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Analysis and Control of a Gonorrhea Dynamic Model

Abstract:
Gonorrhea is a serious global health problem with more than 80 million new cases in 2020. It is possible for infants born to infected mothers to acquire the infection during the birthing process. In infants, it is not uncommon for gonorrhoea to affect the eyes. It is necessary to understand the dynamics and develop strategies to be able to control the spread of this disease. In this work, bifurcation analysis and multiobjective nonlinear model predictive control (MNLMPC) calculations are performed on a gonorrhea transmission model. Bifurcation analysis is a powerful mathematical tool used to deal with the nonlinear dynamics of any process. The MATLAB program MATCONT was used to perform the bifurcation analysis. Several factors must be considered, and multiple objectives must be met simultaneously. The MNLMPC 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 branch points in the model. The branch points were beneficial because they enabled the multiobjective nonlinear model predictive control calculations to converge to the Utopia point in both problems, which is the most beneficial solution.

Key Words: gonorrhea; optimization; bifurcation; control

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Introduction:

Lajmanovich et al (1976)[1] developed a deterministic model for gonorrhea in a nonhomogeneous population, Hooper et al (1978)[2] performed a cohort study of venereal disease, studying the risk of gonorrhea transmission from infected women to men. Kretzschmar et al (1996)[3] developed prevention strategies for gonorrhea and Chlamydia using stochastic network simulations. Garnett et al (1999)[4], studied the transmission dynamics of gonorrhoea, modelling the reported behaviour of infected patients from Newark, New Jersey. Mushayabasa et al (2011)[5] , modelled gonorrhea and HIV co-interactions. Hethcote et al (2014)[6] investigated gonorrhea transmission dynamics and developed control strategies to minimize the damage. Chan et al (2016)[7], researched the extragenital infections caused by Chlamydia trachomatis and Neisseria gonorrhoeae. Grad et al (2016)[8]_ provided strategies to improve control of antibiotic-resistant gonorrhea by integrating research agendas across disciplines. Oyeniyi et al (2017)[9] developed a mathematical model of syphilis in a heterogeneous setting with complications. Adamu et al.(2018)[10] developed a mathematical model for the dynamics of Neisseria gonorrhea disease with natural immunity and treatment effects.

Gumel et al (2018)[11] investigated the mathematics of a sex-structured model for syphilis transmission dynamics. Bonyah et al (2019)[12] modelled the effects of heavy alcohol consumption on the transmission dynamics of gonorrhea with optimal control. Adediipo et al (2020)[13] performed bifurcation and stability analysis of the dynamics of gonorrhea disease in the population. David et al (2020)[14] developed a co-interaction model of HIV and syphilis infection among gay, bisexual men. Newman et al (2021)[15] performed a thorough QT study to evaluate the effect of zoliflodacin, a novel therapeutic for gonorrhea, on cardiac repolarization in healthy adults. Asamoah et al (2023)[16], developed a fractional Caputo and sensitivity heat map for a gonorrhea transmission model in a sex structured population. Asamoah et al (2023)[17] studied the optimal control dynamics of Gonorrhea in a structured population.

This work aims to perform bifurcation analysis and multiobjective nonlinear control (MNLMPC) studies on a gonorrhea transmission dynamic model described in Asamoah et al (2023)[17]. 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 (MNLMPC). The results and discussion is then presented, followed by the conclusions.

Gonorrhea Transmission Model Equations:

In this model, sf, sm, icf, icm, isf, ism, rf, rm represent the symptomatic, icubative, treated, and recovered male and female population. The control variables u1, u2, u3 and u4 are educating people about gonorrhea and its transmission, physical contraceptive use, vaccination against the contraction of gonorrhea, and treatment in both populations.

The model equations are

$$
\begin{aligned}
\frac{d(sf)}{dt} &= \theta_f - \left(\left(1-(u1+u2+u3)\right)\beta_{mf}\left((\eta_{sm}ism)+(\eta_{cm}icm)\right)sf\right)+\left(\rho_f rf\right)-\left(\mu_f sf\right)\\
\frac{d(icf)}{dt} &= \left(\left(1-(u1+u2+u3)\right)\beta_{mf}\left((\eta_{sm}ism)+(\eta_{cm}icm)\right)*sf\right) - \left((\gamma_f+\mu_f)icf\right)+\left((1-\mu_f)k_f rf\right)\\
\frac{d(isf)}{dt} &= \left(\gamma_f icf\right)-\left((u4+\mu_f+\xi_f)isf\right)\\
\frac{d(rf)}{dt} &= u4isf - \left(\left(\rho_f+\left((1-\rho_f)k_f\right)+\mu_f\right)rf\right)\\
\frac{d(sm)}{dt} &= (\theta_m)-\left(\left(1-(u1+u2+u3)\right)\beta_{fm}\left((\eta_{sf}isf)+(\eta_{cf}icf)\right)sm\right)+(\rho_m rm)-(\mu_m sm)\\
\frac{d(icm)}{dt} &= \left(\left(1-(u1+u2+u3)\right)\beta_{fm}\left((\eta_{sf}isf)+(\eta_{cf}icf)\right)sm\right) - \left((\gamma_m+\mu_m)icm\right)+(\mu_m k_m rm)\\
\frac{d(ism)}{dt} &= (\gamma_m icm)-\left((u4+\mu_m+\xi_m)ism\right)\\
\frac{d(rm)}{dt} &= u4ism-\left(\left(\rho_m+\left((1-\rho_m)k_m\right)+\mu_m\right)rm\right)
\end{aligned}
\tag{1}
$$

The base parameter values are

$$
\begin{aligned}
&\theta_f = 0.45;\ \theta_m = 0.3; \eta_{sm} = 0.4; \mu_f = 0.04; \mu_m = 0.04; \alpha_f = 0.03; \alpha_m = 0.4;\\
&k_f = 0.01; \beta_{fm} = 0.0625; \xi_f = 0.001;\ \beta_{mf} = 0.15; \eta_{cf} = 0.65; \eta_{sf} = 0.65; \eta_{cm} = 0.4;\\
&\rho_f = 0.04; \rho_m = 0.04; k_m = 0.01; \xi_m = 0.001;\ \gamma_f = 0.2; \gamma_m = 0.26;\\
&u1 = 0.1; u2 = 0.1; u3 = 0.1; u4 = 0.1.
\end{aligned}
$$

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(Dhooge Govearts, and Kuznetsov, 2003[18]; Dhooge Govearts, Kuznetsov, Mestrom and Riet, 2004[19]). This program detects Limit points(LP), branch points(BP), and Hopf bifurcation points(H) for an ODE system

$$\frac{dx}{dt} = f(x, \alpha) \tag{2}$$

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

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

$$Aw = 0 \tag{3}$$

Where A is

$$A = [\partial f / \partial x \quad | \partial f / \partial \alpha] \tag{4}$$

where $\partial f / \partial x$ is the Jacobian matrix. For both limit and branch points, the Jacobian matrix $[\partial f / \partial x]$ must be singular. The n+1 th component of the tangent vector w_{n+1} = 0 for 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

$$\begin{aligned} Az &= 0 \\ Aw &= 0 \end{aligned} \tag{5}$$

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 w and v 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,

$$\det(2 f_x(x, \alpha) @ I_n) = 0 \tag{6}$$

@ 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 Kuznetsov (1998[20]; 2009[21]) and Govaerts [2000] [22].

<u>Multiobjective Nonlinear Model Predictive Control(MNLMPC)</u>

The rigorous multiobjective nonlinear model predictive control (MNLMPC) method developed by Flores Tlacuahuaz et al (2012)[23] is 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

$$\frac{dx}{dt} = F(x, u) \tag{7}$$

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

$$\min\left(\sum_{j=1}^{n}\left(\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i)-q_j^*\right)\right)^2 \qquad (8)$$
$$subject\ to\ \frac{dx}{dt}=F(x,u);$$

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.

Pyomo (Hart et al, 2017)[24] 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 IPOPT (Wächter And Biegler, 2006)[25]and confirmed as a global solution with BARON (Tawarmalani, M. and N. V. Sahinidis 2005)[26].

The steps of the algorithm are as follows

1. Optimize $\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i)$ and obtain q_j^*.
2. Minimize $\left(\sum_{j=1}^{n}\left(\sum_{t_{i=0}}^{t_i=t_f} q_j(t_i)-q_j^*\right)\right)^2$ and get the control values at various times.
3. Implement the first obtained control values
4. 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.

Sridhar (2024)[27] demonstrated that when the bifurcation analysis revealed the presence of limit and branch points tthe 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 equation (Upreti, 2013)[18]. 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 MNLPMC calculations will minimize the function $(q_1-q_1^*)^2+(q_2-q_2^*)^2$. The multiobjective optimal control problem is

$$\min \quad (q_1-q_1^*)^2+(q_2-q_2^*)^2 \quad subject\ to\ \frac{dx}{dt}=F(x,u) \qquad (9)$$

Differentiating the objective function results in

$$\frac{d}{dx_i}((q_1-q_1^*)^2+(q_2-q_2^*)^2)=2(q_1-q_1^*)\frac{d}{dx_i}(q_1-q_1^*)+2(q_2-q_2^*)\frac{d}{dx_i}(q_2-q_2^*) \qquad (10)$$

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

$$\frac{d}{dx_i}((q_1 - q_1^*)^2 + (q_2 - q_2^*)^2) = 0 \tag{11}$$

The optimal control co-state equation (Upreti; 2013)[28] is

$$\frac{d}{dt}(\lambda_i) = -\frac{d}{dx_i}((q_1 - q_1^*)^2 + (q_2 - q_2^*)^2) - f_x \lambda_i; \quad \lambda_i(t_f) = 0 \tag{12}$$

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

$$\frac{d}{dt}(\lambda_i) = -f_x \lambda_i; \lambda_i(t_f) = 0 \tag{13}$$

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 and Discussion:

The bifurcation analysis, with u1 as the bifurcation parameter, for the gonorrhea model revealed the existence of two branch points at (sf, sm, icf, icm, isf, ism, rf, rm, u1) values of

(11.25, 0, 0, 0, 7.5, 0, 0, 0, 0.581951) and (11.25, 0, 0, 0, 7.5, 0, 0, 0, 1.018049)

Both the branch points are shown in Fig.1

For theMNLMPC calculations sf(0)=0.7, isf(0)=0.1, icf(0)=0.2, rf(0)=0, sm(0)=(0.8), icm(0)=0.1),ism(0)=0.1, rm(0)=0

$\sum_{t_i=0}^{t_i=t_f} isf(t_i), \sum_{t_i=0}^{t_i=t_f} icf(t_i), \sum_{t_i=0}^{t_i=t_f} ism(t_i), \sum_{t_i=0}^{t_i=t_f} icm(t_i), \sum_{t_i=0}^{t_i=t_f} rf(t_i), \sum_{t_i=0}^{t_i=t_f} rm(t_i)$ was minimized individually and each of them led to a values of 0.1, 0.2, 0.1,0.1, 0 and 0. The overall optimal control problem will involve the minimization of

$$(\sum_{t_i=0}^{t_i=t_f} isf(t_i) - 0.1)^2 (\sum_{t_i=0}^{t_i=t_f} icf(t_i) - 0.2)^2 + (\sum_{t_i=0}^{t_i=t_f} ism(t_i) - 0.1)^2 + (\sum_{t_i=0}^{t_i=t_f} icm(t_i) - 0.1)^2$$
$$+ (\sum_{t_i=0}^{t_i=t_f} rf(t_i) - 0)^2 + (\sum_{t_i=0}^{t_i=t_f} rm(t_i) - 0)^2$$

was minimized subject to the equations governing the model. This led to a value of zero (the Utopia solution. The various concentration profiles for this MNLMPC calculation are shown in Figs. 2-7.

The control profiles for u2 and u3 were identical to u1. The profiles of u1 and u4 exhibited noise

using the Savitzky-Golay Filter to produce the smoothed-out versions of these profiles (u1sg, u4sg) as shown in Fig. 6 and Fig. 7.The MNLMPC control values of u1, u2 and u3 were 0.27986 each. The MNLMPC control value of u4 was 0.29932. The presence of the branch points is beneficial because they allow the MNLMPC calculations to attain the Utopia solution.

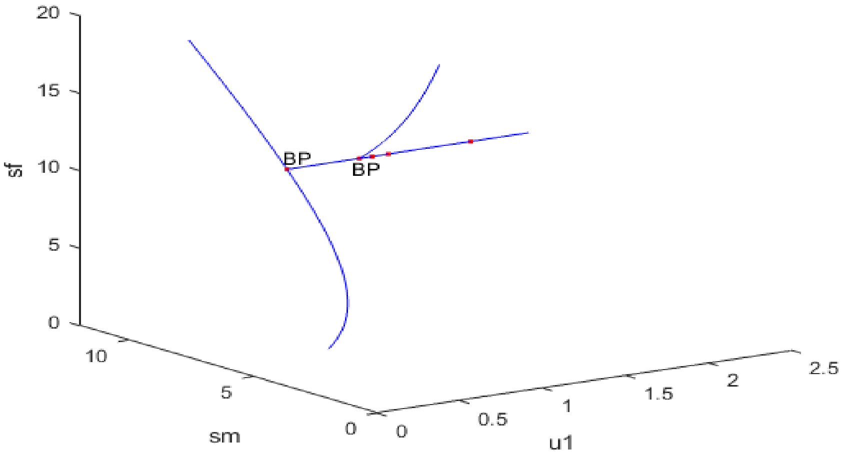

Figure 1: *Bifurcation Diagram for the gonorrhea model, indicating two branch points*

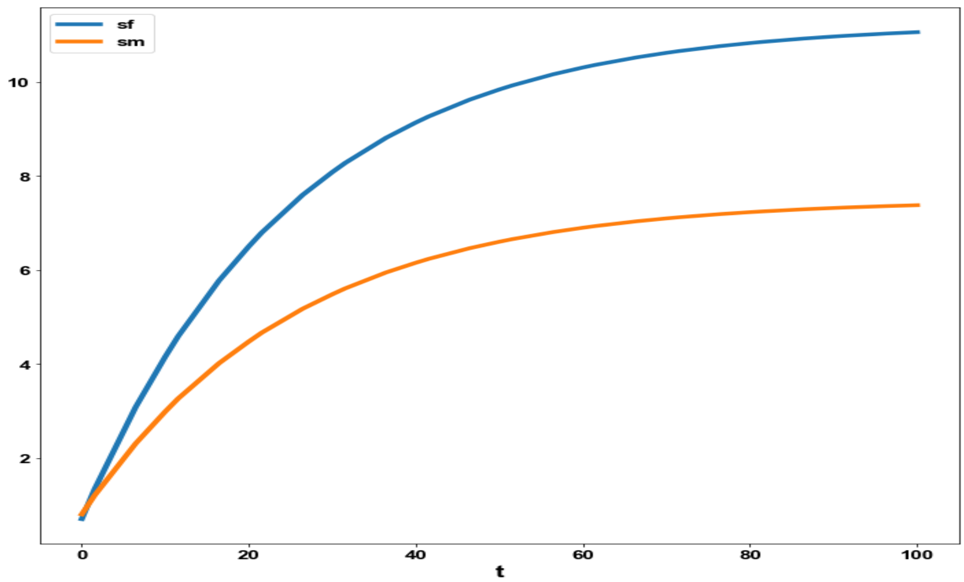

Figure 2 : *MNLMPC of gonorrhea model, sf sm vs t.*

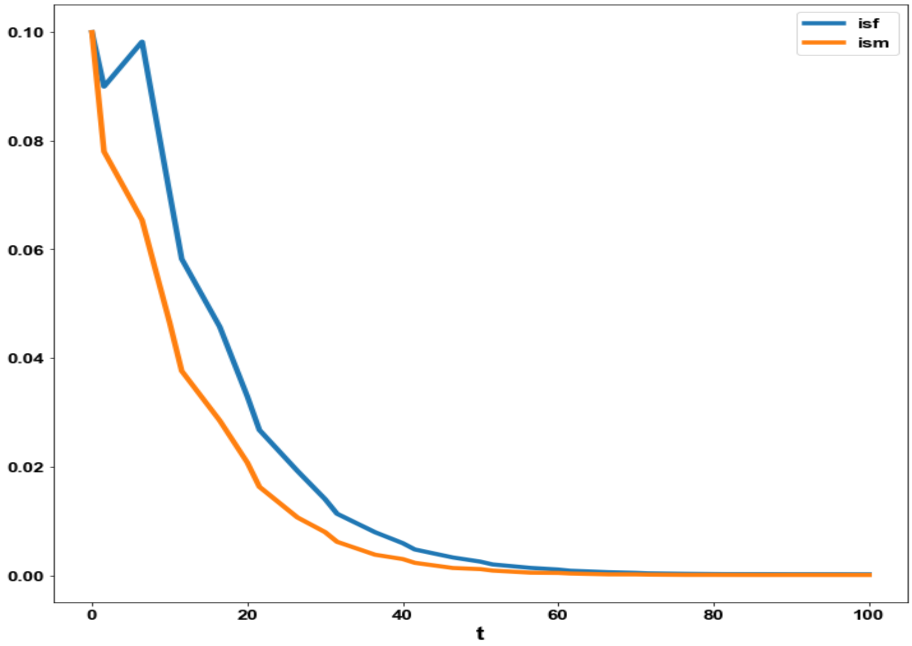

Figure 3: *MNLMPC of gonorrhea model, isf ism vs t*

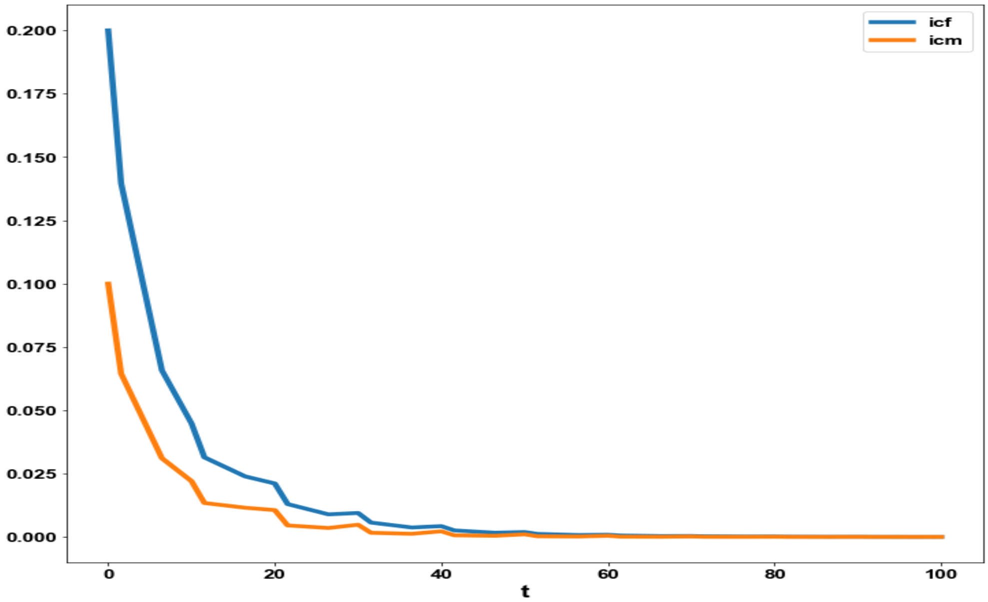

Figure 4: *MNLMPC of gonorrhea model icf icm vs t.*

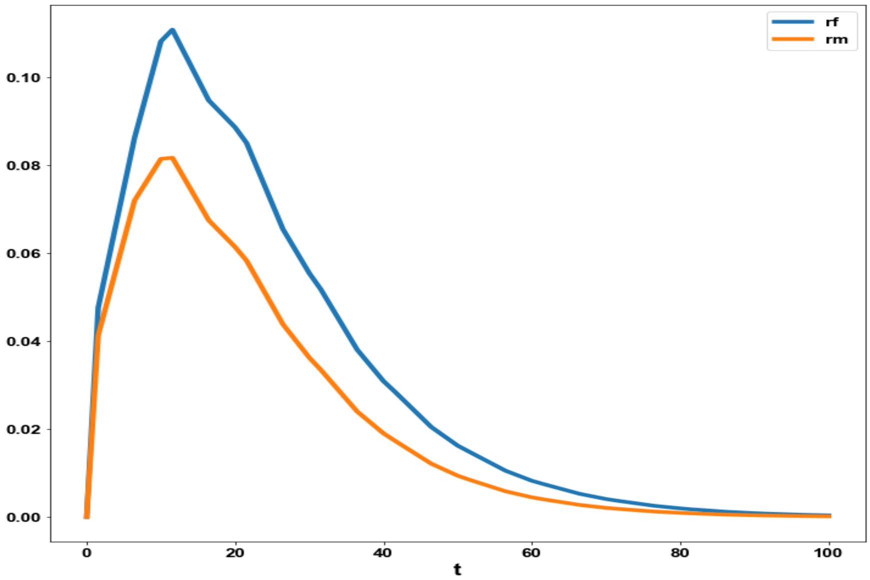

Figure 5: *MNLMPC of gonorrhea model, rf rm vs t.*

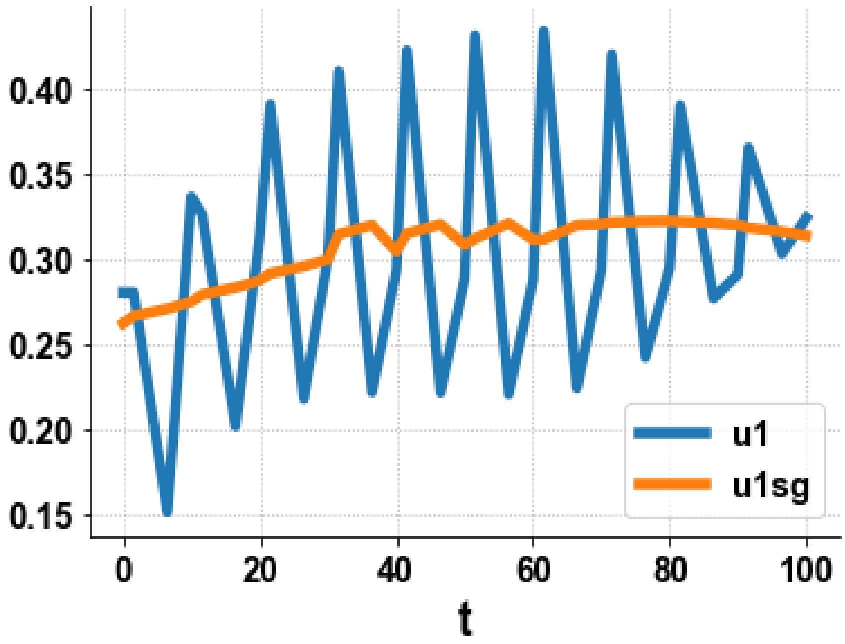

Figure 6 : *MNLMPC of gonorrhea model, u1, u1sg vs t.*

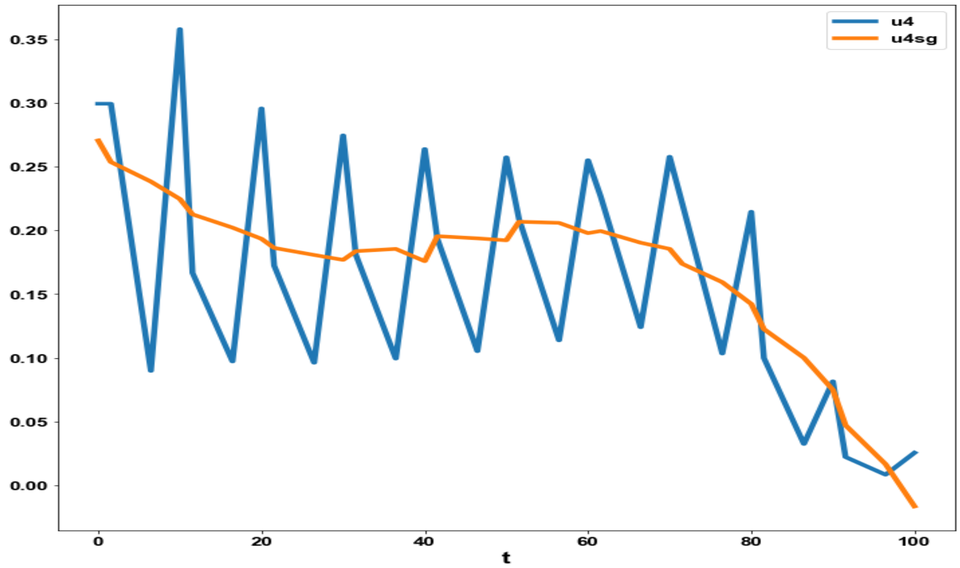

Figure 7: *MNLMPC of gonorrhea model, u4, u4sg vs t.*

Conclusions

Bifurcation analysis and Multiobjective nonlinear model predictive control calculations were performed on a dynamic model involving the transmission of gonorrhea. The bifurcation analysis revealed the existence of branch points. The branch points (which produced multiple steady-state solutions originating from a singular point) are very beneficial as they caused the multiojective nonlinear model predictive calculations to converge to the Utopia point (the best possible solution) in both models. A combination of bifurcation analysis and multiobjective nonlinear model predictive control for the gonorrhea transmission 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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