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Optimal Control of a Coastal Ecosystem Through Neural Ordinary Differential Equations

C. Coelho [1], M. Fernanda P. Costa [1], L.L. Ferrás [1,2],

[1] *Centre of Mathematics, University of Minho, Braga, Portugal*

[2] *Department of Mechanical Engineering (Section of Mathematics) and CEFT - Centro de Estudos de Fenómenos de Transporte - FEUP, University of Porto, Portugal*

CMARTINS@CMAT.UMINHO.PT, MFC@MATH.UMINHO.PT, LFERRAS@FE.UP.PT

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Abstract

Optimal control problems (OCPs) are essentials in various domains such as science, engineering, and industry, requiring the optimisation of control variables for dynamic systems, along with the corresponding state variables, that minimise a given performance index. Traditional methods for solving OCPs often rely on numerical techniques and can be computationally expensive when the discretisation grid or time horizon changes. In this work, we introduce a novel approach that leverages Neural Ordinary Differential Equations (Neural ODEs) to model the dynamics of control variables in OCPs. By embedding Neural ODEs within the optimisation problem, we effectively address the limitations of traditional methods, eliminating the need to re-solve the OCP under different discretisation schemes. We apply this method to a coastal ecosystem OCP, demonstrating its efficacy in solving the problem over a 50-year horizon and extending predictions up to 70 years without re-solve the optimisation problem.

Keywords: Optimal Control; Neural Ordinary Differential Equations; Numerical Methods; Climate;

1. Introduction

An optimal control problem (OCP) is a constrained optimisation problem aimed at finding a set of control variables $u(.) \in U$ for a dynamic system, along with the corresponding state variables $x(.)$, that minimise a given performance index or cost functional, $J(x(.), u(.))$. The application domains of OCPs are diverse, encompassing fields such as science, engineering, and industry, among others (Todorov, 2006; Yin S, 2023).

For example, an OCP in *Lagrange form* is defined as follows:

$$
\begin{aligned}
J^* = \min_{u(t)\in U} J(x(t), u(t)) &\equiv \int_{t_0}^{t_f} f(t, x(t), u(t))\, dt \\
\text{subject to: } \dot{x}(t) = g(t, x(t), u(t)), &\quad \text{for } t \in [t_0, t_f] \\
x(t_0) = x_0, &\quad x(t_f) = x_f
\end{aligned}
\tag{1}
$$

where $U = \{u(t) : u(t) \text{ is measurable}, u_{\min} \leq u(t) \leq u_{\max},\ t \in [t_0, t_f]\}$ is the admissible control set, and $u_{\min}$ and $u_{\max}$ are fixed real constants with $u_{\min} < u_{\max}$.

In general, $f(.)$ and $g(.)$ are continuously differentiable functions in all three arguments. $u(.)$ is piece-wise continuous and the associated state variables $x(.)$ are piece-wise differentiable. In (1) the value of $x(t_f)$ is restricted, i.e, $x(t_f) = x_f$. However, other problems may consider the value of $x(t_f)$ free.

It is important to note that there are well-known equivalent formulations for describing an OCP, namely the Lagrange, Mayer, and Bolza forms (Todorov, 2006). However, solving OCPs precisely and efficiently can be challenging. The majority of real-life OCPs lack explicit solutions and rely heavily on numerical methods. OCPs can be solved using indirect or direct methods.

Indirect methods apply the first-order necessary conditions from Pontryagin's maximum principle to reformulate the original OCP into a boundary-value problem. In these methods, it is mandatory to calculate the Hamiltonian, the adjoint equations and the optimality and transversality conditions. One of the most well-known indirect methods is the backward-forward sweep method (Lenhart and Workman, 2007). Conversely, direct methods eliminate the need for explicitly deriving first-order necessary conditions. Direct methods solve the OCP directly by approximating it with a finite-dimensional optimisation problem (OP) obtained through the discretisation of control and state variables. This transformation allows the use of efficient and well-established optimisation methods to find the solution (Betts, 2010). In direct methods, control variables are always discretised, but the treatment of state variables can vary (Diehl et al., 2006). The Direct Sequential approach transcribes the OCP into an OP by discretising only the control variables while embedding the Ordinary Differential Equations (ODEs) within the OP (Schlegel et al., 2005). This results in relatively small-scale OPs. The dynamic system is solved using an ODE solver to obtain the state values required for the optimisation process. Consequently, simulation and optimisation are performed sequentially. In contrast, the Direct Simultaneous approach discretises both control and state variables, which can lead to large-scale OPs (Hanson et al., 2010). However, in these approaches, using a different discretisation scheme, it is required to solve an entire new OP, which is computationally expensive.

Neural ODEs (Chen et al., 2018) are a specialised neural network (NN) architecture with continuous depth. Unlike traditional NNs, which have a discrete sequence of layers and fit a time-independent function to data, defined by the NN architecture, Neural ODEs fit the solution's of a time-dependent function, a initial value problem, to data using an ODE (or system of ODEs). This enables Neural ODEs to handle irregularly sampled data and, once trained, provide predictions across the entire time domain. In this work, we propose a novel approach by embedding a Neural ODE into the OP to model the dynamics of the control variables, given a system with known dynamics. In our approach, we model the dynamics of the control variables with a Neural ODE, allowing us to solve the resultant system of ODEs to obtain the control variable values at all desired time points once training is complete. This method overcomes a major limitation of traditional methods by eliminating the need to re-solve the OCP if the discretisation or the time horizon changes. This approach is used to solve a coastal ecosystem OCP, originally formulated in Mandal et al. (2021).

This paper is organised as follows. In Section 2, we briefly describe the motivation and the OCP herein proposed to be solved. Section 3 introduces our approach using Neural ODEs. Section 4 presents the numerical results and includes a brief discussion on the solution of the OCP. The paper ends with the conclusions in Section 5.

2. Coastal Ecosystem OCP

Over the past two centuries, unchecked population growth, modernisation, industrialisation, and urbanisation and deforestation have significantly increased greenhouse gas (GHG) emissions. This rise in GHG levels leads to destructive natural phenomena impacting human societies and ecosystems. Carbon Capture and Storage (CCS) techniques, including polymeric amines and desulphurization processes, are increasingly used in industries, potentially reducing CO_2 emissions by 20% by 2050 and mitigating acid rain. However, deforestation and excessive GHG emissions persist, reducing forested areas. Solutions like greenbelts, coastal afforestation, reforestation, and advanced CO_2 capture methods offer promising strategies for GHG reduction (Varghese and Karanikolos, 2020; Babbar and Babbar, 2018; Krótki et al., 2020; Mandal et al., 2021).

In Mandal et al. (2021) the authors proposed an OCP to study the dynamics of GHG emissions on climate change and coastal ecosystems over 50 years, using a coastal greenbelts process ($u_1(t)$) to reduce the concentration of GHGs by absorbing atmosferic CO_2, and a desulphurization process ($u_2(t)$) to prevent the release of harmful sulphur components to limit industrial GHG emissions. More details can be found in Mandal et al. (2021). Let $G(t)$ represent the GHGs emitted by various industrial activities and man-made sources, $T(t)$ the atmosferic temperature which changes the earth's climate, $H(t)$ the human population in coastal regions which worsens deforestation, and $F(t)$ the forest ecosystems near coastal areas which are being damaged due to rapid climate change and concentrations of GHGs. In our work we consider the OCP defined as:

$$
\begin{aligned}
\underset{\boldsymbol{u}}{\text{minimize}} \quad & J(u_1, u_2) = \int_0^{T_p} \left[G + u_1^2 + u_2^2\right] dt \\
\text{subject to} \quad & \frac{dG}{dt} = \alpha_1 G + \delta_1 HG - \delta_2 FG + \delta_3 T - (u_1 + u_2)G, \\
& \frac{dT}{dt} = \alpha_2 T + \theta_1 GT + \theta_2 HT - \theta_3 FT - u_1 GT, \\
& \frac{dH}{dt} = \alpha_3 H \left(1 - \frac{H}{k_1}\right) - \psi_1 GH - \psi_2 TH + \psi_3 FH, \\
& \frac{dF}{dt} = \alpha_4 F \left(1 - \frac{F}{k_2}\right) - \epsilon_1 HF + \frac{\epsilon_2 F}{a + G} - \epsilon_3 TF + (u_1 + u_2)F, \\
& \boldsymbol{u}_{\min} < \boldsymbol{u}(t) \leq \boldsymbol{u}_{\max}, \ \forall t \in [0, T_p]
\end{aligned}
\tag{2}
$$

with the following initial conditions

$$
G_0 = G(0) > 0, T_0 = T(0) > 0, H_0 = H(0) \geq 0, F_0 = F(0) \geq 0.
$$

T_p is a predefined time period over which the controls are applied and α_1, α_2, α_3 and α_4 are respectively the natural growth rate of G, T, H, and F. The term $\delta_1 HG$ is the concentrations of GHGs caused by human activities, $\theta_1 GT$ is the increase in atmosferic temperature, $\psi_1 GH$ is the decline in the human population, and $\frac{\epsilon_2 F}{a+G}$ is the promotion of coastal forest ecosystems due to the rapidly rising concentrations of GHGs. The term $\theta_2 HT$ is the rise in atmosferic temperature and $\epsilon_1 HF$ is the decline in coastal ecosystems, due to humans activities. $\psi_2 TH$ presents the decrease in human population and $\epsilon_3 TF$ presents the destruction of coastal ecosystems, due to rapid global warming. Finally, $\delta_2 FG$ and $\theta_3 FT$ present the absorption of $G(t)$ and $T(t)$ respectively by forest ecosystems, and $\psi_3 FH$ is the increase in human population made possible by the support of forest ecosystems. For a detailed description of all parameters see Table 1 in Mandal et al. (2021).

3. Neural ODEs for Optimal Control

Neural ODEs are a special class of a NN architecture that fits the solution of a initial value problem:

$$\frac{d\boldsymbol{h}(t)}{dt} = \boldsymbol{f_\theta}(\boldsymbol{h}(t), t) \quad \text{with} \quad \boldsymbol{h}(t_0) = \boldsymbol{h}_0, \tag{3}$$

to data (Chen et al., 2018). Here, $\boldsymbol{h}_0$ is the initial condition at the initial time t_0, t is the time at which the solution is being computed, $\boldsymbol{f_\theta}$ is a NN with parameters $\boldsymbol{\theta}$, and $\boldsymbol{h}(t) = \boldsymbol{h}_t$ is the solution at time t.

In contrast to traditional NNs with a discrete layer-by-layer structure, Neural ODEs model the dynamics of data through a continuous-time dynamical system. This continuous-time approach introduces some key advantages over traditional NNs such as the ability to handle irregularly-sampled data and making predictions at any point in the time domain. To achieve this, Neural ODEs are composed of two main components: a NN, $\boldsymbol{f_\theta}$, with parameters $\boldsymbol{\theta}$, which approximates the right-hand side of an ODE or system of ODEs; a numerical method ($ODESolve$) that computes the solution of (3) as an initial value problem (Chen et al., 2018):

$$\{\boldsymbol{h}(t)\}_{t=t_0,t_1,\ldots,t_f} = ODESolve(\boldsymbol{f_\theta}, \boldsymbol{h}_0, (t_0, t_1, \ldots, t_f)),$$

where $(t_0, t_1, \ldots, t_f)$ is the vector of times for which a solution is desired.

Neural ODEs are trained using the same process as traditional NNs, and the result of training a Neural ODE is an ODE or a system of ODEs, which can be used to make predictions by solving the initial value problem at the desired times.

In this work, we propose using Neural ODEs for the OCP (2). Our approach employs a Neural ODE to fit a system of ODEs to the control variables dynamics:

$$\frac{d\boldsymbol{u}(t)}{dt} = \boldsymbol{f_\theta}(\boldsymbol{u}(t), t) \text{ with } \boldsymbol{u}(t_0) = \boldsymbol{u_0}, \tag{4}$$

where $\boldsymbol{u}(t) = (u_1(t), u_2(t))$.

To find the optimal parameters $\boldsymbol{\theta}$, we minimise the objective functional subject to the constraints (2). First, we define the loss function to train our Neural ODE for the optimal control approach (2), for all time steps, given by [1],

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{u}(t)) = \sum_{t=0}^{T_p} G(t) + u_1(t)^2 + u_2(t)^2. \tag{5}$$

In our approach, we propose obtaining $u_1(t)$ and $u_2(t)$ by numerically solving (4):

1. In this work, we do not use the weighting factors for the coastal greenbelt and desulphurisation costs as in Mandal et al. (2021) since these prevented the NN from training successfully.

$$\boldsymbol{u}(t) = ODESolve(\boldsymbol{f_\theta}, \boldsymbol{u}_0, (0, T_p)).$$

Then the state variables $G(t), T(t)), H(t), F(t)$ are obtained by solving the ODE system (2), which receive $u_1(t)$ and $u_2(t)$ from the numerical method $ODEsolve$.

Thus, the Neural ODE is trained by minimising (5), and the result of training is a system of ODEs that can be discretised at any desired points in time to obtain the optimal control values $u_1(t)$ and $u_2(t)$.

According to Mandal et al. (2021), the coastal greenbelt and desulphurisation control variables have limit bounds $u_1(t) \in (0, 0.02]$ and $u_2(t) \in (0, 0.0025]$. To satisfy these bounds, we constrain the Neural ODE's output by applying the exponential function $e^{-\boldsymbol{u}^2}$ and multiply it by 0.02 and 0.0025 for u_1 and u_2, respectively.

The advantage of this approach over traditional optimal control methods lies in its modelling of the dynamics of $\boldsymbol{u}(t)$ as a continuous-time function (the solution of (4)). This means that we only need to solve the optimal control problem once. Even if the time domain $[0, T_p]$ changes, we can easily discretise $\boldsymbol{u}(t)$ at the desired times to obtain the optimal control variables for the problem.

4. Results and Discussion

We conduct numerical experiments by solving the coastal ecosystem OCP using control variables $u_1(t)$ and $u_2(t)$, making the Neural ODE learn the dynamics of the system of ODEs $\frac{d\boldsymbol{u}(t)}{dt}$. This involves learning the optimal control dynamics for both the coastal greenbelt $u_1(t) \in (0, 0.02]$ and the desulphurization $u_2(t) \in (0, 0.0025]$. The OCP is solved for an end time of 50 years, $T_p = 50$, with initial conditions $u_1(t_0) = 0.02, u_2(t_0) = 0.0025$ for the control variables, and $G_0 = 0.04, T_0 = 0.07, H_0 = 1.1, F_0 = 8.75$ for the system variables, as in Mandal et al. (2021).

We then analyse and compare the results obtained before and after implementing the control strategies by plotting the system state variables over time in Figure 1. To examine how the control is applied, we also plotted the control variables over time in Figure 2.

For the Neural ODE, the NN architecture $\boldsymbol{f_\theta}$ is composed of: an input layer with two neurons with a hyperbolic tangent (tanh) activation function; a hidden layer with 32 neurons and a tanh activation function; and an output layer with two neurons. The Adam optimiser was used with a learning rate of 1e-5 (Kingma and Ba, 2014) and the training stopping criteria was given by the maximum number of iterations, 10000.

The coastal greenbelt control variable $u_1(t)$ is constantly used at its maximum value for roughly 20 years, declining to zero afterwards. Conversely, the desulphurisation control variable $u_2(t)$ is gradually reduced over the 50 years until it approaches zero.

Under this control strategy, GHGs emission significantly decline compared to the no-control scenario, consequently influencing atmosferic temperature changes. With control, the temperature rise is kept below 0.5ºC over the next 50 years, while without control, the temperature would rise by more than 2.0ºC over the same period. During the first 20 years, when GHGs concentration are at their lowest, human population growth increases sharply. Additionally, the reduction in GHGs emission leads to a higher growth rate of the forest ecosystem compared to the no-control dynamics. However, the decrease in GHGs emission

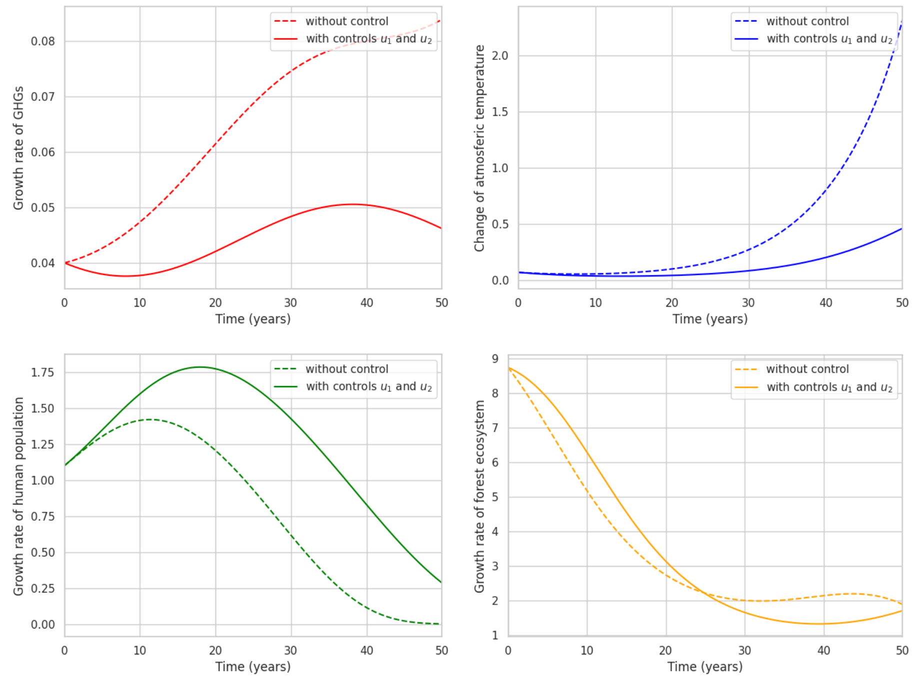

Figure 1: Numerical results for the system with and without the control strategy for the next 50 years.

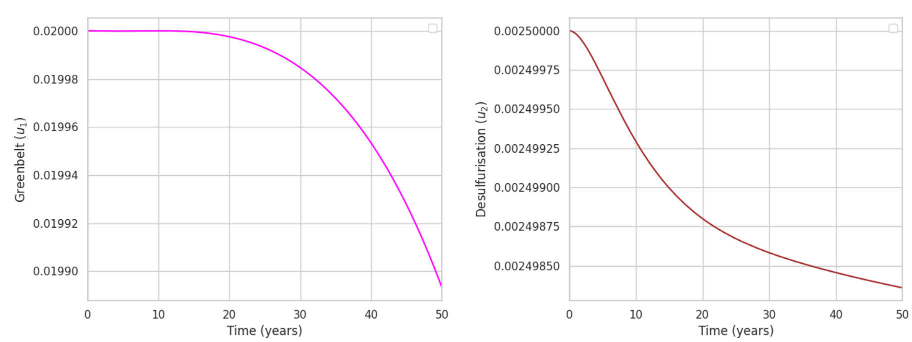

Figure 2: Optimal control profiles for the next 50 years.

also results in a reduction of the forest ecosystem, after 25 years, due to lower atmosferic CO_2 levels, which reduces photosynthetic activity and, consequently, the number of plants.

Extrapolation Our approach fits a system of ODEs to model the control variables of the system $u_1(t)$ and $u_2(t)$. As a result, solving the OCP yields a system of ODEs that can be discretised to obtain the variables' values at desired times without needing to re-solve the problem for different discretisations.

To demonstrate the effectiveness of our method in extrapolating the future beyond the solving time horizon, we discretise $\boldsymbol{u}(t)$ for 70 years and plot the system dynamics in Figure 3 and control variables over time in Figure 4.

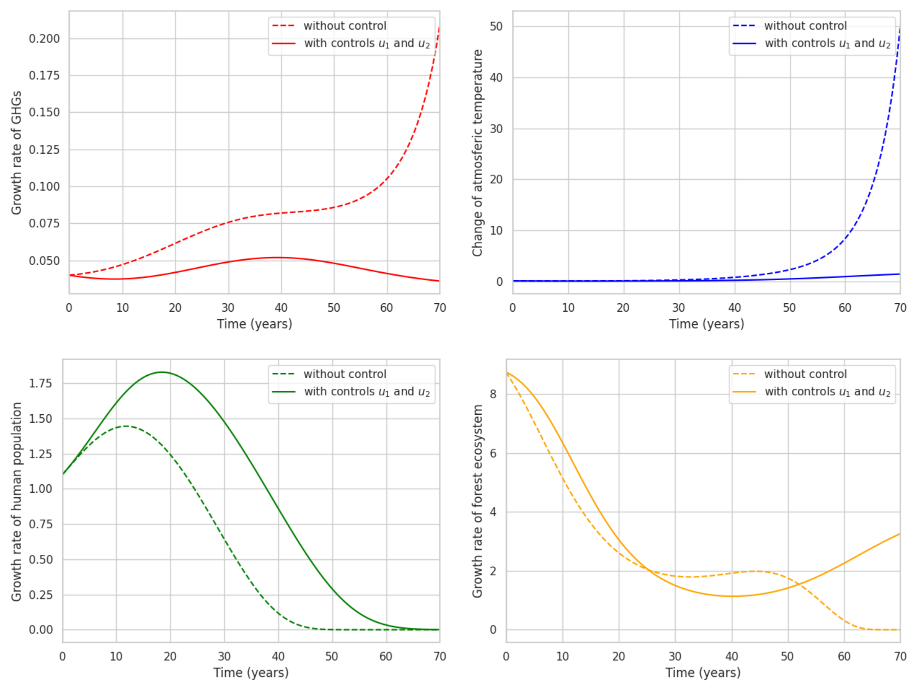

Figure 3: Numerical results for the system with and without the control strategy for the next 70 years.

From Figure 4 we can see that the control strategy for the coastal greenbelt continues to approach zero. However, the desulphurisation control variable starts to rise slightly after 50 years, showing a tendency to increase.

From Figure 3, we observe that over the next 70 years, GHGs emission continue to drop, reaching a growth rate lower than the current one. Consequently, atmospheric temperature does not increase significantly compared to the no-control scenario. After 60 years, the human population in coastal areas will stabilise, with a growth rate of zero. This stabilisation directly affects the increase of the forest ecosystem, which helps reduce GHG emissions by absorbing CO_2. This explains the reduced need for the coastal greenbelt.

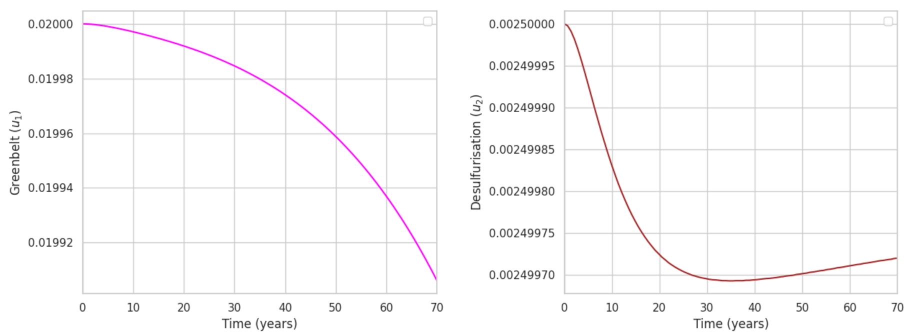

Figure 4: Optimal control profiles for the next 70 years.

5. Conclusion

In this work, we proposed solving the coastal ecosystem optimal control problem defined by Mandal et al. (2021) using a novel approach. We propose using a Neural ODE to learn the control variable dynamics of the coastal greenbelt u_1 and desulphurisation u_2 by fitting a system of ODEs. Once the training process was completed, we analysed the system dynamics with control by discretising the resultant system of ODEs over the desired time interval. This approach overcomes a major limitation of traditional optimal control methods by eliminating the need to re-solve the problem if the discretisation or time horizon changes.

The numerical results demonstrate that our approach successfully solved the coastal ecosystem optimal control problem for the next 50 years, addressing the complexities of these systems. Furthermore, without the need to re-train or re-solve the optimal control problem, we computed the system dynamics for the next 70 years, showing that our approach produces a generalised control strategy.

In future work, we aim to explore the proposed approach with different optimal control problems and compare the results obtained by extrapolating the learnt ODE with those obtained by re-solving the optimal control problem using a longer time horizon discretisation.

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