, the model equations are presented, followed by a discussion of the numerical techniques involving bifurcation analysis and multiobjective nonlinear model predictive control (MNLMP). The results are then presented, followed by the discussion and conclusions.

Model Equations¹⁰

In this model, sv , $uv1$, $uv2$, ev , and zv represent susceptible individuals, drug users, drug users in treatment, individuals in a state of self-protection, and the information density. The model equations are

$$\frac{d(sv)}{dt} = \Lambda - sv\beta1(uv1) - \mu(sv) + \theta(ev) - u1\rho(sv)(zv)$$

$$\frac{d(uv1)}{dt} = \beta1(sv)uv1 - u2(uv1) + \beta2(uv1)uv2 - (\mu + \delta1)uv1$$

$$\frac{d(uv2)}{dt} = u2(uv1) - \beta2(uv1)uv2 - (\mu + \delta2)uv2$$

$$\frac{d(ev)}{dt} = u1\rho(sv)(zv) - (\mu + \theta)ev$$

$$\frac{d(zv)}{dt} = \frac{a(uv1)}{(1+b(uv1))} - a0(zv)$$

$$\Lambda = 0.7; \beta1 = 0.01; \beta2 = 0.0008; \mu = 0.07; \rho = 0.04; \delta1 = 0.05; \delta2 = 0.06; \theta = 0.001; a = 0.01; b = 1.0; a0 = 0.06; u1 = 0; u2 = 0.$$

Bifurcation Analysis

The MATLAB software MATCONT is used to perform the bifurcation calculations. Bifurcation analysis deals with multiple steady states and limit cycles. Multiple steady states occur because of the existence of branch and limit points. Hopf bifurcation points cause limit cycles. A commonly used MATLAB program that locates limit points, branch points, and Hopf bifurcation points is MATCONT^{11,12}. This program detects Limit points (LP), branch points (BP), and Hopf bifurcation points(H) for an ODE system

$$\frac{dx}{dt} = f(x, \alpha)$$

$x \in R^n$ Let the bifurcation parameter be α . Since the gradient is orthogonal to the tangent vector,

The tangent plane at any point $w = [w_1, w_2, w_3, w_4, \dots, w_{n+1}]$ must satisfy

$$Aw = 0$$

Where A is

$$A = [\partial f / \partial x \quad | \quad \partial f / \partial \alpha]$$

where $\partial f / \partial x$ is the Jacobian matrix. For both limit and branch points, the Jacobian matrix $J = [\partial f / \partial x]$ must be singular.

For a limit point, there is only one tangent at the point of singularity. At this singular point, there is a single non-zero vector, y , where $Jy=0$. This vector is of dimension n . Since there is only one tangent the vector

$$y = (y_1, y_2, y_3, y_4, \dots, y_n) \quad \text{must align with}$$

$$\hat{w} = (w_1, w_2, w_3, w_4, \dots, w_n). \text{ Since}$$

$$J\hat{w} = Aw = 0$$

the $n+1$ th component of the tangent vector $w_{n+1} = 0$ at a limit point (LP).

For a branch point, there must exist two tangents at the singularity. Let the two tangents be z and w . This implies that

$$Az = 0$$

$$Aw = 0$$

Consider a vector v that is orthogonal to one of the tangents (say w). v can be expressed as a linear combination of z and w ($v = \alpha z + \beta w$). Since $Az = Aw = 0$; $Av = 0$ and since v and w are orthogonal, $w^T v = 0$. Hence $Bv = \begin{bmatrix} A \\ w^T \end{bmatrix} v = 0$ which implies that B is singular.

Hence, for a branch point (BP) the matrix $B = \begin{bmatrix} A \\ w^T \end{bmatrix}$ must be singular. At a Hopf bifurcation point,

$$\det(2f_x(x, \alpha) @ I_n) = 0$$

@ indicates the bialternate product while I_n is the n -square identity matrix. Hopf bifurcations cause limit cycles and should be eliminated because limit cycles make optimization and control tasks very difficult. More details can be found in Kuznetsov¹³⁻¹⁵.

Hopf bifurcations cause limit cycles. The tanh activation function (where a control value u is replaced by) $(u \tanh u / \varepsilon)$ is used to eliminate spikes in the optimal control profiles¹⁶⁻¹⁹. Sridhar²⁰ explained with several examples how the activation factor involving the tanh function also eliminates the Hopf bifurcation points. This was because the tanh function increases the oscillation time period in the limit cycle.

Multiobjective Nonlinear Model Predictive Control(MNLMPC)

The rigorous multiobjective nonlinear model predictive control (MNLMPC) method developed by Flores Tlacuahuaz, et al.²¹ was used.

Consider a problem where the variables $\sum_{t_i=0}^{t_i=t_f} q_j(t_i)$ ($j=1, 2..n$) have to be optimized simultaneously for a dynamic problem

$$\frac{dx}{dt} = F(x, u)$$

t_f being the final time value, and n the total number of objective variables and u the control parameter. The single objective optimal control problem is solved individually

optimizing each of the variables $\sum_{t_i=0}^{t_i=t_f} q_j(t_i)$. The optimization of $\sum_{t_i=0}^{t_i=t_f} q_j(t_i)$ will lead to the values q_j^* . Then, the multiobjective optimal control (MOOC) problem that will be solved is

$$\min \left(\sum_{j=1}^n \left(\sum_{t_i=0}^{t_i=t_f} q_j(t_i) - q_j^* \right)^2 \right)$$

$$\text{subject to } \frac{dx}{dt} = F(x, u);$$

This will provide the values of u at various times. The first

obtained control value of u is implemented and the rest are discarded. This procedure is repeated until the implemented and the first obtained control values are the same or if the Utopia

point where $(\sum_{t_i=0}^{t_i=t_f} q_j(t_i) = q_j^*)$ for all j is obtained.

Pyomo²² is used for these calculations. Here, the differential equations are converted to a Nonlinear Program (NLP) using the orthogonal collocation method. The NLP is solved using IPOPT²³ and confirmed as a global solution with BARON²⁴.

The steps of the algorithm are as follows

Optimize $\sum_{t_i=0}^{t_i=t_f} q_j(t_i)$ and obtain q_j^* .

Minimize $(\sum_{j=1}^n (\sum_{t_i=0}^{t_i=t_f} q_j(t_i) - q_j^*))^2$ and get the control values at various times.

Implement the first obtained control values

Repeat steps 1 to 3 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 $\sum_{t_i=0}^{t_i=t_f} q_j(t_i) = q_j^*$ for all j .

Sridhar²⁵ demonstrated that when the bifurcation analysis revealed the presence of limit and branch points the MNLMPC calculations to converge to the Utopia solution. For this, the singularity condition, caused by the presence of the limit or branch points was imposed on the co-state equation²⁶. If the minimization of q_1 lead to the value q_1^* and the minimization of q_2 lead to the value q_2^* . The MNLMPC calculations will minimize the function $(q_1 - q_1^*)^2 + (q_2 - q_2^*)^2$. The multiobjective optimal control problem is

$$\min (q_1 - q_1^*)^2 + (q_2 - q_2^*)^2 \quad \text{subject to} \quad \frac{dx}{dt} = F(x, u)$$

Differentiating the objective function results in

$$\frac{d}{dx_i} ((q_1 - q_1^*)^2 + (q_2 - q_2^*)^2) = 2(q_1 - q_1^*) \frac{d}{dx_i} (q_1 - q_1^*) + 2(q_2 - q_2^*) \frac{d}{dx_i} (q_2 - q_2^*)$$

The Utopia point requires that both $(q_1 - q_1^*)$ and $(q_2 - q_2^*)$ are zero. Hence

$$\frac{d}{dx_i} ((q_1 - q_1^*)^2 + (q_2 - q_2^*)^2) = 0$$

The optimal control co-state equation

$$\frac{d}{dt}(\lambda_i) = -\frac{d}{dx_i} ((q_1 - q_1^*)^2 + (q_2 - q_2^*)^2) - f_x \lambda_i; \quad \lambda_i(t_f) = 0$$

λ_i is the Lagrangian multiplier. t_f is the final time. The first term in this equation is 0 and hence

$$\frac{d}{dt}(\lambda_i) = -f_x \lambda_i; \quad \lambda_i(t_f) = 0$$

At a limit or a branch point, for the set of ODE $\frac{dx}{dt} = f(x, u)$ f_x is singular. Hence there are two different vectors-values for $[\lambda_i]$ where $\frac{d}{dt}(\lambda_i) > 0$ and $\frac{d}{dt}(\lambda_i) < 0$. In between there is a vector $[\lambda_i]$ where $\frac{d}{dt}(\lambda_i) = 0$. This coupled with the boundary condition $\lambda_i(t_f) = 0$ will lead to $[\lambda_i] = 0$. This makes the problem an unconstrained optimization problem, and the optimal solution is the Utopia solution.

Results

Bifurcation analysis revealed the existence of a branch point at, $(sv, uv1, uv2, ev, zv, \delta1)$ values of $(10, 0, 0, 0, 0, 0.03)$. For the MNLMPC calculations $sv(0)=30$, $uv1(0)=15$, $\sum_{t_i=0}^{t_i=t_f} uv1(t_i)$ was minimized and produced a value of 15 and $\sum_{t_i=0}^{t_i=t_f} zv(t_i)$ was maximized led to value of 2000. $u1, u2$ were the control parameters. The multiobjective optimal control problem will involve the minimization of $(\sum_{t_i=0}^{t_i=t_f} zv(t_i) - 2000)^2 + (\sum_{t_i=0}^{t_i=t_f} uv1(t_i) - 15)^2$ subject to the equations governing the model. This led to a value of zero (the Utopia solution) (Figure 1a). The MNLMPC control values of $u1$ and $u2$ were 0.0045 and 0.5. (Figures 2a-2f) show the various MNLMPC profiles. The profile of the control variable $u1$ exhibited a lot of noise, which was remedied using the Savitsky-Golay filter to produce the smooth profile $u1sg$. $u2$ had a uniform value of 0.5 throughout.

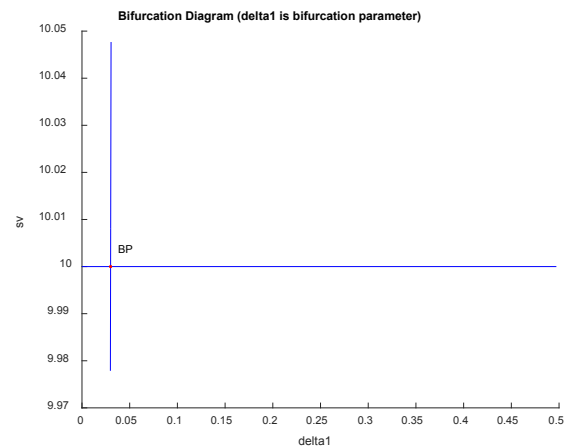


Figure 1a: Bifurcation diagram when $\delta1$ is bifurcation parameter.

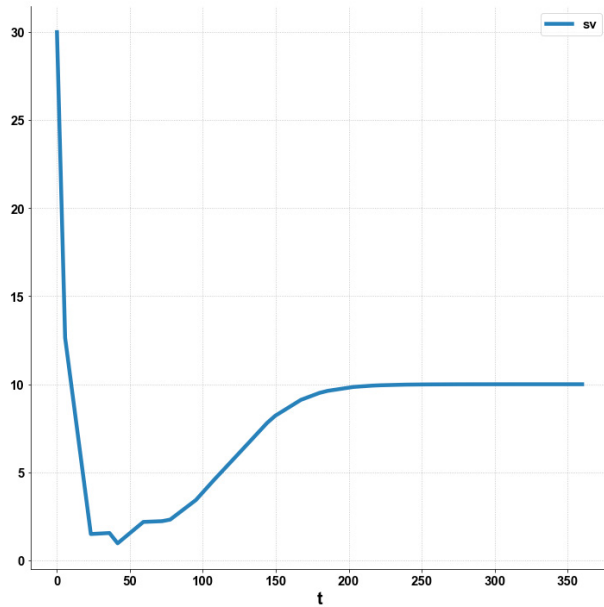


Figure 2a: MNLMPc sv vs t.

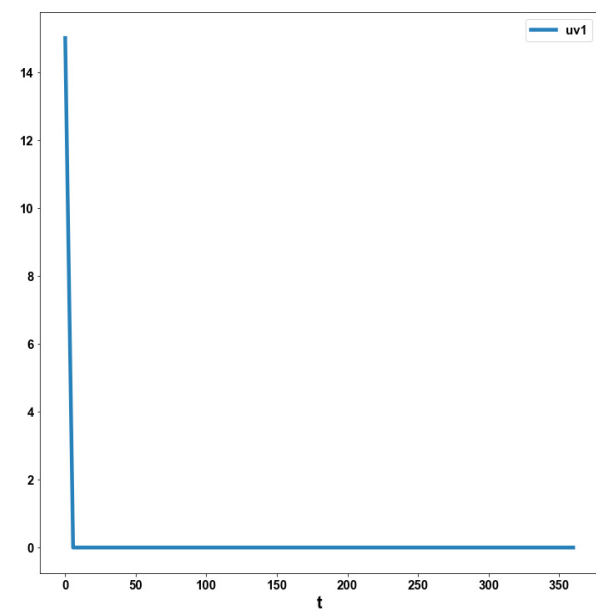


Figure 2b: MNLMPc uv1 vs t.

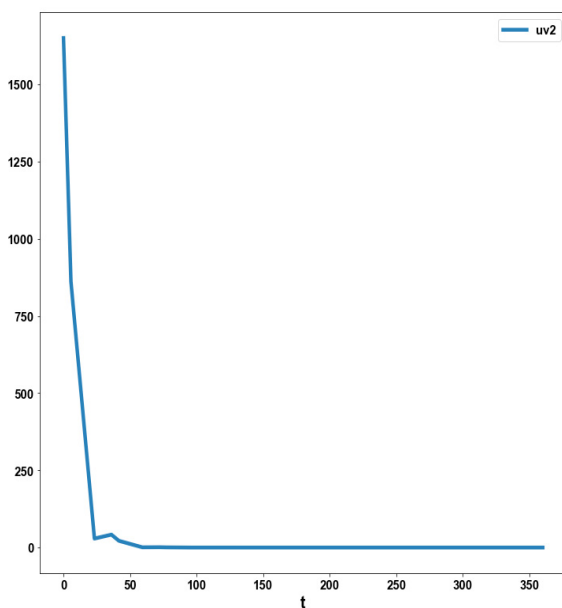


Figure 2c: MNLMPc uv2 vs t.

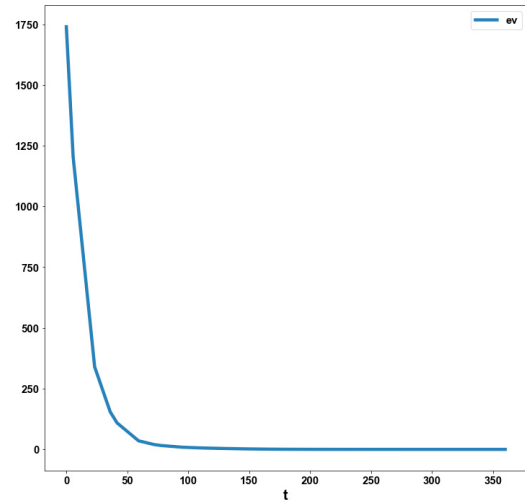


Figure 2d: MNLMPc ev vs t.

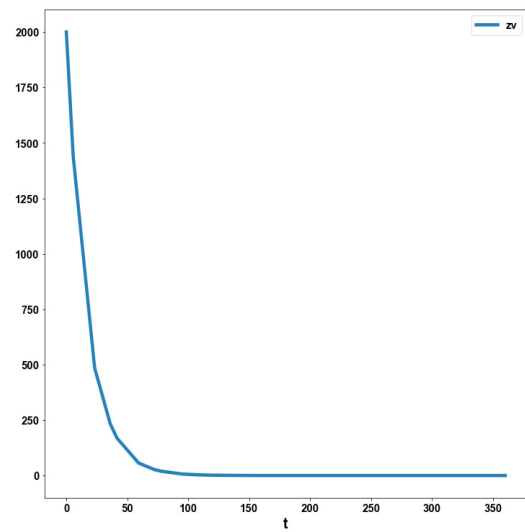


Figure 2e: MNLMPc zv vs t.

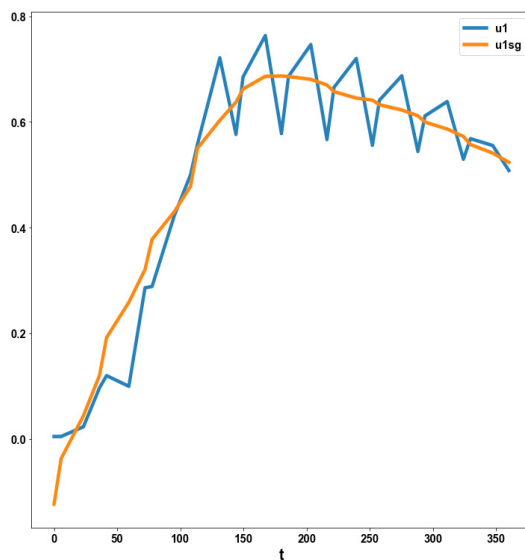


Figure 2f: MNLMPc u1, u1sg vs t.

Discussion of Results

Theorem

If one of the functions in a dynamic system is separable into two distinct functions, a branch point singularity will occur in the system.

Proof

Consider a system of equations

$$\frac{dx}{dt} = f(x, \alpha)$$

$x \in R^n$. Defining the matrix A as

$$A = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} & \frac{\partial f_1}{\partial x_4} & \dots & \frac{\partial f_1}{\partial x_n} & \frac{\partial f_1}{\partial \alpha} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} & \frac{\partial f_2}{\partial x_4} & \dots & \frac{\partial f_2}{\partial x_n} & \frac{\partial f_2}{\partial \alpha} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \frac{\partial f_n}{\partial x_3} & \frac{\partial f_n}{\partial x_4} & \dots & \frac{\partial f_n}{\partial x_n} & \frac{\partial f_n}{\partial \alpha} \end{bmatrix}$$

α is the bifurcation parameter. The matrix A can be written in a compact form as

$$A = \left[\frac{\partial f_p}{\partial x_q} \mid \frac{\partial f_p}{\partial \alpha} \right]$$

The tangent at any point x ; ($z = [z_1, z_2, z_3, z_4, \dots, z_{n+1}]$) must satisfy

$$Az = 0$$

The matrix $\left\{ \frac{\partial f_p}{\partial x_q} \right\}$ must be singular at both limit and

branch points. The $n+1$ th component of the tangent vector $z_{n+1} = 0$ at a limit point (LP) and for a branch point (BP) the matrix

$$B = \begin{bmatrix} A \\ z^T \end{bmatrix} \text{ must be singular.}$$

Any tangent at a point y that is defined by $z = [z_1, z_2, z_3, z_4, \dots, z_{n+1}]$ must satisfy

$$Az = 0$$

For a branch point, there must exist two tangents at the singularity. Let the two tangents be z and w . This implies that

$$Az = 0$$

$$Aw = 0$$

Consider a vector v that is orthogonal to one of the tangents (say z). v can be expressed as a linear combination of z and w ($v = \alpha z + \beta w$). Since $Az = Aw = 0$; $Av = 0$ and since

z and v are orthogonal, $z^T v = 0$. Hence $Bv = \begin{bmatrix} A \\ z^T \end{bmatrix} v = 0$

which implies that B is singular where $B = \begin{bmatrix} A \\ z^T \end{bmatrix}$

Let any of the functions f_i are separable into 2 functions

ϕ_1, ϕ_2 as

$$f_i = \phi_1 \phi_2$$

At steady-state $f_i(x, \alpha) = 0$ and this will imply that either $\phi_1 = 0$ or $\phi_2 = 0$ or both ϕ_1 and ϕ_2 must be 0. This implies that two branches $\phi_1 = 0$ and $\phi_2 = 0$ will meet at a point where both ϕ_1 and ϕ_2 are 0.

At this point, the matrix B will be singular as a row in this matrix would be

$$\left[\frac{\partial f_i}{\partial x_k} \mid \frac{\partial f_i}{\partial \alpha} \right]$$

However,

$$\left[\frac{\partial f_i}{\partial x_k} = \phi_1 (=0) \frac{\partial \phi_2}{\partial x_k} + \phi_2 (=0) \frac{\partial \phi_1}{\partial x_k} = 0 (\forall k = 1, \dots, n) \right]$$

$$\frac{\partial f_i}{\partial \alpha} = \phi_1 (=0) \frac{\partial \phi_2}{\partial \alpha} + \phi_2 (=0) \frac{\partial \phi_1}{\partial \alpha} = 0$$

This implies that every element in the row $\left[\frac{\partial f_i}{\partial x_k} \mid \frac{\partial f_i}{\partial \alpha} \right]$ would be 0, and hence the matrix B would be singular. The singularity in B implies that there exists a branch point.

The branch point occurred at $(sv, uv1, uv2, ev, zv, \delta 1)$ values of $(10, 0, 0, 0, 0, 0.03)$

Here, the two distinct functions can be obtained from the second ODE in the model

$$\frac{d(uv1)}{dt} = \beta 1(sv)uv1 - u2(uv1) + \beta 2(uv1)uv2 - (\mu + \delta 1)uv1$$

The two distinct equations are

$$uv1 = 0$$

$$\beta 1(sv) - u2 + \beta 2uv2 - (\mu + \delta 1) = 0$$

Since $\delta 1 = 0.03$, $\mu = 0.07$; $\beta 1 = 0.01$; $u2=0$; $uv2=0$, both distinct equations are satisfied, validating the theorem. The MNLMPC calculations converge to the Utopia point, validating the analysis in Sridhar²⁵.

Conclusions

Bifurcation analysis and multiobjective nonlinear control (MNLMPC) studies were conducted on a heroin dynamic model. The bifurcation analysis revealed the existence a branch point. The branch point (which causes multiple steady-state solutions from a singular point) is very beneficial because it enables the Multiobjective nonlinear model predictive control calculations to converge to the Utopia point (the best possible solution) in the model. It is proven (with computational validation) that the branch point was caused because of the existence of two distinct separable functions in one of the equations in the model. A theorem was developed to demonstrate this fact for any dynamic

model. A combination of bifurcation analysis and Multiobjective Nonlinear Model Predictive Control(MNLMPC) for a heroin dynamic model is the main contribution of this paper.

Data Availability Statement

All data used is presented in the paper.

Conflict of interest

The author, Dr. Lakshmi N Sridhar has no conflict of interest.

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