An Evolutionary Algorithm Approach to Ecological Optimal Control Problems

Amy-Rose Westcott

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An Evolutionary Algorithm Approach to Ecological Optimal Control Problems

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Abstract

There are several challenges associated with applying conventional (hereafter *classic*) optimal control (OC) methods to ecological optimal control problems (OCPs). Conditions required by these methods, including differentiability and convexity, for example, are not always met, and ecological problems do not always adhere to solvable OCP formulations. Moreover, mathematically optimal solutions do not always translate to optimal ecological strategies in practice. Despite this, alternative OC approaches are relatively under-explored.

Evolutionary algorithms (EAs) circumvent many of the complex aspects of classic OC methods and have been successfully applied to diverse OCPs. Nevertheless, EAs have seldom been applied to ecological OCPs. The viability of an EA approach to ecological OCPs was therefore investigated in the current study, facilitated by four case studies of increasing complexity and a genetic algorithm (GA) as a representative EA approach.

To ascertain the accuracy of a GA approach, comparisons between a GA and classic OC methods were conducted in the first three case studies. The GA generated near-optima in these comparisons, comparable to the corresponding classical solutions, whilst avoiding non-trivial mathematical theory. Supported by these results, an unconventional OCP, that arguably cannot be solved using classic OC methods, was formulated in the fourth case study, and solved using a GA approach. The resulting solution was feasible and further conformed with strategies found to be successful in practice. Additionally, the GA approach was relatively simple to apply in all case studies.

These collective outcomes demonstrated the viability of a GA as an OC method in ecological OCPs, thereby supporting the use of an EA approach as an alternative to classic OC methods in ecological OCPs. The feasibility of an EA approach to atypical OCPs was further demonstrated, which may act to increase realism in OC applications. Further investigation in this regard is thus warranted by this study.

Keywords: optimal control, ecological optimal control problems, optimal control methods, evolutionary algorithms, genetic algorithms

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Abbreviations

BTCS	**B**ackward in **T**ime-**C**entred in **S**pace
CPFT	**C**entral **P**lace **F**oraging **T**heory
CS	**C**omposite **S**impson's method
EA	**E**volutionary **A**lgorithm
FBSM	**F**orward-**B**ackward **S**weep **M**ethod
FTCS	**F**orward in **T**ime-**C**entred in **S**pace
GA	**G**enetic **A**lgorithm
HJB	**H**amilton-**J**acobi-**B**ellman
LDT	**L**ong **D**istance **T**ranslocation
NLP	**N**on-**L**inear **P**rogramming problem
OC	**O**ptimal **C**ontrol
OCP	**O**ptimal **C**ontrol **P**roblem
OCT	**O**ptimal **C**ontrol **T**heory
ODE	**O**rdinary **D**ifferential **E**quation
ORVS	**O**ral **R**abies **V**accination **S**trategies
PDE	**P**artial **D**ifferential **E**quation
PMP	**P**ontryagin's **M**aximum **P**rinciple
R-K	**R**unge-**K**utta method
R-K4	Explicit **R**unge-**K**utta method of order **4**
RS	left **R**iemann **S**um

Chapter 1

Research Context

1.1 Introduction

Optimal control theory (OCT) emerged as an independent mathematical field in the 1950s; a powerful tool with which to drive systems towards an optimal state (Pesch and Plail, 2009). Although developed in the engineering disciplines, its widespread applicability quickly facilitated its use elsewhere, incorporating and aided by developments made in varied fields, notably that of computational advances (Pesch and Plail, 2009).

Essentially, OCT utilises mathematical knowledge of a system to embed controls within the system in such a way that their manipulation is able to effect change on the outcome of a system in order to best obtain a desired objective or so-called optimal result (Lenhart and Workman, 2007). This is especially valuable in ecological fields as it allows decision-makers to simulate the imposition of measures on organisms at lower cost and with fewer ethical considerations (Lachish, Jones and McCallum, 2007).

In order to apply optimal control (OC), various conditions, like differentiability for example, should be met by certain functions in the optimal control problem (OCP) (Lenhart and Workman, 2007). These conditions are not always attainable in practice (Engelbrecht, 2007). In some instances, problem complexity or the OCP formulation itself may render *classic OC methods* (Section 2.2.3) inapplicable (Hamblin, 2013; Wang, Chen, Wang and Cao, 2017) or require complex mathematical knowledge (Lachish et al., 2007).

Depending on the nature of the OCP, standard OC methods may need to be supplemented with rigorous mathematical proofs (Ratković, 2016) or systems may have to undergo the requisite problem-specific reformulation in order to implement solution procedures (Zhang, Qiao, Wen and Julius, 2016). This may result in the OCP becoming unduly complicated (Bara, Djouadi, Day and Lenhart, 2017) and excessively challenging to the interdisciplinary researcher through the requirement of non-trivial mathematical expertise (Sargent, 2000).

Evolutionary algorithms (EAs), possessing fewer mathematical restrictions, offer an alternative to classic OC methods, allowing the user more flexibility (Fleming and Purshouse, 2002) and requiring less intensive mathematical knowledge (Engelbrecht, 2007). Although an optimal solution is not guaranteed using EAs (Engelbrecht, 2007), the stochastic nature thereof ensures their capability of locating global optima (Balsa-Canto, Banga, Egea, Fernandez-Villaverde and de Hijas-Liste, 2012). Changes to problem formulation can easily be implemented in EAs, without having to recast the problem as is the case in classic OC methods, making EAs better suited to use in practice (Blueschke and Savin, 2017).

To date, EAs have been successfully applied in many fields, including OC. Typically, EA usage in OC occurs in engineering-type OCPs, with applications ranging from renewable energy (Wang et al., 2017) to road design (Babapour, Naghdi, Ghajar and Mortazavi, 2018), but rarely ecological OCPs. Applying EAs to selected ecological OCPs, particularly when classic OC methods require mathematical expertise and thus become unavailable to the interdisciplinary researcher, therefore appears warranted.

The premise of the current research is based on examining the under-explored potential displayed by EAs for OC in ecology. This is formalised in Section 1.2, where both the research question and hypothesis are presented. Thereafter, the research question is decomposed into supporting aims and objectives in Section 1.3, followed by the methodology used in Section 1.4. Scope limitations are then discussed in Section 1.5, and the envisaged contribution of the proposed research, given in Section 1.6. Lastly, Section 1.7 outlines the dissertation layout.

1.2 Research Problem and Statement

Although classic OC methods are renowned for producing optimal solutions, theoretically-derived OC solutions do not always translate well in practice, particularly in ecology where discrepancies between mathematical assumptions and reality cannot reasonably be consolidated (Loehle, 2006). Optimal solutions can therefore have limited relevance as control strategies in ecology, as evidenced by the degradation of ocean fisheries (Loehle, 2006), for example. This motivates the reviewing of aspects of OC in ecology. This research proposes to investigate the feasibility of one such alternative approach, namely that of EAs.

The increased flexibility and reduced theoretical requirements of EAs may be well-suited to ecological applications of OC, and may even avoid some of the challenges of classic OC methods in ecological modelling. The success of EAs elsewhere (Sections 2.4.2 and 2.5.2) lends support to this notion, however, EA usage in ecological OCPs is still uncommon (Gobeyn et al., 2019). The research problem that this study will address is thus the limited extent of investigation into the viability of EA usage in ecological OCPs.

By contrasting the performance of EAs and classic OC methods through the use of comparisons within this study, this research proposes that a reasonable conclusion as to the viability of EAs in ecological OCPs may be derived. Thereafter, should promising results be attained, subsequent ecological applications may be advocated, particularly under the circumstances wherein classic OC methods encounter challenges. The overarching research question of this study is thus:

"Is an evolutionary algorithm approach a viable alternative to classic optimal control methods in ecological optimal control problems?"

In order to investigate the research question, a suitable implementation of an EA, namely a genetic algorithm (GA), will be applied to several ecological OCPs. The GA results will then be compared to results obtained using classic OC schemes. These comparisons will be used to gauge the quality of GA solutions, the outcomes of which will form the main criteria by which the research question will be investigated.

What constitutes the viability of an EA approach is arguably subjective and may embody a number of facets requiring consideration. To investigate this, the research question was further deconstructed into supporting aims and objectives, as stipulated in Section 1.3, which seek to provide tangible criteria by which to address the posed research question.

It is further hypothesised in this study that an EA approach could potentially increase the ease of implementing OC in ecology, whilst producing satisfactory results. Since complexity is difficult to quantify, this hypothesis will not be explicitly tested, however comments to this effect will be made. These processes and associated factors are elaborated on in the respective sections following.

1.3 Aims and Objectives

An EA approach to ecological OCPs will be investigated in a two-fold manner in this study. Firstly, the assertion that an EA can produce results analogous to classic OC methods will be examined. Thereafter, the ability of an EA to circumvent challenging aspects of classic OC schemes, whilst performing sufficiently, will be determined. The aims and objectives of this study were thus formulated to encompass these aspects, requiring a sub-division into two aims and their respective supporting objectives.

The main aim of this research seeks to establish whether an EA can adequately replicate classically-obtained OC results, providing a useful alternative to traditionally used methods in ecological OCPs. To operationalise this, objectives and related sub-questions, associated with achieving the main aim, were fashioned and are as follows:

1. **Review literature regarding classic OC solution methods and identify their associated caveats.** From this review, select the methods that will be used in the current study in conducting comparisons;
2. **Nominate ecological case studies.** Select case studies so as to cover a broad range of OCP formulations with which to then make the comparisons;
3. **Evaluate the outcome of applying an EA to the selected ecological OCPs.** Determine whether the EA will be able to reproduce classical results. Furthermore, is the EA able to circumvent any difficulties associated with the classical approach?
4. **Draw conclusions and possibly recommendations.** Identify the advantages and disadvantages of the two approaches. Does the EA increase the ease of implementing OC whilst adequately meeting the objectives of the OCP? Does the type of problem or its formulation have an effect on the performance of the EA?

The secondary aim of the study is concerned with identifying circumstances, if such exist, where classic OC methods become disproportionately complicated and it is tenable to use EAs instead. This aim therefore seeks to formulate an OCP as realistically as possible within the scope of the study, that cannot be or is exceptionally difficult to solve classically, and obtain a solution using an EA, which would appear to translate well in practice. Due to scope constraints and the anticipated complexity of formulating such an OCP, only a single case study will be examined. The examination of the second research aim is further dependent on the first being fulfilled. The objectives associated with achieving the second aim are thus:

1. **Identify an appropriate ecological case study.** The case study should demonstrate characteristics indicative of areas where difficulties in classic OC methods arise;
2. **Formulate an OCP which exploits the insensitivity of EAs to restrictions of classic OC methods.** Develop an OCP to address an ecological issue, incorporating the circumstances wherein conventional schemes display innate complexity;
3. **Evaluate the solution(s) produced by the EA.** Determine the feasibility and robustness of the results. Are the EA solutions realistic and implementable in practice?

Upon application of an EA to selected ecological OCPs, this study endeavours to ascertain whether EAs reduce the complexity of solving OCPs whilst producing satisfactory solutions. The methods used to address the aims and objectives are introduced next.

1.4 Methodology

Comparisons between different classic OC methods are frequently conducted via application to benchmark problems, which are typically of an engineering nature (Frego, 2014; Vanderbei, 2001). In recent comparisons with classic optimisation algorithms, EAs have produced promising results to engineering-based problems (e.g. Notte, Pedemonte, Cancela and Chilibroste, 2016; Theo, Lim, Ho, Hashim and Lee, 2017), thus motivating further investigation.

An experimental-type methodology will be adopted in the current research, whereby several ecological case studies will be used to facilitate comparisons between classic OC methods and an EA. Diverse case studies, designed to incorporate common OCP formulations, will be selected. These will be investigated in order of increasing complexity. Attention will be drawn to caveats of classic OC methods in order to ascertain whether EAs increase application ease. This will seek to address the main aim and supporting objectives of the study.

To address the second aim, a realistic ecological case study will be developed wherein it is inordinately complicated to apply classic OC methods. An EA will then be applied under these circumstances to determine whether an EA can be used, and if it is beneficial to use an

EA as an alternative OC method in such cases. The outcomes from this case study will be evaluated to ascertain the success of EA application.

Numerical schemes (Section 2.2.5.5), for both the EA and classical components, will be selected as per the literature review and applied to each case study using suitable computational algorithms (Section 3.4). OC solutions will then be analysed and compared to establish the viability of an EA approach. Limitations of the current study are discussed next.

1.5 Limitations

Various scope limitations will be introduced to constrain the content covered and maintain tractability. To this end, several case studies will be chosen to broadly represent OC applications in ecology. The anticipated feasibility of EAs may therefore have reduced generalisability in applications differing from those chosen herein. Furthermore, only three classic OC methods will be compared to a single EA in this study. Consequently, conclusions drawn from these comparisons cannot necessarily be extended to alternative classic OC methods or EAs.

Likewise, a variety of numerical integration methods are used in classical approaches. For practicality, only a subset of numerical methods, tailored to this study, will be used. This may, in turn, affect results. These limitations are however deemed essential to prevent the alteration of too many factors masking both observations and the core essence of the research.

To examine the potential of an EA approach to ecological OCPs, only a single, representative EA, namely a GA, will be used, so as to restrict the scope of the research. GAs have been extensively applied, their popularity and ubiquitous use a testament to their capability (Yang, 2014), prompting their usage in this study. Furthermore, the built-in GA function of MATLAB (2018), with default parameter settings, will be used to conduct the EA component of the research. The effect parameter settings may have on results obtained will not be examined in the current study due to scope limitations and is thus deferred to future work. Additionally, due to the dynamic nature of ecological systems (Jørgensen and Fath, 2011), continuous rather than discrete dynamical systems (Oruh and Agwu, 2015) will be employed.

Not all classical results will be derived and/or reproduced classically within the current study. In these instances, classical results will be extracted from existing literature and presented. The impacts of not reproducing these results will be discussed pertaining to conflicting literature, and mention made of the techniques used in obtaining the classical results.

1.6 Expected Outcomes and Contribution

Having seldom been applied to ecological OCPs, EAs may provide an alternative approach to classic OC methods, but have shortcomings associated with them (Blueschke and Savin, 2017). An appraisal of EAs in ecological OCPs would thus contribute to existing research, determining several advantages and disadvantages of their use in an ecological setting. Difficulties arising in classic OC methods in ecology have been identified (Bara et al., 2017), but to the best of the author's knowledge, comparative handling thereof by EAs has not been examined. This study seeks to address this gap in research.

EAs have been successfully applied across a range of topics and disciplines. Similarly, OC techniques are widely applicable and therefore any knowledge gained in this research may be transferable in some measure to seemingly unrelated disciplines. If an EA is shown to be an effective alternative, this research would further advocate EA use in OCPs where classic OC methods are predominantly favoured. The impact thereof could then be to potentially improve the accessibility of OC to ecologists.

In a study by Notte et al. (2016), an EA was found to perform marginally less well than classic OC methods, locating near-optimum solutions, but with the additional benefit of producing diverse solutions. EAs have also produced robust solutions when applied to non-linear programming problems (NLPs) (Singh, 2012), a formulation closely associated with and regularly followed in OC (Biral, Bertolazzi and Bosetti, 2016). The outcome of the current study would thus be an extension of the above-mentioned research, its aim being to apply an EA to OCPs, not merely in a comparative capacity, but to demonstrate the ability of EAs to overcome shortcomings associated with classic OC methods.

Investigating the feasibility of EAs as an alternative OC method in ecology would thus contribute to advancing scientific research, addressing several of the complexities of classic OC methods and evaluating the performance of EA under these circumstances. One such consideration is whether EAs may to an extent avoid the simplifications frequently ascribed under classical frameworks to enable specific solution procedures (Blueschke and Savin, 2017). Additionally, the need for review of conventional applications of OC in ecology (Loehle, 2006) is to a small extent attempted by consideration of this alternative approach.

1.7 Dissertation Layout

The structure of this dissertation is separated into theoretical, application, and concluding components. Firstly, context and theory are given, providing supporting literature and methodological considerations. Comparative case studies are then presented in order to address the main aim of this study. An experimental case study in which an EA is applied to an OCP in an exploratory capacity as a means of addressing the secondary aim follows, concluding the application component. Finally, a summary of research findings and recommendations for future research are given. A more detailed outline of each chapter is as follows:

- **Chapter 2** presents literature pertaining to OC, ecological OC, and EAs, in order to provide a comprehensive basis for the investigation proposed in this research.
- In **Chapter 3**, an overview of the methods adopted in this research is given, based on considerations raised in the literature review.
- **Chapter 4**, the first of two comparative chapters, addresses the main aim of the study in relation to ordinary differential equation (ODE) models; namely to ascertain whether a GA is able to replicate classical results, and the ease with which this is accomplished. Two ODE case studies will be used to facilitate comparisons.
- In **Chapter 5**, the main aim is further investigated by applying both a GA and classic OC method to a partial differential equation (PDE) model and comparing the results.
- **Chapter 6** pursues an experimental approach to address the secondary aim of the study. An OCP is formulated, to which classic OC methods cannot be applied, or are excessively complex to apply, and a GA approach is used to solve the resulting model.
- **Chapter 7** collates the findings obtained throughout the course of this dissertation to deliberate the aims, hypothesis and research question posed. Finally, concluding remarks and recommendations for future work are made.

Chapter 2

Related Literature

2.1 Introduction

The evolution of OC has largely been facilitated through the support of computational advances. EAs offer further potential for the evolving of OC in an ecological capacity, but are as yet under-explored. In order to form a comprehensive basis with which to explore this potential presented by EAs, literature relating to both classic OC and evolutionary methods is reviewed in this chapter, with emphasis on ecological applications and research needs.

To contextualise this research, the literature review commences with the historical context from which OC has arisen and follows the developments it has undergone until the present time (Section 2.2). An overview of ecological OC ensues (Section 2.3), followed by literature concerning EAs (Section 2.5); their strengths, weaknesses, and potential in ecological OC.

2.2 Optimal Control Theory

Building on the theory of static optimisation and the calculus of variations, OCT employs *dynamic optimisation* - using unknown functions or control variables, rather than state variables, to optimise functionals (Frego, 2014; Ratković, 2016). Formalised as an independent discipline in the 1950s (Pesch and Plail, 2009), OCT has undergone a continual evolution ever since. As challenges have arisen, so have solutions been sought, with OC developments frequently taking inspiration from computational advances. Faced with challenges in ecological OCPs, this research endeavours to do the same. Consequently, a brief history of OC follows.

2.2.1 A Brief History

The first documented prototypes of OCPs appeared as early as the 1600s, and many prominent mathematicians have lent their expertise to the development of OCT through the passage of time since (Sargent, 2000). As a result of this collaborative effort spanning decades, the burgeoning field of OCT was systematically fleshed out with the components that would later form the essence of the theorems fundamental to OCT today (Sargent, 2000).

Where early strides were bolstered by a synergistic approach between mathematicians of the time, later developments were cultivated as proceeds of war. The invention of the digital computer, a product of World War II (Krotov, 1996), facilitated the devising of numerical methods, leading to the rapid expansion of OCT during the Cold War (Pesch and Plail, 2009). Mathematicians enlisted in the war effort consolidated the theoretical findings of their predecessors into theorems (Sargent, 2000), forming the backbone of the independent field now known as OCT. Significant contributions were made by both the US and the USSR during this period (Pesch and Plail, 2009), with substantial advances attributed largely to the pioneering, albeit separate, work of Bellman and Pontryagin (Frego, 2014).

Arising from the calculus of variations to tackle the aerospace dilemmas of the Cold War, and supported by the new problem-solving capabilities of the computer (Sargent, 2000), OC has experienced a pattern of necessity driving innovation throughout its existence (Krotov, 1996). Initially, the absence of numerical methods rendered OCPs unsolvable (Pesch and Plail, 2009). Subsequently, linearisation became obsolete in the face of increasing aircraft speeds demanding non-linearity be taken into account (Pesch and Plail, 2009; Ratković, 2016). Similarly, constraints and inequalities were met with extreme complexity in the existing methods, requiring a reversion to NLP which allowed for their inclusion (Frego, 2014).

Even with the prolific number of algorithms available today, adaptations to existing methods and the creation of innovative solving procedures are of ongoing importance as new complexities and advances in OCT come to light (Theo et al., 2017). Borne predominantly as a means to solve problems in the engineering disciplines (Loehle, 2006), applications in this field are still outpacing theoreticians in devising mechanisms to overcome obstacles encountered in OC applications (Fleming and Purshouse, 2002).

Meta-heuristic[1] algorithms have shown promise as both a flexible and capable alternative

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[1] Stochastic algorithms that use a combination of randomisation and local searches to equip them for global optimisation (Yang, 2014).

OC solution procedure (Barbour et al., 2016). This recent work has allowed EAs, a class of nature-inspired meta-heuristics, to be used in conjunction with deterministic schemes, thereby avoiding specific complexities presented by classic OC methods and successfully aiding classic OC methods to more efficiently locate optimal solutions (Balsa-Canto et al., 2012). The hybrid algorithms that have evolved from this re-conceived methodology, as well as the successful applications of EAs, lends weight to the investigation proposed in this study.

In addition, although successful in many disciplines, OC has had a more modest outcome in ecology, with derived policies sometimes failing to achieve optimal results in practice (Loehle, 2006). In some instances, this is as a result of altering OCPs to ensure compatibility with mathematical theory (Rodrigues, Monteiro and Torres, 2009). Typically this occurs in complex OCPs, as is characteristic of ecology. Indifferent to the rigid requirements of classic OC methods, the flexible meta-heuristics may be better suited under such circumstances, however, there are also occasions when classic OC methods are more appropriate (Barbour et al., 2016). Prior to investigating the viability of EAs in ecological OCPs, an understanding of OCT is therefore needed. Correspondingly, the OCP formulation is next outlined.

2.2.2 The Optimal Control Problem

The purpose of an OCP is to maximise or minimise some criteria of a system subject to the dynamics of the system itself, and any constraints placed on the system. The OCP is formulated accordingly, a general, unconstrained example of which, adapted from Stengel (1994) and given in *Lagrange* form (Subchan and Żbikowski, 2009), is as follows:

$$\underset{U}{\text{maximise}} \text{ or } \underset{U}{\text{minimise}}\ J(\bar{u}(t)) = \int_T \ell(\bar{x}(t), \bar{u}(t), t)\, dt \tag{2.1}$$

subject to:

$$\dot{\bar{x}}(t) = \bar{f}(\bar{x}(t), \bar{u}(t), t), \tag{2.2}$$

$$\bar{x}(t_0) = \bar{x}_0. \tag{2.3}$$

The optimality criterion which best quantitatively represents the desired outcome or the overarching reason for pursuing the optimal functioning of a system, is given by an *objective function*[2], denoted $J(\bar{u}(t))$ in Equation (2.1). The associated cost of achieving such an outcome is typically factored into the function $\ell(\cdot)$. Inputs in the form of *controls*, $\bar{u}(t)$ from a

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[2] Used interchangeably with the terms cost function, performance index, optimal criterion or functional.

set U, are used to manipulate the *state*, given by vector function $\bar{x}(t)$, towards producing an output that optimises the objective. This requires the formulation of a dynamical system, represented by state equations in Equation (2.2), describing the characteristics of the system considered, into which the controls are inserted with the capacity to influence the system's dynamics. Initial ($\bar{x}(t_0)$, Equation (2.3)), or terminal conditions are attached, as are constraints on the states and/or controls of the system (not shown in the OCP formulation).

The controls should be feasible, which requires them to be *admissible* and satisfy all constraints on the entire time interval (T) considered (Lenhart and Workman, 2007). The response the controls effect from the system should too be defined over T (Pontryagin, Boltyanskii, Gamkrelidze and Mishchenko, 1962). Upon satisfaction of these requirements, the OCP is fully specified. The formulation and anticipated functioning thereof is further dependent on the *observability* and *controllability* of the system (Bryson and Ho, 1975).

The dynamical system can be in the form of ODEs (as shown), PDEs, difference equations or even stochastic differential equations (Lenhart and Workman, 2007), each of which requires altered optimality principles (Stengel, 1994). Controls are varied dynamically to drive the state towards achieving an optimum (Subchan and Żbikowski, 2009) and dependence on time is factored into the objective by featuring a final time condition to be optimised, or in the form of an integral (Stengel, 1994). Once formulated, an optimal solution to the OCP can be obtained using specialised schemes, the classic methods of which, are outlined next.

2.2.3 Classic Optimal Control Methods

The cornerstone methods used to solve OCPs can chiefly be accredited to the seminal works of Pontryagin, Bellman and their colleagues at the time (Frego, 2014). Throughout this text, these, and other, conventional methods used to solve OCPs will be termed *classic OC methods*, indicating that the method is rooted in mathematics or makes use of standard optimisation results, as opposed to modern computational methods like meta-heuristics.

Classic OC methods can almost exclusively be categorised as indirect, direct or dynamic programming methods (Biral et al., 2016); each of which is next outlined. Central to all methods, is the devising of conditions that will facilitate the attaining of optimality. Results generated using classic OC methods, or a *classical* approach, will be referred to as *classical results* in the remainder of this text, unless the method itself is specified.

2.2.3.1 Indirect Methods

The indirect methods are synonymous with Pontryagin's Maximum Principle[3] (PMP) (Pontryagin et al., 1962); a theorem which employs *adjoint* functions (or *co-state equations*), and their associated *transversality* conditions to facilitate the absorbing of the objective into the system of equations to be solved (Ghosh, Lashari and Li, 2013). This is accomplished by formulating a *Hamiltonian*, from which the necessary (*optimality*) conditions of PMP are derived (Balsa-Canto et al., 2012; Sargent, 2000). An explicit expression for the optimal control is then obtainable from the necessary conditions (Biral et al., 2016).

This routine first optimises and then discretises, converting the OCP into a boundary value problem (BVP) from which solutions to the adjoint and state variables can be obtained (Balsa-Canto et al., 2012). Maxima produced by solving the BVP are verified against sufficiency conditions to determine whether a global optimum has been found in the extrema produced (Rao, 2010; Ratković, 2016). Should all necessary, sufficient, existence and uniqueness conditions be satisfied, a global optimum is guaranteed. Equivalently, PMP can be stated as Pontryagin's Minimum Principle, from which minima are obtained analogously.

Ample complexities are attached to the indirect methods, arising largely in the form of theoretical conditions (Subchan and Żbikowski, 2009). As OCPs increase in complexity, so too does the derivation of optimality conditions (Rao, 2010). This is exacerbated in the presence of inequality constraints (Subchan and Żbikowski, 2009) which add considerable complexity to the solution procedure (Frego, 2014; McAsey, Mou and Han, 2012). Significant expertise may then be required to deal with the resulting issues, such as discontinuity, that the indirect method can bring about (Sargent, 2000; Subchan and Żbikowski, 2009). Computationally, the size of the system can become a formidable factor as the addition of adjoint variables doubles the number of equations in the system (Bertolazzi, Biral and Da Lio, 2006).

The primary techniques for solving OCP-derived BVPs are centred around shooting, finite difference, and collocation methods (Morrison, Riley and Zancanaro, 1962; Rao, 2010). Once solved, validating sufficiency conditions to establish global optimality can present substantial difficulty (Schwartz, 1996). Hence, global optimality is often assumed rather than proved. However, as dynamic optimisation methods, the indirect methods are capable of locating global optima and can (under specific conditions) admit analytical solutions (Frego, 2014).

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[3] Lenhart and Workman (2007) gives both autonomous and non-autonomous versions of PMP.

Whilst the theoretical knowledge and understanding of the OCP gained using indirect schemes remains possibly the most informative of the approaches, the inherent difficulties of the method obstruct solution procedures, requiring the devising of sophisticated mechanisms for implementation in realistic applications (Sargent, 2000), acting to reduce its usage by non-mathematicians. Recent literature seldom considers the indirect methods in isolation (McAsey et al., 2012), but rather in combination with the direct methods, or in a comparative capacity, in an effort to mitigate the complications of applying this approach to the increasingly complex OCPs formulated nowadays (Goryanin and Goryachev, 2011).

2.2.3.2 Dynamic Programming

Analogous to the indirect methods, dynamic programming can be used to achieve global optimality in OCPs (Zanetti, Aprile, Kum, Scoccia and Motta, 2020). Specific OC configurations, namely a quadratic objective and linear states, can also easily and accurately be solved using dynamic programming (Bellman, 1971; Zhang, Li and Liao, 2019). Similarly, however, its implementation is hampered by frequently requiring expertise and innovative adaptations (Talpaz, 1982). Differences in the dynamic programming approach include solving the OCP as a family of OCPs by restricting and optimising the OCP on subintervals (Frego, 2014).

The premise of Bellman's (1967) Principle of Optimality revolves around viewing the optimal trajectory as composed of sections of optimal sub-arcs (Frego, 2014). The Hamilton-Jacobi-Bellman (HJB) equation, a PDE central to the method, is then solved iteratively on each of the restricted subintervals (Frego, 2014). This can cause a compounding increase in dimension, or the *curse of dimensionality*, even in relatively simple problems (Sahashi, 2002), and can cause intractability, particularly in higher dimensions (Bertolazzi et al., 2006). Compared to both the indirect and direct methods, dynamic programming requires far greater computational effort to obtain equivalent accuracy (Biral et al., 2016).

A feasible solution to the HJB equation is required to obtain a solution to the OCP using dynamic programming (Bryson and Ho, 1975). Elementary problems where the HJB equation can be solved analytically excepted, a numerical approximation to the equation is typically required (Beeler, Tran and Banks, 2000). Iterative processes are usually used in this respect, which produce a series of approximations that generally converge to a satisfactory approximation. Alternatively, an OCP can be transformed into a related formulation, from which a suboptimal solution to the OCP can be obtained (Beeler et al., 2000).

This is not unlike the passage from the indirect methods to the direct methods, with the former habitually considering iterative processes that upon decreasing the discretisation step length, may converge to the true solution, whereas the latter, discussed next, transforms the problem into a NLP formulation which can at best converge to a suboptimal solution.

2.2.3.3 Direct Methods

The direct methods were developed to reduce the complexity involved in incorporating constraints and inequalities in OCPs cast as BVPs (Balsa-Canto et al., 2012). Reverting to static optimisation by transcribing an OCP into a NLP which can more easily handle challenges of BVPs, a wide body of research, optimisation solvers, and resources become available to assist in solving OCPs (Frego, 2014). Proof of the equivalence between the OCP and the corresponding NLP is first required however, and upon obtaining a solution, the necessary conditions should be verified to evaluate the fidelity of the results (Bertolazzi et al., 2006).

A coordinate transformation is typically used to convert an infinite dimensional OCP into a finite dimensional NLP (Schwartz, 1996). A number of routines exist to accomplish this. Complete parameterisation schemes parameterise both the controls and states, requiring large computational resources, whereas control vector parameterisation methods parameterise only the controls (Hirmajer, Fikar, Balsa-Canto and Banga, 2008) and are thus able to handle large NLPs more efficiently (Balsa-Canto et al., 2012). In both approaches, the OCP control variables are incorporated as decision variables in the corresponding NLP (Schwartz, 1996).

Upon indefinitely decreasing the discretisation step length (step size $h \to 0$), the Karush-Kuhn-Tucker necessary conditions of the associated NLP converge to the necessary conditions of PMP, and can thus be viewed as the discrete equivalent of PMP's Euler-Lagrange equations (Bara et al., 2017). In spite of this, global optima cannot be guaranteed and are not necessarily obtained using this approach, as static optimisation runs the risk of getting trapped in local optima. This may, in part, be attributed to the gradient-based, deterministic local search methods often used to locate optima (Balsa-Canto et al., 2012). The extrema located are further dependent on initialisation and should be analysed to ensure that convergence does not occur simply to the closest local optimum (Zhang, Wen and Julius, 2012).

While the direct methods address many of the challenges faced by the indirect methods, such as constraint handling (Subchan and Żbikowski, 2009), solution quality is dependent on the approach taken to solving (Rao, 2010), with more accurate methods coming at a high computational cost (Frego, 2014). Scrutiny of results is thus crucial due to the dependency of their merit on the numerical methods used in obtaining them (Ratković, 2016).

Reliance on an appropriate *solver* (specialised optimisation or OC software) can be critical to the direct approach and customary solvers may even fail to produce solutions (Biral et al., 2016). The direct methods are thus constrained by limitations such as the increase in difficulty when handling non-linearity (Balsa-Canto et al., 2012), and dimensionality (Bertolazzi et al., 2006). Consequently, there is a continuing need to improve solution schemes.

2.2.4 Implementing Classic Optimal Control Methods

OC has seen widespread applicability since its inception with varying degrees of success. Arguably, this can in part be attributed to how OC is implemented across various disciplines. Where OC may be used in the designing or building of systems, based on components well-studied and easily modelled in some, in others, such as ecological disciplines, the user has limited controllability and observability of the system at hand (Loehle, 2006). As a result, opposing schools of thought exist concerning the functionality of OC (Locatelli, 2001).

On one hand, OC is perceived as idealised and its applicability overestimated, provoking an equally extreme view on the other hand, of its futility, believing it to have purely theoretical value (Locatelli, 2001). There are also disagreements as to the best-suited methods, and factors that should be taken into consideration when solving an OCP. This may complicate the decision-making of the user, particularly if they are from a non-mathematical field. Accordingly, assessing the limitations of classic OC methods is pertinent to effectively applying OCT (Locatelli, 2001) and thereby producing useful solutions (Barbour et al., 2016). To this end, challenges associated with applying optimal control are dealt with next.

2.2.5 Challenges Associated with Applying Optimal Control

The determination of optimality within traditional frameworks, developed for early OCPs, has become somewhat outdated in the presence of the complex OCPs now formulated (Barbour et al., 2016). Consequently, emphasis should be placed on examining the limiting effects factors such as model conceptualisation, implementation or uncertainty may have on optimal strategies, and whether these suitably represent the intended problem (Barbour et al., 2016). In order to produce useful OC solutions (Bellman, 1971), these factors were next examined.

2.2.5.1 Assumptions and Simplifications

The derivation of an OCP to describe a real-world problem requires various assumptions and simplifications in order to capture the essence of a system within a mathematically tractable form (Gumowski and Mira, 1968), examples of which are given in Table 2.1. Excessive simplification, however, can lead to significant discrepancy between a real-world system and its theoretical counterpart, rendering a theoretical exercise with little to no practical value (Gumowski and Mira, 1968). Adjusting the degree of simplification to one wherein a reasonable level of complexity is maintained, while also including necessary assumptions, is critical to adequately representing the system mathematically (Evans, Norris and Benton, 2012).

Table 2.1: Examples of typical simplifications made during model development.

Measure	**Reason**	**Outcome**
Grouping several of the dynamic states of a system together	To decrease computational requirements, or through limited understanding of intermediate dynamics (Terfve and Saez-Rodriguez, 2012)	Compromised solution accuracy, e.g. classic OC methods may fail to produce global optima (Zanetti et al., 2020)
Discarding of noise and approximation by linear models	System has specific properties, e.g. asymptotically stable equilibria, that allow it to be simplified	Satisfactory results can be obtained from idealised models (Gumowski and Mira, 1968)

On many occasions, simplifications allow effective solutions, particularly when modelling well-understood components. Simplifying wind turbine models in renewable energy OCPs, for example, is both imperative, and results in successful implementations (Wang et al., 2017). An in-depth understanding of components allows the researcher to determine where processes can be simplified and where complexity or detail are necessary, enabling simplifications and assumptions in a manner that maintains the integrity of an OCP (Zanetti et al., 2020).

Recognising the necessity of assumptions highlights the importance of frequently re-evaluating models and the effects of their application (Beddington, 1974). Models created with the purpose of providing insight into the behaviour of a system are formulated from a position of incomplete system understanding, and thus error introduced through discarding components deemed non-critical, may propagate through to model outputs (Clark, Galpin, Gilmore, Guerriero and Hillston, 2012). Outputs should thus be analysed in conjunction with the assumptions upon which the model was built, as their validity is dependent on the abstractions assumed by the researcher (Evans et al., 2012; Terfve and Saez-Rodriguez, 2012).

Whether a system is well or poorly understood, concessions have to be made in order to describe it mathematically. A distinction arises between assumptions made to model systems (e.g. regarding dynamic behaviour or noise) and those adopted to fit an OCP to a solution framework (Fleming and Purshouse, 2002). In many cases, the derivation of mathematical equations to describe a system are tailored to fit the rigid requirements of established theory (Bellman, 1971; Blueschke and Savin, 2017), favouring theoretically-aligned solutions with advantageous mathematical properties rather than realism (Evans et al., 2012). A typical example of this is the artificial alteration of the objective function, discussed next.

2.2.5.2 Artificial Objective Function Formulation

The process of determining an expression for the objective can be demanding, balancing the importance of often conflicting designer goals, and maintaining a structural form within the mathematical parameters of an OCP which suitably represent the application (Locatelli, 2001). The inability to achieve these goals simultaneously may therefore encourage adjusting the objective to facilitate pursuing a particular solution framework, such as in the OCPs of Bara et al. (2017) and Rodrigues et al. (2009), for example.

Furthermore, objective functions are often non-linear and non-convex; depriving OC methods of convergence to global optima (Bi, Chen, Wu and Ben-Arieh, 2020). The objective can be altered to enable a solution procedure, but this is unlikely to translate well in practice (Gumowski and Mira, 1968). This can include constraining the objective to ensure convexity, or rewriting inequality constraints into the objective, as many OC methods are ill-equipped to deal with state constraints (Cardoso, da Cruz, Wanner and Takahashi, 2009).

The optimal solution to an OCP is inextricably linked to the objective (Barbour et al., 2016). Alteration of the objective's structure thus critically affects the OCP and directly impacts the optimal strategy (Runge and Johnson, 2002). Typically, sensitivity can be an important indicator of realism (Gumowski and Mira, 1968). Effort should thus be devoted to deriving a suitable objective, which is often non-trivial (Finn, Levine and Abbeel, 2016).

Several equally important, often incompatible, objectives often exist in real-world systems, and that most suited to a system can be indistinguishable from others (Fleming and Purshouse, 2002). Multiple objective functions are thus routinely trialled to determine that best-suited to an application. Blueschke and Savin (2017), for instance, explored four alternatives, implementing each one in MATLAB, concluding that individual examination is needed in every OCP. Both assigning a mathematical formulation to represent a system, and selecting a form that can be absorbed into an OCP, can present difficulties (Finn et al., 2016).

Formulating an explicit objective function introduces limitations in accurately reflecting system properties (Finn et al., 2016; Gumowski and Mira, 1968); presented next. This essential requirement of classic methods (Barbour et al., 2016) is not required by many modern algorithms (Gumowski and Mira, 1968) which are able to drive a OCP towards an optimal state without restricting the objective to a particular structural form (Finn et al., 2016).

2.2.5.3 System Representation

The relationship between the mathematical representation of a system and its real-world counterpart can be described as a many-to-one mapping (Bellman, 1971). However, real-world systems frequently contain more elements than is possible to model, and the characteristics thereof are not necessarily captured in classical formulations (Bellman, 1971). Consequently, it is vital to use the most appropriate abstraction available when formulating a mathematical system, that will best accomplish the aims of the OCP and avail the most suited methods (Andersson, Gillis, Horn, Rawlings and Diehl, 2019; Bellman, 1971).

The diverse techniques available should be reviewed to ensure a suitable model is selected (Jørgensen and Fath, 2011). However, an appropriate system representation is not always clear-cut in ecology (Runge and Johnson, 2002). Selecting a survival function in population models, for example, can present the challenges given in Figure 2.1. Deriving models according to the behaviour of ecological systems should thus supersede satisfying statistical fit, and the predictive capability of models should be investigated (Runge and Johnson, 2002).

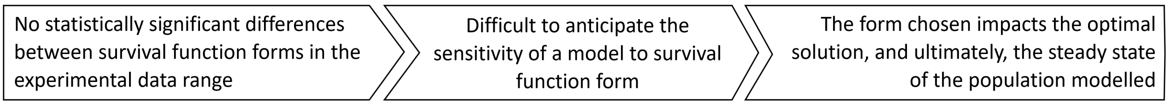

Figure 2.1: Challenges associated with choice of survival function (Runge and Johnson, 2002)

Dynamical System

The dynamical system used is critical to the suitability of an OCP to a real-world system. The importance of including spatio-temporal dynamics or age structure in ecological OCPs, for example, can be addressed by employing PDEs. This is evident in malaria modelling, where a mosquito population's age structure affects disease progression and transmission (Ghosh et al., 2013). Although PDEs can improve the predictive capability of models, the mathematical and computational complexity increases concurrently (Alexanderian et al., 2011).

PDE usage in OCPs is limited, and therefore has minimal formal theory at its disposal, requiring the derivation of conditions for each OC application (Miller Neilan, 2009). There is, for example, no provision for inequality constraints, and thus significant expertise is required to solve a constrained OCP (Jang, Kwon and Lee, 2020). Extensions to PMP exist that can be used to devise either analytical or numerical solutions to OCPs cast as PDEs, but the computational and theoretical requirements increase from that required by ODEs (Akkouche, Maidi and Aidene, 2014). Furthermore, analysis of optimal solutions becomes increasingly complex (Alexanderian et al., 2011). An adjustment to boundary conditions alone can produce substantially different OC strategies (Kelly, Xing and Lenhart, 2016).

To simplify PDE-based OCPs, researchers may elect to implement only a single control (Xiang, Liu and Fang, 2018), or use constant biological (Kelly et al., 2016), or diffusion (Jang et al., 2020) rates. Similarly, assuming constant, rather than dynamic domains, simplifies the PDE system and has been shown to produce adequate solutions (Kelly et al., 2016). Differences in scale between temporal and spatial domains further requires assumptions and problem-specific adaptations to facilitate solution procedures (Jang et al., 2020).

Deterministic methods are not always sufficient, and it is often necessary to incorporate stochasticity (Terfve and Saez-Rodriguez, 2012). Models of biological reactions with slow reaction times or few components, for instance, are more suitably modelled using stochastic equations (Terfve and Saez-Rodriguez, 2012). Although technical expertise is required to produce optima under noisy circumstances, the resulting model is more robust to formulation errors (Vanaja, Feinberg and Levchenko, 2012). Injecting noise into an OCP can thus act to:

1. Include random occurrences while generating tolerable results (Vanaja et al., 2012),
2. Account for many of the forces acting on real-life systems that are excluded when formulating a mathematical model (Goryanin and Goryachev, 2011),
3. Benefit the predictive capabilities of a model (Goryanin and Goryachev, 2011).

Many authors thus promote stochasticity as a more accurate reflection of real-life systems.

This is evident in biological systems that exhibit noisy behaviour, resulting in stochastic experimental data (Vanaja et al., 2012). Accordingly, parameters cannot be estimated without a large degree of uncertainty (Sharma and Samanta, 2014). This, in turn, affects any optimal solutions produced (Runge and Johnson, 2002). Similarly, insensitivity of a model to parameter values can obscure the best values and impact predictive capability (Terfve and Saez-Rodriguez, 2012). This is a cause for concern in classic OC methods as model changes require the redefining and re-solving of the entire OCP. When applying indirect methods, even a minor alteration requires the system be reformulated (Blueschke and Savin, 2017), whereas in an EA, the relevant component can simply be altered and the solution scheme re-run (Section 2.5). The solution framework should therefore be carefully considered.

2.2.5.4 Solution Frameworks

The suitability of OC methods, and the numerical methods and *quadrature* used to integrate numerically in OC methods, can have a meaningful effect on optimal solutions (Blueschke and Savin, 2017; Rao, 2010). It may be necessary, for example, to apply the indirect methods so as to obtain sufficient accuracy, but the algebraic computation required, hinders their applicability (Bertolazzi et al., 2006). Since dynamic programming is frequently excluded from consideration due to the *curse of dimensionality*, the onus falls on the direct methods (Bertolazzi et al., 2006) – the approach utilised in the majority of OCPs (Biral et al., 2016).

Direct Approach

Preference for OC solution techniques reside with the direct methods, with around 90% of solvers and solution approaches in literature favouring their use (Biral et al., 2016). Solution schemes employed to solve the resulting NLP are classified as either local or global methods, with the former generally gradient-based and the latter, heuristic (Rao, 2010).

Unique solutions can be found using local deterministic methods when the NLP in question is convex (Balsa-Canto et al., 2012). As is characteristic of classic OC methods, constrained and highly non-linear OCPs present substantial obstacles to obtaining optimal solutions, and gradient determination can be challenging in complex environments (Chehouri, Younes, Perron and Ilinea, 2016). Moreover, local methods may converge to local optima in multi-modal OCPs, which becomes increasingly likely when initial estimates are located far from global optima (López Cruz, Van Willigenburg and Van Straten, 2003). Noise, present in a system or introduced by the quadrature, also impedes local methods (Balsa-Canto et al., 2012).

Global methods are able to bypass these limitations through a number of mechanisms, depending on whether a deterministic, stochastic or hybrid approach is used. In order to guarantee convergence to a global optimum using deterministic methods, the OCP should possess particular differentiability, smoothness and structural properties, conducive to the method (Balsa-Canto et al., 2012). Increasing dynamical system size can exacerbate the computational burden of using global methods (Balsa-Canto et al., 2012).

A high computational cost is arguably the most prominent disadvantage of stochastic methods, which although capable of speedily locating the region containing the global optimum, demand significant computational resources to refine the solution (Balsa-Canto et al., 2012). Nevertheless, although convergence to a global optimum is not guaranteed, stochastic methods like the meta-heuristic algorithms, are capable of obtaining global optimality (Balsa-Canto et al., 2012). Notably, near-optima located using meta-heuristic algorithms such as EAs, are often indistinguishable from global optima in practice (Whigham and Fogel, 2003).

Consequently hybrid methods, which combine the strengths of deterministic and stochastic methods, improve efficiency and better handle issues like noise, discontinuity and non-smoothness (Balsa-Canto et al., 2012). Generally, a stochastic algorithm is used to determine the locality of a global optimum and a deterministic algorithm used in the reduced *search space* (the domain containing all feasible solutions) to improve the possibility of locating or obtaining close proximity to a global optimum (Hirmajer et al., 2008). Although hybrid methods are effective and enhance solution quality in solvers, additional advances are needed to treat the complexity and scale of models in ecology (Balsa-Canto et al., 2012).

While dynamic programming is severely limited by dimensionality, in a vast number of OCPs, the indirect and direct methods perform equivalently (Biral et al., 2016). Inclination to select the direct methods could arguably be attributed to the ease of applying OC using this approach, as a solver may be selected, with little expertise required. This can impede correct application in solvers with opaque functionality, where results may be produced without full realisation of the impact the error propagation or accuracy of schemes used may have had (Subchan and Żbikowski, 2009). To produce valid results, both OC and solver knowledge is needed to correctly apply software and verify results (Subchan and Żbikowski, 2009).

Solvers

Solvers are primarily categorised as BVP or NLP solvers, associated with the indirect methods or direct methods respectively. Solution techniques often employed therein are given in Table 2.2. BVP solvers are frequently ill-equipped to deal with formulation complexities, like unstable adjoint equations, and sophisticated mathematics is then required to circumvent these occurrences, which is often unsuccessful (Zhang et al., 2012).

Table 2.2: Examples of popular solution methods used to solve OCPs.

Shooting Methods	**Multiple-Shooting Methods**	**Collocation Methods**
• One of the first methods used to solve OCPs (Pytlak, 1999) • Seldom used as they suffer from propensity to be unstable and are reliant on accurate initialisation (Bertolazzi et al., 2006)	• Requires accurate initial estimates to ensure convergence (Rao, 2010), accurate to two decimal places in some instances (Burlirsch, Nerz, Pesch and von Stryk, 1993) • Estimating initial adjoint values is complex when a physical interpretation is not apparent (Subchan and Żbikowski, 2009) • Mathematical and problem-specific expertise required to obtain successful results using this process discourages applications (Burlirsch et al., 1993)	• Reduce the complexity of gradient determination and constraint incorporation in OCPs (Schwartz, 1996) • Specialised collocation methods substantially improve numerical integration accuracy (Rao, 2010) • Increased problem size (from introduced variables (Schwartz, 1996)) and computational cost that accompany the better accuracy, deter its usage (Frego, 2014)

Successful solver usage requires an understanding of both OC methods and the solver itself (Subchan and Żbikowski, 2009). Since solvers do not readily discern infeasible solutions from feasible solutions (Vanderbei, 2001), documentation should be reviewed to determine whether a solver is suited to an OCP formulation, as this can impact the ability of a solver to produce adequate solutions (Dussault, 2014). The user should also be reminded that:

- the solver-produced solution is an optimal solution to the discretised OCP, which may not concur with a discretised version of the true optimal solution (Dussault, 2014),
- implementation choices, including quadrature selection, can impact solver performance and accuracy (documentation advocates trialling multiple options) (Wächter, 2009),
- sensitivity to initial estimates should be investigated (Chehouri et al., 2016), as reliance on initial values can be critical to solver performance (Vanderbei, 2001).

Furthermore, many solvers require initialisation from a narrow range of values, constrained to a small region around the optimum, in order to produce solutions (Vanderbei, 2001). This is true of the interior-point *IPOPT* software, wherein initial values can determine whether the algorithm will converge and if so, whether to an infeasible solution or a local optimum

(Wächter, 2009). *IPOPT* generally performs both robustly and efficiently in benchmark tests, and tactics can be used to obtain adequate initial parameter estimates (Wächter and Biegler, 2006). Imposing iterative refinement can alleviate dependence on initialisation, but is not always tractable as it increases computational requirements (Wächter and Biegler, 2006), and computational resources are often an obstacle in NLP (Chehouri et al., 2016).

Many extremely efficient OC solvers exist, which, under appropriate application, yield OC strategies suitable for practical application (Balsa-Canto et al., 2012). The relevance of a solver to a particular OCP is often overlooked and may significantly affect the solution obtained (Balsa-Canto et al., 2012). Depending on the form of an OCP, some solvers may fail to produce solutions, whereas others are able to cultivate solutions to a range of OCP formulations (Dussault, 2014). Heed must thus be taken of the numerical execution of a solver (Subchan and Żbikowski, 2009) and the suitability of methods employed therein.

The variability of reported optimal results is arguably greater than is often acknowledged. Rodrigues, Monteiro and Torres (2013) and Schreppel and Chudej (2018), for example, both applied direct method solvers to the same OCP and found different optima. Factors contributing to this variability include numerical methods, control formulation and implementation measures such as step size, which are not solver-specific considerations, but feature in all OC solution schemes. Consequently, these factors are outlined next.

2.2.5.5 Numerical Implementation Factors

Numerical methods are vital to the execution of OCT (Krotov, 1996). Only a small subset of OCPs, possessing simple state equations, objectives and constraints (Bryson and Ho, 1975) can be solved analytically (Rao, 2010). Numerical schemes are thus needed to accompany most realistic OC applications (Oruh and Agwu, 2015). This simultaneously enables OC to be applied in complex situations and further adds complexity through its interaction with mathematical theory (Subchan and Żbikowski, 2009).

Despite method comparisons confirming that differences in results can be attributed to the quadrature used (Dal Bianco, Bertolazzi, Biral and Massaro, 2019), no standardised numerical approach exists. This likely stems from the problem-specific competition between retaining the best possible accuracy at the least computational expense (Bostan, Akhtari, Bonakdari and Jalili, 2019). To this end, many researchers advocate for accuracy (Schwartz, 1996), whereas others champion reducing computational requirements (Rodrigues et al., 2009).

Dynamical System: Precision and Efficiency of Numerical Methods

In the literature reviewed, authors elected to use either first, second, third or fourth-order methods. Typically, either Euler's Method ($O(h)$) or the fourth-order ($O(h^4)$) Runge-Kutta method (R-K4) (Burden and Faires, 2011) are used to solve ODE systems, and primarily second-order finite difference methods in PDE systems. Where low-order methods are used, motivation for such frequently cites reduced computational time (Rodrigues et al., 2009) but rarely deals with accuracy considerations; a factor criticised by Frego (2014).

Numerical methods, usually selected at the user's discretion, can have a determining effect on the accuracy of results (Rao, 2010) and should thus be taken into account when evaluating OC solutions (Ratković, 2016). Differences between solutions found using the indirect and direct methods, for example, can be due to the numerical methods used (Bertolazzi et al., 2006). Although low-order methods may appear to produce solutions with lower cost, the decrease in accuracy and increase in discretisation error may falsely claim an optimal solution (Nezhadhosein, Heydari and Ghanbari, 2015). Perhaps counter-intuitively, higher-order quadrature is often capable of solving OCPs with greater efficiency (Schwartz, 1996).

OCPs regularly entail sizeable systems of equations, and thus computational resources are a critical consideration (Bertolazzi et al., 2006). As a result, authors often elect to use low-order methods like Euler's Method. When controlling large systems, Euler's Method maintains a suitable level of efficiency without having to compromise model complexity by simplifying models to decrease computational requirements (Hur, 2018). These findings are not unanimous however, and apart from elementary OCPs, Euler's Method has been found to be inadequate, especially in constrained OCPs (Subchan and Żbikowski, 2009). Furthermore, Euler's Method is inefficient in many OCPs (Schwartz, 1996), requiring a step size four times less than that of the R-K4 to achieve equivalent accuracy (Burden and Faires, 2011).

High-order numerical methods are not without disadvantages. When used in conjunction with interior-point solvers, particularly when a fine discretisation is used, high-order methods can induce *ringing* (Vanderbei, 2001); outlined in Figure 2.2. While low-order methods may appear preferable in such cases, they are less likely to detect singularity (resulting from division by zero) and infeasibility than higher-order methods (Vanderbei, 2001).

The use of high-order numerical methods has been criticised by Rodrigues et al. (2009) on the basis of increasing both computer processing time and the number of iterations required

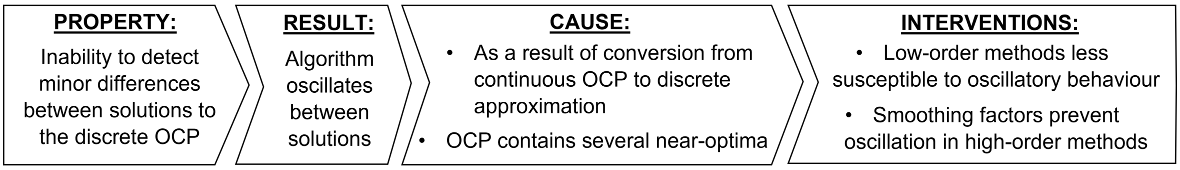

Figure 2.2: Ringing property in algorithms (Vanderbei, 2001)

to obtain solutions, without sufficient benefit to the optimal solution. Asserting that there is no clear advantage to employing more accurate methods, Rodrigues et al. (2009) adopted similar sentiments in later work where computational efficiency was emphasised over accuracy (Rodrigues, Monteiro and Torres, 2010). This viewpoint has been contended by Frego (2014), who states that factors such as the number of iterations should not be used comparatively as different frameworks are used within solvers, many of which refine solutions through iterative processes. Instead, solution accuracy should be central to any comparison (Frego, 2014).

The concepts of method efficiency or accuracy are rarely discussed in PDE-based OCPs, where existing literature is heavily weighted towards theoretical rather than numerical elements. In the literature reviewed, the extent of discussion relating to computational factors was limited to decreasing computational expenditure by using constant rates to approximate system components (Kelly et al., 2016), applying only a single control to simplify and increase feasibility (Xiang et al., 2018), and determining convergence criteria (Akkouche et al., 2014).

Due to the lack of PDE-based optimality theorems in OCT, employing PDEs in OCPs is a theoretically comprehensive and challenging exercise. Indirect methods are almost exclusively used, with substantial mathematics required to derive optimality conditions (e.g. Jang et al., 2020; Kelly et al., 2016; Miller Neilan, 2009). A combination of first and second-order finite difference methods are often applied, using first-order schemes on the temporal domain, and second-order schemes on the spatial domain (Kelly et al., 2016; Xiang et al., 2018). Occasionally, finite element methods are used on the spatial domain, and a lower-order finite difference method, on the temporal domain (Jang et al., 2020).

Objective Function Evaluation

The formulation of an objective typically seeks to account for the behaviour of a system over space or time (Barbour et al., 2016), and the cost associated with obtaining a desired optimal state. Because of the pivotal nature of the objective, the methods used to aggregate these costs over time play a role in dictating optimal solutions (Barbour et al., 2016).

Moreover, solution quality is often judged by the numerical value assigned to the objective, which is usually an approximation to its true value (Nezhadhosein et al., 2015). This is of particular concern when using solvers as the methods involved in approximating the objective are not always explicit to the user (Frego, 2014). Consequently, there is a possibility that solutions appearing superior, have in reality underestimated (when minimising) the optimum through approximation error (Frego, 2014). This has been demonstrated when OC solutions obtained using low-order methods have been verified against real-world data, and have been found to have underestimated the true (minimum) optimum (Bertolazzi et al., 2006).

Quadrature of equal order to that used to integrate the dynamical system should be used to evaluate the objective (Rao, 2010; Sweilam, Tharwat and Abd El Moniem, 2019). Hence, previous arguments regarding numerical integration order are applicable to the quadrature used to evaluate the objective. For this reason, integration schemes of $O(h^4)$ are commonly used, as low-order methods are often too inaccurate to be of use (Bara et al., 2017). These findings were reiterated by Dussault (2014), who found that low-order methods may even produce false optima and thus recommended methods of at least $O(h^2)$. High-order methods are however accompanied by a concurrent increase in complexity (Bertolazzi et al., 2006).

Authors advocating the use of the low-order, Euler's Method have correspondingly used the $O(h)$ rectangular method to evaluate the objective (Schreppel and Chudej, 2018). As per previous arguments, the rectangular method has been criticised as too inaccurate to be of use in practice (Stengel, 1994). As the natural counterpart of R-K4 (Golub and Ortega, 1992), authors applying the R-K4 usually employ the $O(h^4)$ Composite Simpson's method (CS) to evaluate the objective (McAsey et al., 2012; Nezhadhosein et al., 2015). Objective evaluation was not covered in any of the PDE-based OCPs reviewed. It was thus assumed that equivalent orders of quadrature and numerical integration methods would be most appropriate.

Additional Numerical Factors

Whether first discretising an OCP and then optimising, characteristic of the direct method, or the reverse, typical of the indirect approach, the consistency of an approximation is critical to obtaining adequate solutions (Polak, 1993). Consistency, in this context, refers to the converging of the global (local) optima of the approximate solutions to the global (local) optima of the OCP as discretisation step size is reduced ($h \to 0$) (Schwartz, 1996). The numerical methods applied to an OCP should thus ensure consistent approximations which are both stable and converge to the true solution (Rao, 2010). In addition, the direct methods either require the NLP equivalent of the OCP to be consistent (Polak, 1993), or make use of an iterative approach to obtain consistent approximations (Schwartz, 1996).

Consistency of OC solutions[4] using the Runge-Kutta (R-K) methods[5] has been established, subject to R-K parameter constraints (Schwartz, 1996), guaranteeing that an approximate solution of equal order to the R-K algorithm used is obtained (Hager, 2000). Compellingly, the explicit R-K4 (henceforth referred to simply as R-K4) obtains solutions of high-order accuracy with greater efficiency than many lower-order algorithms that require variable discretisation to maintain accuracy (Schwartz, 1996). Additionally, the R-K4:

- fulfils all criteria necessary to ensure consistent, $O(h^4)$ solutions (Hager, 2000),
- produces solutions that correspond exceptionally well (possessing insignificant error) with analytical solutions, across diverse OCPs (Oruh and Agwu, 2015),
- is able to surmount instability in system dynamics (Schwartz, 1996).

In conjunction with numerical method selection, control form should be carefully selected as it plays an important role in approximating the optimal solution of an OCP (Pytlak, 1999). Combined with a fine discretisation, high-order quadrature can have an overwhelming effect on the accuracy of numerical solutions, even while using the most rudimentary of control forms (Pytlak, 1999). Numerical integration of the best accuracy, computational resources considered, should thus be selected in a bid to eradicate errors as far as possible.

2.2.5.6 Control Configuration

At the heart of OC lies the use of controls to drive a system towards a desired state. Deriving an optimal control using the indirect methods can be challenging however (Rigatos, Busawon and Abbaszadeh, 2020), and while both the indirect and direct methods can produce explicit controls, it is often necessary to approximate the control(s). This is common in solvers, and is pertinent to the accuracy and/or optimality of OC solutions (Schwartz, 1996).

In addition to the error introduced into an OC solution through choice of quadrature, the error corresponding to a control approximation can further erode the accuracy of a numerical OC solution (Schwartz, 1996). This additional error can to an extent be managed however,

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[4] The criteria for consistent solutions to an OCP differ from that of differential equations (Rao, 2010).

[5] The mathematical derivations of the R-K methods can be found in Burden and Faires (2011).

since manipulation of the control representation and numerical integration scheme can alter the accuracy of approximate numerical solutions to an OCP (Pytlak, 1999; Schwartz, 1996).

Depending on the OCP at hand, a minimal set of choices for control configuration may be available. Typically, piecewise constant functions are used (Sussmann, 1990), however, higher order piecewise polynomial functions can also be employed (Balsa-Canto et al., 2012), provided they are at least one degree lower than the order of the numerical integration used in the OCP (Pytlak, 1999; Schwartz, 1996). The presence of constraints on either the control or state further limits the degree of polynomial that can be applied, with recommendations that polynomials should not exceed second degree when constraints are imposed, regardless of the order of numerical integration used (Schwartz, 1996).

Moreover, high-degree polynomials can act to over-parameterise the control, thereby aggravating solution error (Schwartz, 1996). Comparisons to benchmark OCPs have however found piecewise linear control functions to be as accurate as higher-degree piecewise polynomial controls at a statistically significant level, in terms of error in the estimated objective function (Nezhadhosein et al., 2015), further supporting the use of low-degree controls.

Piecewise constant controls can potentially introduce greater error when approximating solutions than high-degree polynomials, but do not violate constraints, as the use of higher-degree polynomials can (Schwartz, 1996). Numerous solvers, such as the DOT_{CVP} software (Hirmajer et al., 2008), configure piecewise constant controls (Rodrigues, Monteiro and Torres, 2014). This not only simplifies the solution procedure but in practical applications such as dosage scheduling, is better suited than theoretically-derived optimal controls (Bara et al., 2017). Since constrained OCPs are seldom able to obtain an order of accuracy greater than one (Schwartz, 1996), selecting piecewise constant controls becomes the simplest choice.

The control form may interact with an OCP's structure, and ultimately, the accuracy of solutions (Frego, 2014; Schwartz, 1996). Inaccuracy introduced through the choice of control can be reduced by adjusting the discretisation. When a fine discretisation is used, the order of a numerical integration scheme has a dominating effect on the errors in an OC solution, overshadowing and, in part, *integrating out* the error produced by even the simplest of control forms from the system dynamics (Pytlak, 1999; Schwartz, 1996). Alternatively, the order of quadrature can be increased (Pytlak, 1999). In all PDE cases reviewed, an indirect approach was pursued which specifies the optimal control(s), bypassing the need for approximation.

2.2.6 Overview of Optimal Control Applications

Successful OC applications have largely occurred when the methods employed are suited to the idiosyncrasies of an OCP. The robustness of direct methods, for example, is dependent on whether or not they are applied to conducive OCP types (Rao, 2010). Similarly, dynamic programming is well-suited to handling constrained, mixed integer, and stochastic OCPs, when conditions such as smoothness are satisfied, but requires significant mathematical expertise and is restricted by large problem dimensions (Bellman, 1971; Biral et al., 2016).

OCT, as it stands, is ill-equipped to manage many of the complex OCPs developed today, particularly in systems that are not easily mathematically described or understanding thereof is limited (Fleming and Purshouse, 2002). Many systems are too complex to adequately model using current mathematical tools, and thus OC is applied simply to improve system understanding (Bara et al., 2017). Real-world systems are not, however, decreasing in complexity. Improved system understanding should thus be used to refine OC methods and improve their capacity in complex systems (Barbour et al., 2016), or investigate alternatives.

As a result, attention is increasingly being drawn to alternative methods, such as meta-heuristic algorithms, which are better-suited to complex OC formulations (Chehouri et al., 2016; Fleming and Purshouse, 2002). Ecological systems, harbouring complexity at both a micro and macro-scale, and subject to both internal and external influences, present a challenge to OC methods (Barbour et al., 2016), and thus an opportunity to investigate the potential of meta-heuristic algorithms therein. Consequently, ecological OC is now presented.

2.3 Controlling Ecological Systems

The transitioning of ecology into an interdisciplinary science in which complex systems can be engineered and predictions for future events made, has largely been facilitated by mathematical and computational advances (Goryanin and Goryachev, 2011). As it now stands, theoretical ecology draws from the sciences of living organisms, such as biology, and non-living components, like geology, to model the interrelationships between biotic and abiotic components in an environment (Bolton, 2019), using a combination of mathematics, statistics and computational methods (Hastings and Gross, 2012).

Procedures routinely followed to engineer systems however, are not readily transferable to ecology, due to innate differences in the design, observability and controllability of engineered versus ecological systems (Kaltenbach and Stelling, 2012). Similarly, findings borrowed from various disciplines do not necessarily have equivalent applicability in theoretical ecology (Holling, 1973). Methods derived from classical physics and used in ecology for example, are hampered by uncertainty, external influences (Holling, 1973), and assumptions included in model formulation, often stemming from incomplete system understanding, requiring sophisticated schemes to tailor techniques to ecological systems (Goryanin and Goryachev, 2011).

For the purposes of this research, ecological modelling will be defined as the modelling of interactions between organisms and their environment, encompassing both biotic and abiotic components, so as to characterise the behaviour exhibited by the system as a whole. Consequently, an ecological model should encapsulate the dynamic behaviour of a system, subject to appropriate spatio-temporal dimensions, and facilitate predictions of future behaviour (Whigham and Fogel, 2003). To this end, a combination of experimental techniques, mathematical modelling and computational tools are needed to both understand the ecological systems being studied and further make predictions based on the knowledge gained (Jopp, Reuter and Breckling, 2011; Jørgensen and Fath, 2011). Theoretical findings should then be refined in tandem with experimental data and observations (MacPherson and Gras, 2016).

2.3.1 Ecological Management Strategies

The demand for strategies to address the factors driving environmental change, including, amongst others, escalating pollution levels, diminishing biodiversity and land degradation, is a pressing issue in ecological research (Lek and Guégan, 1999). To successfully manage the ecological problems facing society, a synthesis between theoretical and applied ecology is needed (MacPherson and Gras, 2016). In a chiefly empirical discipline, ecologists are often faced with discerning the tractability of solutions to increasingly complex problems using sophisticated mathematics in which they are not versed (Ruxton and Beauchamp, 2008).

From numerical and statistical schemes to artificial intelligence, modern computational advances have provided ecological researchers, often with introductory level mathematics, access to advanced mathematical techniques to address these challenges (Lek and Guégan, 1999; May and McLean, 2007). While computational developments have advanced ecological research (Lek and Guégan, 1999), it is critical to retain caution when interpreting outcomes as they are dependent on assumptions made during model creation (May and McLean, 2007).

A variety of techniques have been developed over the years to effectively model ecological systems (Jopp et al., 2011). A modelling technique matching both the complexity required and the ease and limitations involved in applying the approach, should be selected to best solve a posed ecological problem (Jopp et al., 2011; Jørgensen and Fath, 2011). This requires significant understanding of the natural systems modelled (Müller, Breckling, Jopp and Reuter, 2011). Correspondingly, an overview of ecological modelling is now given.

2.3.2 Ecological Modelling

Predicting the behaviour of a real-world ecological system can theoretically be achieved by altering elements of the system and subsequently observing the long-term effects this incurs (Evans et al., 2012). The scale of such an experimental approach is severely constrained by implementation, monetary and ethical factors, thereby limiting inferences that can be made from this process (Evans et al., 2012; Lachish et al., 2007). Ecological modelling can thus be used as a means of extracting distinguishing traits from an ecological system and utilising it to better understand and describe characteristics of the system (Jørgensen and Fath, 2011).

While real-life systems are not completely describable by way of modelling, they are also not completely observable and, hence, models collating all available system information, mathematical and otherwise, are pertinent to developing an understanding of the complex relations in ecological systems (Jørgensen and Fath, 2011). The viability of management strategies in ecology is therefore best investigated through the use of ecological models (Evans et al., 2012; Lachish et al., 2007), which have aided developments in ecology (Morrall, 2003).

Substantial knowledge of the behaviour, characteristics, and relationships of organisms with one another and their environment, is a key requirement of ecological modelling, and should precede, and further accompany the model development process (Müller et al., 2011). The stringent nature of mathematical techniques in ecological modelling is in contrast to the dynamic nature of ecosystems themselves (Jørgensen and Fath, 2011). Consequently, typical mathematical methods used in ecology may require adaptations to create a synergistic combination of mathematical theory and ecology that is able to sufficiently capture an abstraction of an ecological system and provide a useful model (Jopp et al., 2011).

Whilst many template models for ecological processes exist, substantial knowledge is required to assimilate and consolidate the hypothesis of a system under investigation with available frameworks (Jopp et al., 2011). Thus, where analytic models can be used in many disciplines as precursors to design in the building of systems, ecological modellers are required to work within a framework of what is observable, identifiable and controllable (Loehle, 2006).

When formulating an ecological model, model complexity should be balanced with the level of reliance on the model expected (Jopp et al., 2011). Assumptions should be made accordingly; to reduce model complexity and select the most appropriate system representation, by including spatio-temporal dynamics, for example (Müller et al., 2011). When high predictive accuracy is required, stricter conditions on the quality of data and degree of detail incorporated in the model should exist (Jopp et al., 2011). Both model and ecological outcomes should then be compared to deduce where adaptations in current modelling methods are required to better understand and represent ecological systems (Barbour et al., 2016).

2.3.2.1 Typical Ecological Models

From its origins in predator-prey modelling, ecological modelling has undergone distinct development stages, traversing population dynamics, environmental management and culminating in ecosystem modelling (Lek and Guégan, 1999). Each of these stages has been accompanied by increased model complexity and concurrent advances in the tools and techniques available to find and analyse solutions to the modelled systems (Lek and Guégan, 1999).

The behaviour of ecological systems is typically characterised using model types including, but not limited to, population dynamic, stochastic, agent or individual-based, fuzzy, artificial neural networks and spatial models (Jørgensen and Fath, 2011). These models apply PDEs, ODEs, stochastic differential equations, or discrete equations, and can take into account adaptive behaviour, uncertainty and randomness, or a combination of all the aforementioned factors (Jørgensen and Fath, 2011). In many instances, model types rely on different principles, but the same underlying logic, to formulate equations modelling ecological processes. For example, population dynamic models have been utilised in individual-based models for the translocation of rhinoceroses (Dunn, Hearne and McArthur, 2007). In line with the scope constraints imposed in the current study and the widespread use of population dynamic models, population dynamic models will serve as a focal point of the current research.

Population dynamic models can be used to describe a variety of ecological processes (Jørgensen and Fath, 2011). Many researchers use the Lotka-Volterra equations[6] as a basis,

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[6] Originally reaction-kinetic equations, they also describe predator-prey interactions where the species are equivalent to the chemical components of reaction-kinetic equations (Murray, 2002; Svirezhev, 2008).

with minor alterations as required (Jørgensen and Fath, 2011; Murray, 2002), depending on whether predator-prey interactions or epidemiology, for example, is being modelled. Harvesting can be modelled by the simple addition of harvesting terms, and factors such as age or size structure included, as is commonly used in fishery models (Jørgensen and Fath, 2011).

Whilst of the most widely used in ecology, these models have limited realism and applicability, but can be used to better understand systems (Jørgensen and Fath, 2011). The analysis of mathematical properties of the systems, such as stability, are of little relevance when applied to ecological systems (Murray, 2002; Svirezhev, 2008), as environmental interrelations and interactions, generally not modelled within the system, are needed to describe realistic stability properties thereof (Jørgensen and Fath, 2011). However, models such as the Lotka-Volterra model, have inspired informative lines of investigation that have led to increased model relevance to real-world applications (Murray, 2002). Furthermore, although the predictive capability of models may be limited upon practical application, they assist in identifying concerns of both the model and system (Murray, 2002).

Certain fundamental assumptions have been ingrained in ecological models since their inception. The Lotka-Volterra equations, for example, which are based on chemical reaction kinetics, are criticised as insufficient for application (Murray, 2002) and yet are widely used. Conservation laws, used to describe the random reactive and diffusive behaviour of atoms in the equations, fail to sufficiently capture the cognitive and complex behaviour of organisms (Svirezhev, 2008). Even when spatial patterns are adequately captured, inherently non-linear processes in ecological systems require adaptations that are all but depleted using available conventional frameworks (Svirezhev, 2008).

Although these early models aided in validating ecological theory and laid the groundwork for predictive models, advances in ecological modelling have stagnated in recent years (Morrall, 2003). Moreover, complexities arise naturally when modelling the highly adaptive, non-linear, multivariate and often unpredictable dynamics of ecological systems (Whigham and Fogel, 2003). Additionally, obtaining parameter estimates capable of maintaining adequate model predictions outside of observable data ranges, within traditional modelling frameworks (Morrall, 2003), makes ecological modelling an inherently challenging task.

There is thus an opening to reimagine the methods and approaches to solve ecological problems to more suitably represent such systems using existing mathematics (Svirezhev, 2008), and perhaps modern adaptive methods such as EAs (Morrall, 2003). Modern methods are increasingly equipped to handle the spatio-temporal and non-linear dynamics exhibited by ecological systems, and with the potential and capabilities of developments in computation at their disposal, better able to cater for changing ecosystems (Lek and Guégan, 1999).

2.3.3 Ecological Optimal Control

Ecological OC applications, although somewhat more scarce than OCPs in disciplines such as engineering, have grown steadily over the last two decades (Jørgensen and Fath, 2011). Numerous applications can be found in epidemiology, with typical problems including the development of optimal vaccination strategies for the control of disease transmission (Rodrigues et al., 2014), optimal drug dosage scheduling (Bara et al., 2017), and optimal vector control (Rodrigues et al., 2013; Schreppel and Chudej, 2018).

Several researchers have considered the optimal control of circadian rhythms, subsequently deriving techniques to cater for unstable adjoint equations using the indirect approach when confronted by limitations of the scheme (Zhang et al., 2016). Resource harvesting OCPs, whether for commercial purposes, such as animal products (Beddington, 1974) and forestry (Sahashi, 2002), or biodiversity purposes (Mwakiwa et al., 2013) have also been examined. What ultimately constitutes optimality in an ecological system, however, can be difficult to define and subsequently describe mathematically (Barbour et al., 2016). OC usage in ecology has therefore had mixed results (Loehle, 2006), instances of which are given next.

2.3.3.1 Challenges Associated with Optimal Control in Ecology

Successful OC outcomes have been obtained in agricultural settings such as forestry (Loehle, 2006), and in chemotaxis systems (Kaltenbach and Stelling, 2012), whereas in others, complexity has reduced the effectiveness of OC (Loehle, 2006) and it has thus been used solely to better understand the mechanisms underlying the control application (Bara et al., 2017). Although OCPs are frequently proposed in areas such as disease control or drug scheduling, the development into policy or practical use thereof is rarely dealt with. Practical benefits arising from optimal strategies, in addition to theoretical findings, are thus difficult to gauge.

More detrimental aspects of OC have seen the collapse of oceanic fisheries, where fish stocks were over-harvested in accordance with OC strategies concerning their management (Holling, 1973; Loehle, 2006). Ineffective optimal strategies implemented as policy, have too failed to restore endangered species (Loehle, 2006). Caution should thus be advised as the components of ecological systems do not necessarily behave in a predictable, easily controllable, nor observable manner (Loehle, 2006). These factors may be responsible for the discrepancy between theoretically optimal solutions and their less successful applications in practice, and should therefore be factored into OC-derived policy (Loehle, 2006).

Poor management, lack of data or the inherent characteristics of ecological systems, such as noise or non-linearity, can all contribute to a lack of observability or controllability (Loehle, 2006). Specifically, the innate, complex nature of ecological systems makes relating specific outcomes from the system to internal processes difficult (Barbour et al., 2016), thereby hindering the observability of the system. Non-linearity in ecological systems, coupled with this limited observability, further inhibits the accurate estimation of parameters from the observable outcomes of an ecological system (Loehle, 2006). This is demonstrated by the extensive use of optimisation in ecology as a means of obtaining optimal parameter values in a parameter estimation capacity (Balsa-Canto et al., 2012). Similarly, inputs that can alter the final state of the ecological system are limited by what is achievable in practice and are not always easily manipulated. Hence, ecological systems are often not controllable (Loehle, 2006).

2.3.3.2 Arguments Underpinning Unsuccessful Ecological Control

Ecological OC applications can only be as successful as the abstraction used to model the ecological system is at representing system behaviour (Barbour et al., 2016). Beddington (1974), for example, argues that using simplistic techniques, such as logistic equations to model population growth, are too artificial to be of use, and assumptions imposed such as the insensitivity of demographic parameters to environmental effects, further limit model applicability. Problems then ensue when the, at best suboptimal, and at worst infeasible, OC solutions found are treated as optimal, regardless of the incorporated assumptions and unsuitability of the model (Barbour et al., 2016; Loehle, 2006).

In a similar vein, Holling (1973) argues that the focal point of controlling ecological systems is fundamentally concerned with their behaviour at equilibria. This stance may produce mathematical systems that are easier to analyse and predict future behaviour from, but does not account for ecological systems whose behaviour is susceptible to external or random influences, and can behave erratically (Holling, 1973; Svirezhev, 2008). Consequently, management strategies relying on equilibrium behaviour have been poorly informed and have inadvertently increased extinction probability in fisheries, for example (Holling, 1973).

Although no longer deemed sufficient, an equilibria-skewed approach provided insight integral to the formulation of theoretical ecology (Holling, 1973; Lek and Guégan, 1999). Similarly, computational advances inspired by natural processes (Yang, 2014) have led to the development of sophisticated parallel algorithms, conveniently placed to model the ecological systems their very own structures are based on (Lek and Guégan, 1999). Researchers have begun exploring this potential, applying techniques such as artificial neural networks in areas such as disease, ecosystem and population modelling, for example (Lek and Guégan, 1999).

Traditional OC approaches in ecology have lacked transferability to real-world systems (Holling, 1973; Loehle, 2006), and yet, utilisation of alternative techniques has been largely stagnant. Successful OC tools in other disciplines may need to be reconditioned to be fully applicable in ecology (Loehle, 2006; Svirezhev, 2008). The development of new and innovative methods, as well as manipulation of current techniques should thus be addressed (Jopp et al., 2011). To this end, recent advances could be used to alter conventional practices in order to formulate better-suited approaches in ecology (Goryanin and Goryachev, 2011). Consequently an overview of recent OC developments is now given.

2.4 Recent Developments in Optimal Control Applications

When addressing an ecological issue, limitations exist as to what can be controlled, modelled and feasibly achieved using management strategies. In lieu of this, conventional OC approaches require adaptations to better reflect the changing and altogether new demands placed on them (Barbour et al., 2016). Classic OC methods, however, impose constraints of their own. Attention has been devoted to exploiting the mathematical properties of systems, such as sparsity (Rao, 2010), or symmetry (Murray, 2002), in a bid to streamline existing algorithms and increase the accuracy and efficiency of OC methods. In systems which do not warrant complex models, classic OC methods are therefore successful (Barbour et al., 2016).

Real-world systems, however, seldom satisfy the fundamental conditions of smoothness, convexity and differentiability under which deterministic methods produce good solutions (Balsa-Canto et al., 2012). Whereas many OCPs may merely be inconveniently difficult or require particular expertise in order to derive robust optimal solutions (Sargent, 2000), some OCPs are intractable using conventional approaches (Wang et al., 2017). Consequently, there has been a gradual move towards incorporating modern computational methods.

2.4.1 Meta-Heuristics

One such powerful advance in computational techniques has been that of meta-heuristics. The co-joining of meta-heuristics and deterministic methods to form a hybrid approach, in particular, is increasing in popularity, and has been instrumental in improving the ability of conventional algorithms to locate global optima (Hirmajer et al., 2008). This has spilled over to direct-based solvers, with software such as DOT_{CVP} recommending hybridising the approach with stochastic methods (Hirmajer et al., 2008).

Although disadvantages of classic OC methods are avoided using hybrid algorithms, classical knowledge is still required. The versatility of meta-heuristic algorithms however, has allowed global optimality to be achieved in mathematically unfavourable conditions, with complete disregard for the quintessential classical requirements of convexity, continuity and differentiability (Huang, 2017). While reducing method complexity, the capacity to capture complex ecology is increased by using meta-heuristics (Barbour et al., 2016). Moreover, restrictions regarding objective and constraint formulations are dispensed with (Huang, 2017).

Meta-heuristics have been extensively applied in optimisation. Current optimisation methods are classified as either modern or conventional, with modern schemes predominantly meta-heuristic based (Theo et al., 2017). These modern approaches have been shown to be suitable for dealing with many of the challenges of conventional methods, such as non-linear constraints, and have been able to maintain sufficient accuracy and efficiency, even in problems of large dimensions (Theo et al., 2017). As a result, optimisation problems have seen a drastic increase in successful use of non-conventional techniques, in particular, that of EAs.

2.4.2 Motivation for Evolutionary Algorithms

The flexibility of EAs is well-suited to the increasing complexity of formulating systems in an adaptive manner, without the assumptive restrictions of classical frameworks, and thus when applied appropriately (Hamblin, 2013), EAs have proved useful (Chehouri et al., 2016; Fleming and Purshouse, 2002). This concept has been embraced in engineering where, despite the success of OC, since the design and building of systems is often founded on analytic models, classic OC methods are in many cases inapplicable (Fleming and Purshouse, 2002) or even intractable (Shakoor, Hassan, Raheem and Wu, 2016). Researchers have therefore turned to EAs, and instead of hybrid approaches, purely EA approaches have been adopted, particularly in highly non-linear and constrained systems (Chehouri et al., 2016).

Engineering applications of EAs have been both extensive and successful, ranging from renewable energy (Shakoor et al., 2016), to road construction (Babapour et al., 2018) and robotics (Fleming and Purshouse, 2002). This has not been true of the ecological domain, where EA usage has mostly involved parameter optimisation (Gobeyn et al., 2019). Expanding the investigation of EAs in OC to an ecological capacity is thus justifiable.

EA applicability in an ecological capacity cannot merely be assumed however, as effective models and principles from various disciplines have often proved unsuitable when applied in ecology (Svirezhev, 2008). Therefore, in view of the fact that EAs have proved proficient in highly constrained, non-linear and non-convex engineering-based OCPs, the current research seeks to examine EA potential in ecological OCPs. Consequently, a review of EAs ensues.

2.5 Evolutionary Algorithms

Inspired by biological evolution, EAs are a class of meta-heuristics that have proved successful in a wide variety of OCPs (Fleming and Purshouse, 2002). A population-based set of optimisation algorithms, EAs are governed by biological principles (Engelbrecht, 2007) and therefore mimic evolutionary processes (Sivanandam and Deepa, 2008). EAs can thus be adapted to problem changes, without requiring reinitialisation, or re-solving, as is often the case with classic optimisation algorithms (Sivanandam and Deepa, 2008).

2.5.1 Evolutionary Algorithm Operation

The operation of a typical EA, illustrated in Figure 2.3, begins with the creation of a population of *individuals*, distributed across the search space, encoding candidate solutions as *chromosomes* (Haefner, 2012). *Genes* (making up chromosomes) represent decision variables, or control variables in the case of OC, each of whose associated value is termed an *allele* (Engelbrecht, 2007). A *fitness function* is then used to determine the quality, or optimality, of an individual by transforming the objective and constraint satisfaction of an individual into a numerical value, termed the fitness of the individual (Engelbrecht, 2007).

To replicate the natural selection mechanisms characteristic of evolution, individuals in an EA population undergo *selection* and *reproduction* to successively generate increasingly *fit* individuals (Engelbrecht, 2007). Selection processes are used to compare chromosomes' fitnesses (Sivanandam and Deepa, 2008) in order to determine the best, or *fittest*, individuals, and in most applications, individuals are ranked according to fitness.

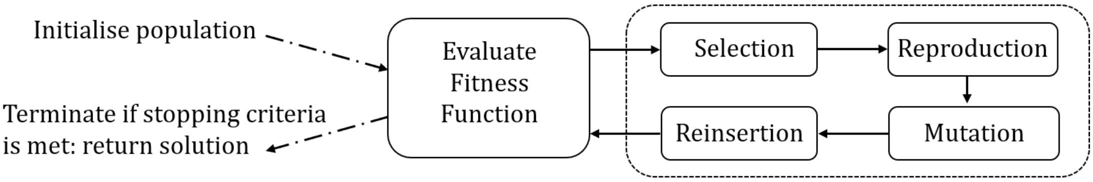

Figure 2.3: The operation of a generic EA, adapted from Fleming and Purshouse (2002)

Reproduction operators are used to facilitate *exploitation* and *exploration*, a combination of which equips an EA with the capability of locating global optima (Yang, 2014). Operating in an exploitation capacity, *crossover* is used to combine the genetic material of *parent* chromosomes to form *offspring*, with individuals of greater fitness rank (when maximising the fitness function) more likely to be used in crossover (Engelbrecht, 2007). Exploitation, or intensification, prioritises generating solutions in proximity to the best solutions obtained thus far, in order to improve upon the current, most optimal solutions (Yang, 2014).

Occurring on a local scale, exploitation is sensitive to how the population is initialised, and while securing high *convergence rates* (iterations until error tolerance met), may inadvertently cause convergence to a local optimum (Yang, 2014). Hence, the exploratory component of the algorithm, namely *mutation*, is required to perturb and diversify solutions, and prevent premature convergence (Yang, 2014). Mutation alters selected alleles with a specified probability, referred to as the *mutation rate*, to generate *diverse* offspring (Engelbrecht, 2007).

Operating on a global scale, exploration, or diversification, facilitates the production of diverse solutions across the entire search space, but decreases convergence rates and consumes valuable computational resources to generate far-from-optimal, and often redundant solutions (Yang, 2014). Balancing exploration and exploitation, termed the *exploration-exploitation* trade-off, is therefore critical to attaining global optimality (Balsa-Canto et al., 2012).

Lastly, reinsertion is used to partially, or completely, replace parent chromosomes with offspring in successive generations (Haupt and Haupt, 2004; Morrall, 2003). Often, a number of *elite* individuals, or the fittest individuals, pass through to the next generation, unchanged (Engelbrecht, 2007). This process (Figure 2.3) continues iteratively until the specified stopping criteria have been met and the algorithm therefore terminates. In line with the research question (Section 1.2), dissimilarities between the operation, characteristics, and associated suitability of EAs versus classic OC and optimisation methods are highlighted next.

2.5.2 Classic Optimisation Algorithms Versus Evolutionary Algorithms

Identifying a suitable OC algorithm is an important part of OC (Barbour et al., 2016). In simpler OCPs, for example, or under favourable mathematical conditions, classic OC methods are capable of greater accuracy and efficiency than EAs (Barbour et al., 2016). This is partly because most classic OC methods operate sequentially, locating optima through the use of gradient information and sequential searches (Engelbrecht, 2007; Maier et al., 2019). In contrast, EAs rely on the fitness of individuals to steer a parallel search across the entire search space, using probabilistic-transitioning rather than gradient information (Engelbrecht, 2007). This has several associated advantages, examples of which are given in Table 2.3.

Table 2.3: Properties of EAs along with their associated advantages.

EA Property	**Result**	**Advantage**
EAs are equipped for computational parallelisation (because of their parallel nature).	Can dramatically reduce running time, depending on the number of processors or computational speed of the computers used (Maier et al., 2019).	Lends itself towards the increasingly complex OCPs formulated nowadays, while maintaining a suitable level of efficiency (Sivanandam and Deepa, 2008).
Do not impose structural or framework constraints, bypassing the conditions prescribed by classic OC methods (Gobeyn et al., 2019).	Acts to reduce the difficulty associated with encoding the properties of a system as an OCP (Blueschke and Savin, 2017); characteristics that assist EAs in maintaining robustness in classically adverse domains (Engelbrecht, 2007).	Beneficial when the ecological characteristics of a system are not fully understood, or the most suitable objective is unclear (Runge and Johnson, 2002), which would otherwise require the examination of multiple models (Blueschke and Savin, 2017).

These properties have been exploited in chemotherapy drug scheduling, for example, where EAs have generated near-optimal solutions on par with leading published classical solutions, while also simplifying and automating the OC process (Tan, Khor, Cai, Heng and Lee, 2002). In this previous work, the EA was able to maintain effectiveness and improve realism without subjecting the objective to the differentiability and convexity conditions typical of gradient-based schemes (Tan et al., 2002). Benchmark comparisons have substantiated these findings by demonstrating that EAs are capable of accurately reproducing classical results, but may require a greater time frame to achieve equivalent results (Blueschke and Savin, 2017).

Thus, when classic OC methods are inapplicable, EAs often become the natural successor

(Shakoor et al., 2016). Typically this occurs in multi-objective, multi-modal, discontinuous, noisy or large systems (Shakoor et al., 2016), for which EAs retain flexibility and robustness (Fleming and Purshouse, 2002). The large number of indispensable design variables, highly-constrained environments and conflicting objectives in wind turbine design, for example, often renders classic OC methods obsolete, and thus EAs are instead applied (Wang et al., 2017).

EAs, however, too experience decreasing efficiency with increased problem size, due to the increase in computation required (Wang et al., 2017). Thus, while the gradient-free and noise-tolerant EAs can effectively obtain global optima in complex OC environments, their search parallelism can reduce efficiency when applied to large, multi-objective or constrained OCPs, if not computationally parallelised (Tan et al., 2002; Wang et al., 2017). Additionally, hyper/meta-parameter tuning (e.g. of mutation or crossover rates) is attached to EA usage, which can introduce complexity (Gobeyn et al., 2019).

Attributes of EAs, demonstrated across various applications, present a good fit for an ecological setting (Whigham and Fogel, 2003). Inevitably, the selection of an algorithm becomes subject to researcher preference (Yang, 2014). Relevant factors in its choosing, including computational requirements, time constraints and the congruity of the problem type with the solution technique, are then dependent on the researcher's proficiency (Yang, 2014).

Increasingly complex applications are arising in theoretical ecology, requiring researchers to improve upon current practices and advance the investigation of EAs in ecology (Gobeyn et al., 2019). As one of the earliest and most popular EAs, GAs are based on the behaviour of ecological systems (Simon, 2013) and have been extensively applied (Sivanandam and Deepa, 2008), which acts to advocate their potential in ecology.

GAs hail as one of the most versatile optimisation algorithms, accredited with handling challenging and often classically-intractable OCPs (Ruxton and Beauchamp, 2008). Compared to classic OC methods, limited problem knowledge (e.g. the physical interpretation of variables) is required by GAs (Pacheco and Segrè, 2021), and GAs have outperformed classic OC methods on occasion (Haupt and Haupt, 2004). Furthermore, a variety of GA toolboxes exist in popular software, for example MATLAB (2018), ensuring the accessibility of a GA approach in ecology. An in-depth analysis of a single algorithm, across multiple settings, could arguably provide insight into its capabilities. To this end, and in line with the scope of the research, only one EA, namely a GA, will be considered, presented next.

2.6 Genetic Algorithms

Based on the Darwinian concept of natural selection and brought into being through the pioneering work of Holland (1975) and De Jong (1975), GAs have been extensively used since their creation in the 1960s (Yang, 2014). Resilient to classically incompatible problem domains, GAs have been successfully applied to a plethora of optimisation problems, gradually developing into the broader class of algorithms, since coined EAs (Yang, 2014). Additionally, GAs have proved proficient in many applications, producing results superior to both the indirect and direct methods (Section 2.2.3) in selected applications, and handling complex OCPs formidable to conventional methods (Nezhadhosein et al., 2015; Yang, 2014).

As an optimisation algorithm, a GA is an iterative search method that is used to evolve solutions to a system towards an optimal state, specified by an objective (Haupt and Haupt, 2004; Sivanandam and Deepa, 2008). Ideally, the search is terminated when there is no further improvement in solution quality and thus convergence occurs (Haupt and Haupt, 2004). An outline of a generic GA, adapted from Yang (2014) and Engelbrecht (2007) is as follows:

```
Generate an initial population, letting $n = 0$ be the generation counter;
while stopping condition(s) not met do
    Evaluate the fitness of each individual;
    Create a new population using selection and reproduction operations;
    Update $n = n + 1$ to advance to the next generation;
end → return fittest individual in the final population.
```

Algorithm 1: Genetic algorithm operation (Engelbrecht, 2007; Yang, 2014)

Analogous to the role of the objective in OC, the fitness function in a GA is pivotal in steering the evolution of the system (Morrall, 2003), as fitness values correspond to the quality of candidate solutions. As a population-based algorithm, multiple individuals are produced at each generation, the parallel paradigm of GAs providing opportunity for diverse, independent and simultaneous exploration of the search space (Yang, 2014).

The mathematical counterparts of biological genetic operators are implemented through crossover and mutation in a GA (Yang, 2014). A selection mechanism based on the fitness of individuals is used to enforce the *survival of the fittest* (Engelbrecht, 2007). The roles of each of these operators in the GA are outlined as follows:

- **Selection** ensures the fittest chromosomes pass their characteristics on to successive generations; in essence, imitating the *survival of the fittest* and enhancing convergence (Yang, 2014). Use of elitism ensures that the most optimal solutions, at any given generation, pass through to the next generation unchanged (Yang, 2014).

- **Crossover** is used to mimic reproduction through the recombination of parent genetic material (Engelbrecht, 2007). Offspring are generated by combining the corresponding segments of genetic material from parent chromosomes (Sivanandam and Deepa, 2008), with probability, termed the *crossover rate*, commonly in the range 0.6 to 0.95 (Yang, 2014). Operating in an exploitative capacity, crossover promotes convergence by allowing the best solutions to dominate in a subspace of the search space (Yang, 2014).

- **Mutation** alters characteristics of a gene(s) within a chromosome, encouraging exploration of the search space and hence solution diversity (Yang, 2014). Mutation can act locally for low mutation rates but usually promotes a global search, with mutation rates generally lying between 0.001 and 0.05 (Yang, 2014).

In keeping with the governing principles of exploitation and exploration, a balance between the stochastic processes of crossover and mutation is needed to locate a global optimum (Yang, 2014). Additionally, factors such as the population size, selection criteria and fitness function, can impact the solutions obtained by a GA (Babapour et al., 2018), and convergence thereto (Yang, 2014). Implementation choices for factors governing GA behaviour, presented next, may thus act either to impede or enhance GA performance.

2.6.1 Implementation Features of a Genetic Algorithm

GAs can be applied to diverse systems and objectives, incorporating discontinuity, noise or non-convexity, provided the operational parameters of a GA are appropriately selected (Yang, 2014). GA population size (number of individuals), for example, can influence the fidelity of results (Sivanandam and Deepa, 2008) and affect the convergence of a GA towards a global optimum (Babapour et al., 2018). The population size should be proportional to the number of control variables encoded in each chromosome (Babapour et al., 2018). Large population sizes facilitate exploration and increase the likelihood of obtaining global optimality, but increase computational time (Engelbrecht, 2007).

The GA population is subjected to selection and reproduction to replace the population in each successive generation (Section 2.5.1). Selection methods can be random, proportional to fitness, or rank-based, amongst others (Engelbrecht, 2007). Typically, chromosomes of greater fitness (when maximising the fitness function) are more likely to be selected to take part in reproduction (Sivanandam and Deepa, 2008). Due to the stochastic nature of the algorithm however, GAs may suffer from sensitivity to the initialised population (Yang, 2014). This is of particular concern in multimodal domains where the initial population generated may not contain solutions in the vicinity of the global optimum (Yang, 2014).

To counteract this, a genetically diverse initial population reflecting the entire search space is required, which may be achieved through random initialisation (Sivanandam and Deepa, 2008). Analysis of the GA results throughout multiple runs of the GA with varied initial populations, or using a stopping criterion that allows the GA enough time to locate a global optimum, irrespective of the initialisation, may help alleviate premature convergence (Yang, 2014). Additionally, the mutation operator can be used to avoid premature convergence.

Mutation can play a pivotal role in the overall success of GA results. Greater mutation rates promote global rather than local optimality (Yang, 2014), but may inadvertently degrade the long-term persistent behaviour of the system by inhibiting convergence (Ruxton and Beauchamp, 2008). Implementing adaptive mutation may address this by decreasing mutation throughout the duration of the algorithm, as the risk of converging to a local optimum dissipates (Ruxton and Beauchamp, 2008). Higher initial mutation is needed to encourage exploration of the search space using this approach, but with the propagation of the best of the diverse solutions with successive generations, lower mutation rates can be sustained.

Many popular software programs containing built-in GA toolboxes, such as MATLAB (2018), implement specific choices for factors such as reproduction or selection operators, which the user can adjust. In addition to operative factors of GAs however, a number of OCP features can prove challenging to GAs (Chehouri et al., 2016). Constraints, for example, may have to be embedded in the fitness function (Engelbrecht, 2007).

Synonymous with processes used in classic OC methods, a constrained OCP can be transformed to an unconstrained equivalent by introducing penalty functions (Engelbrecht, 2007). Penalties introduce considerable complexity into an OCP, particularly in connection with assigning a weight to penalty terms (Chehouri et al., 2016). Chosen too large, and the search will disregard feasible areas of the domain; too small, and infeasible solutions result (Chehouri et al., 2016). Customised tuning of these terms to obtain appropriate weights, however, is a complex issue in both conventional and modern OC methods (Chehouri et al., 2016).

Caution should thus be exercised when applying a GA, as to operational components thereof (Ruxton and Beauchamp, 2008) which can impact results. In a similar vein to classic OC methods, components such as numerical integration schemes used within a GA approach, play a pivotal role in the solutions obtained (Subchan and Żbikowski, 2009). Since a GA approach does not guarantee an optimal solution however, cautious interpretation of results is arguably more important than when employing classic OC methods.

GAs were used to establish a basis for evolutionary computing, and have remained among the most favoured and widely applied EAs today (Yang, 2014). Notably, this popularity extends to NLPs, where the exploratory, parallel nature of GAs allows the handling of complex OCPs, and further circumvents the classic OC requirement of gradient information (Yang, 2014). These design elements of GAs make them ideal candidates for OC applications.

2.6.2 Genetic Algorithms in Optimal Control

GAs have been widely applied to optimisation problems in which persuasive arguments for their broader usage have been made (Theo et al., 2017). Although the relationship between GAs and optimisation can naturally be extended to OCPs, GAs are not widely applied in OC. In accordance with the focus of this research, chiefly OC applications of GAs were considered.

Theory to establish the validity of GA results is sparse (Ruxton and Beauchamp, 2008). Many authors thus rely on comparisons with classic OC methods to establish the accuracy and effectiveness of GA usage. Ranging from agriculture (Singh, 2012) to vehicle racing (Dal Bianco et al., 2019), GAs have been applied to diverse OCPs in which they were compared to a variety of classic OC methods. Some noteworthy mentions by Singh (2012) include:

- GAs demonstrating better efficiency and robustness than direct methods in groundwater management OCPs, while also accurately obtaining global optima and near-optima,
- GAs producing equivalent results to NLP, and even being deemed preferable to NLP, when determining optimal cropping and irrigation patterns.

Displays of preference for GA use in OC are not isolated incidents. Surge tanks, for example, demand a highly constrained, non-linear and discrete environment of large dimension, characteristics ill-suited to gradient-based conventional methods (Bostan et al., 2019). For this reason, GAs are favoured (Bostan et al., 2019), as the demanding computational and governing mathematical requirements of NLP limits its use in many practical applications, demoting these techniques to a supportive capacity in many OCPs (Singh, 2012).

GAs have also performed well in comparisons with non-classic OC methods. In the optimal vertical alignment of road design, for example, GAs have proven capable of:

- generating solutions with less financial cost than those obtained via manual design,
- producing solutions with lower financial cost than particle swarm optimisation[7], particularly as the number of decision variables increases (Babapour et al., 2018).

GA-derived OC strategies, superior to a host of conventional techniques, have been obtained in temperature control applications; a finding that bears favourable ramifications in both medicinal and produce sectors (Gani, Islam and Ullah, 2019). Additionally, minimum lap time OCPs have seen GAs satisfactorily solve complex vehicle problems, albeit slowly (Dal Bianco et al., 2019). In spite of the obvious benefits of GAs, the uptake of GAs in ecological OCPs appears to have been slow, as there were a limited number of applications found in the literature reviewed. These applications are now presented.

2.6.3 Genetic Algorithms in Ecological Optimal Control Problems

The use of GAs in ecology is still in its infancy, with usage predominantly limited to a parameter estimation capacity or optimal experimental design (Balsa-Canto et al., 2012). This was exemplified in a recent systematic review by Wang and Sobey (2020), who found approximately 20 papers of a multi-objective optimisation nature employing GAs in biological fields, over a time period of 30 years; less than 0.8% of GA-based papers in the database.

GA applications in ecological OCPs consider fairly typical model types, and include the management of invasive alien grass species (Taylor and Hastings, 2004) and the development of drug therapy schedules in stochastic HIV models (Saeedizadeh and Moghaddam, 2017). More atypical applications have seen GAs used in conjunction with chaos synchronisation in circadian rhythm phase OCPs – obtaining non-linear controls using a GA and then refining the controls with synchronisation methods (Vo-Tan, Ton-That and Janerio, 2016).

---

[7] A population-based, biologically-inspired, meta-heuristic algorithm (Engelbrecht, 2007; Yang, 2014).

GAs are uniquely placed for diverse applications in ecology, including the evolving of species interactions, self-designing ecosystems, and parameter optimisation (Morrall, 2003). Although devised using principles governing biological phenomena (Simon, 2013), usage in the very same field that inspired the creation of GAs has arguably been limited to mainly parameter optimisation. Possessing characteristics fundamentally suited to obtaining optimal controls in complex and adaptive systems, characteristic of ecological settings (Morrall, 2003), GAs are ideal candidates for which to pursue further investigation in ecology.

2.7 Summary

Humans have had a significant effect on ecological systems, prompting the urgent requirement for methods to predict the impact of external influences and further alter ecological systems to ensure sustainability, amongst other management goals (Morrall, 2003). OCT is comprised of effective methods with which to exert control under such circumstances, but requires expertise to implement and subsequently rely on the results thereof. Additionally, substantial numerical and software understanding is needed to adequately cater for the inherent difficulties involved in correctly applying and analysing an OCP in a realistic setting.

Even when applied appropriately, OC solutions can be far less precise than assumed theoretically, with different approaches frequently yielding different results. Moreover, optimal ecological management strategies are often unsuccessful in practice, primarily due to the inherent assumptions of classic OC methods being unsuitable in an ecological setting. In particular, the rigidity of classic OC methods is ill-suited to the dynamic, evolutionary behaviour of ecological systems, which are in a constant state of adaptation (Jørgensen and Fath, 2011; Morrall, 2003).

EAs, and in particular GAs, are modelled after biological processes and possess the potential to address complex OCPs in ecology. Based upon the very principles governing ecology, with the potential to support the mathematical techniques available to managing ecological systems, GAs have been relatively unexplored in a stand-alone capacity in ecological OCPs. This research thus endeavours to explore this potential by investigating the viability of such an approach. The methods by which this will be examined are presented in Chapter 3.

Chapter 3

Methodology

3.1 Introduction

To establish whether a GA presents a viable alternative to classic OC methods in ecological OCPs according to the aims of the research, an experimental-type approach was adopted, as presented in this chapter. The approach consists of both a comparative component, presented in Section 3.2, and an exploratory component, outlined in Section 3.3.

Several ecological case studies will be used to facilitate this investigation, each of which addresses an ecological issue. Firstly, comparisons will be used to ascertain whether a GA is capable of replicating classical results to a sufficient extent (Chapters 4 and 5). Thereafter, a complex OCP will be developed in an exploratory capacity, and solved using only a GA (Chapter 6). The algorithms and software used to solve the OCPs are presented in Section 3.4, followed by additional numerical factors that were taken into account in Section 3.5. Solution quality is discussed in Section 3.6, followed by concluding remarks in Section 3.7.

3.2 Comparative Component

The ultimate manner in which to establish the viability of a GA approach is through comparisons with analytical solutions (Ruxton and Beauchamp, 2008). Unfortunately, analytical solutions are seldom obtainable (Bostan et al., 2019), as few OCPs can be solved analytically (Rao, 2010). Solutions obtained using classic OC methods are thus often used instead, particularly when establishing the viability of modern computational methods like EAs. Benefits attached to EAs, for example, have been identified in comparisons with classic OC methods across a range of optimisation problems, motivating future studies to increasingly explore the potential of such algorithms (Theo et al., 2017).

Compilations of test OCPs exist whereby comparisons between methods can be made, however, little detail is given as to the processes employed in such studies, which are chiefly engineering-based (Betts, 2015). Moreover, establishing test problems is not widespread amongst all disciplines as the complexity involved in even a single practical application severely restricts the development of benchmark problems in certain disciplines (Betts, 2015).

Consequently, several ecological case studies were used to perform comparisons between a GA and the three classic OC methods considered in the current study. The comparisons were conducted in a similar manner to the experimental research methodology of Singh (2006), with a GA applied as the experimental factor and the classic OC method as the controlled factor. The objective function of the OCP was used as the criterion component (Singh, 2006) in order to determine the efficacy of the GA. This is summarised in Figure 3.1.

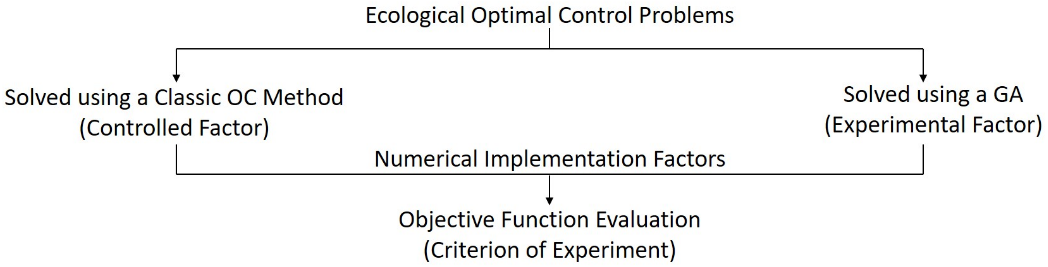

Figure 3.1: The experimental-type approach, adapted from Singh (2006)

3.2.1 Case Study Usage and Selection

The rigorous analysis of cases studies has instigated mathematical discoveries throughout the history of mathematics (Gumowski and Mira, 1968). The repeated and consistent obtaining of patterns and findings have then been generalised and even formalised into corroborating theory (Gumowski and Mira, 1968). Consequently, case studies are routinely used as a means of conducting comparisons between methods in OCT, or comparing modern methods, like the GA, to traditional methods in real case studies (Notte et al., 2016).

An approach akin to that used by Rawlings, Barrera-Martinez and Rico-Ramirez (2020) was implemented in the current study, whereby the merits of a technique are illustrated through applications to successively more complex case studies. Each case study was used to establish whether a GA is capable of reproducing classic OC results and to investigate the effect that increasing complexity had on GA performance. Factors that typically present challenges to classic OC methods, or *caveats*, were incorporated in the case study selection as far as possible, to see whether the added complexity would impact GA performance.

One of the most widely stated obstacles in classic OC methods is the difficulty of solving OCPs with path or inequality constraints. Such an ecological case study could not be found, arguably due to the complexity involved in solving such and so such an OCP was not compared in this study. Instead, GA performance was examined in the presence of non-convexity, since convexity is a critical assumption of classic OC methods. In addition, a PDE-based OCP was considered, as PDEs increase the mathematical complexity of OCPs considerably. Furthermore, case studies were selected from literature wherein both indirect and direct methods (Section 2.2.3) were applied so as to obtain a more comprehensive comparison.

The case studies in the current research follow the development trajectory of ecological modelling. As per its origins, the widely studied predator-prey model, with a harvesting term attached, was used in the first ODE case study (Section 4.2). Thereafter, disease control was investigated in an ODE epidemiology model, wherein a critical classical OC assumption was broken (Section 4.3). A PDE model was then examined (Section 5.3), representative of the increasing importance of including spatio-temporal dynamics. Lastly, the final case study (Chapter 6) addressed the pertinence of wild bee conservation in modern agriculture, and was formulated as an unconventional OCP, and solved in an exploratory capacity.

3.3 Exploratory Component

Since a demand exists for atypical OCP applications (Koryakovskiy et al., 2017), the development of an OCP that is excessively difficult, or intractable to solve using classic OC methods is both relevant, and serves to address the second research aim (Section 1.3). Investigating the use of a GA as an alternative OC method therein, is also consistent with the use of OC tools commonly being illustrated through applications to complex case studies in realistic settings (Subchan and Żbikowski, 2009), with many leading researchers demonstrating the advantages and disadvantages of specialised methods in this manner (Jopp et al., 2011).

By first establishing GA results as comparable with accepted mathematical techniques in test problems, namely the comparative case studies (Section 3.2), the fidelity of a GA approach could be justified in the final case study in the absence of a comparison (Vanderbei, 2001). Results from the comparative case studies were thus used to support and substantiate the viability of GA results in the exploratory component, as illustrated in Figure 3.2. The algorithms and software used to solve the OCPs are presented in the section following.

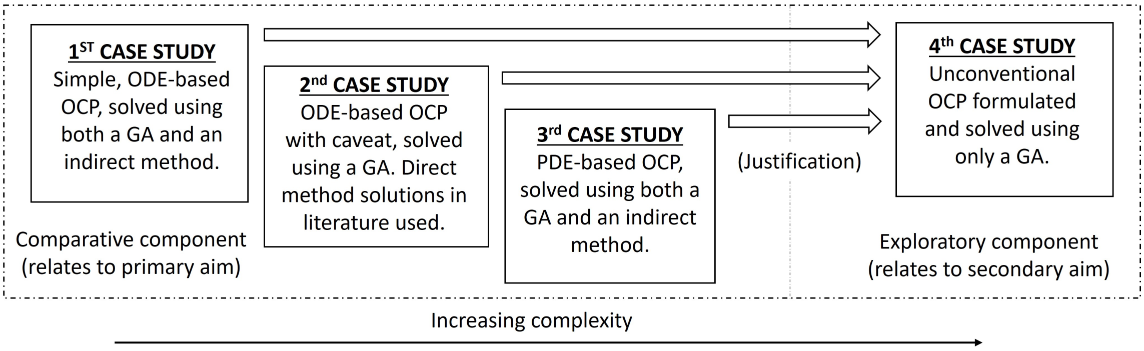

Figure 3.2: Case study progression used in the research methodology

3.4 Algorithms and Software Implementation

Both the classical and GA approaches were implemented in MATLAB (2018) in this study. As per the aims of this research, this ensures a standard algorithm is available to ecological researchers. Moreover, MATLAB is compatible with many solvers and is frequently utilised in literature. Factors specific to the classical approach used in this study are next given, followed by GA considerations. For a more detailed account of the algorithms, the interested reader is referred to Lenhart and Workman (2007) and MathWorks (2017) respectively.

3.4.1 Classic Optimal Control Approach

The indirect Forward-Backward Sweep Method (FBSM) (Lenhart and Workman, 2007) was the only classic OC method (Section 2.2.3) implemented in the current study. To implement the FBSM, the time interval is typically divided into N subintervals, with $N+1$ nodes at which to approximate the solution. A value of $N = 1000$ is commonly found in literature (Schwartz, 1996), provided this elicits suitably small step sizes. After applying PMP (Pontryagin et al., 1962), vector approximations to the adjoint ($\bar{\lambda}$), control ($\bar{u}$) and state ($\bar{x}$) are used to iteratively obtain an optimal solution to the OCP in the FBSM as follows:

```
Estimate initial control values $\bar{u}_{i=0}$, with initial conditions at the $i = 0$ iteration;
    while relative errors $> \delta$ do
        Update $i = i + 1$;
        Solve for $\bar{x}_i$ forward in time, using $\bar{u}_{i-1}$ and the state equations;
        Solve for $\bar{\lambda}_i$ backward in time, using $\bar{u}_{i-1}$, $\bar{x}_i$ and the adjoint equations;
        Input $\bar{x}_i$, $\bar{\lambda}_i$, and $\bar{u}_{i-1}$ into the optimality condition and update $\bar{u}_i$;
        Obtain the relative errors $\frac{\|\bar{x}_i - \bar{x}_{i-1}\|}{\|\bar{x}_i\|}$, $\frac{\|\bar{\lambda}_i - \bar{\lambda}_{i-1}\|}{\|\bar{\lambda}_i\|}$, and $\frac{\|\bar{u}_i - \bar{u}_{i-1}\|}{\|\bar{u}_i\|}$;
    end
```

Algorithm 2: The FBSM, adapted from Lenhart and Workman (2007)

The value assigned to δ acts as the stopping criterion, with Lenhart and Workman (2007) recommending a value of $\delta = 0.001$ to ensure convergence. Classical solutions obtained using the direct methods (reported in Section 4.3.2) were not generated in the current study.

3.4.2 Genetic Algorithm Approach

The GA feature in MATLAB (2018) was used in the current study, with default meta-parameters. To apply the GA, an OCP's control(s) must first be encoded as a chromosome. A population of chromosomes is then generated, and each encoded candidate optimal control is substituted into the OCP, and the OCP is then solved. Selection and reproduction are then performed until the GA terminates (Section 2.6). Since MATLAB minimises the fitness function, the optimal control is given by the chromosome with minimum fitness. This iterative process is illustrated in Figure 3.3, for a population size of 200, and is next described.

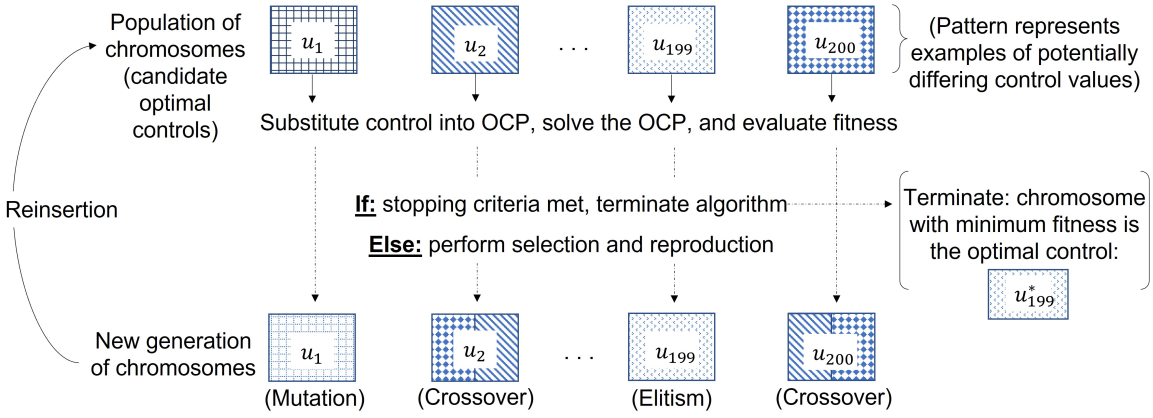

Figure 3.3: An example illustration of the application of a GA to an OCP

The GA function in MATLAB (2018), as applied in this study, randomly generates an **initial population** from the interval of values over which the control is restricted. If the number of variables optimised by the GA, or control variables in this instance, exceeds five, a population size of 200 is used, otherwise, a population of 50 chromosomes is generated. The GA then proceeds iteratively until the stopping criterion is met, as follows:

1. **Evaluation**: The candidate optimal control(s) encoded in each chromosome in the population is substituted into the OCP. The OCP is then solved for every chromosome in the population, and a fitness value related to the OCP's objective is calculated. Consequently, every chromosome has an associated fitness.

2. **Selection**: A combination of uniform sampling and roulette wheel selection (MathWorks, 2017) is implemented with parent chromosomes selected according to scaled fitnesses, proportional to their respective rank in the population. This promotes *survival of the fittest* in successive generations by propagating the fittest individuals.

3. **Reproduction**: A crossover rate of 0.8 is implemented in a random or uniform manner, ensuring genetic material from either parent chromosome can be used.

4. **Mutation**: The default mutation for bounded controls is adaptive mutation which uses a mutation function to generate step lengths and directions within the allele range to adaptively mutate the alleles, while satisfying bounds on the controls.

5. **Reinsertion**: An elite count of 5% of the population size is used, translating to 5% of individuals passing through to the next generation unchanged. The remaining parents are replaced by the offspring generated through reproduction and mutation. The population thus advances to the next generation.

The GA **terminates** when the average relative difference in the fitness of the best individual over 50 generations is less than 1×10^{-6}. The maximum number of generations is further restricted to 100×(number of control variables), regardless of whether convergence occurs. The FBSM stopping criterion of 1×10^{-3} (Section 3.4.1) was not sufficient for the GA to converge and so the default MATLAB value of 1×10^{-6} was kept. Alternative values were not examined due to scope limitations. However, the FBSM requires the relative error of all variables between successive iterations to satisfy this bound, which is not directly comparable to the GA which relies on an average difference in the fitness function over 50 generations.

3.5 Numerical Implementation Factors

Numerical integration methods perform a critical role in OC (Rao, 2010), with appropriate quadrature able to substantially reduce the error incurred in numerically approximating an OCP (Pytlak, 1999). Additionally, control approximation, which is required to pursue a GA approach, impacts on solutions (Schwartz, 1996). Since the user determines the controls and quadrature used, choices can be made to influence solution accuracy. The inclusion of these factors is next outlined. Beyond this, the OC solution approach, or a GA in this instance, may significantly affect the accuracy of solutions (Schwartz, 1996). To comprehensively assess the GA's performance and accuracy as an OC method, the GA was run 30 times for every OCP formulation considered, as is the typical standard (Wang and Sobey, 2020).

3.5.1 Dynamical System

The assumption of continuity is common to ecological models and typically suffices (Svirezhev, 2008). Suited to the fundamentally dynamic nature of ecosystems (Jørgensen and Fath, 2011; Oruh and Agwu, 2015), continuous dynamical systems were thus used in the current study. Numerical integration methods consistent with arguments in literature were then applied.

In all ODE case studies (Chapter 4), the R-K4 was applied, which is assured of achieving $O(h^4)$ accuracy when applied to OCPs and ensures that consistent approximations to OCPs are obtained (Hager, 2000). Furthermore, the R-K4 produces consistent solutions for piecewise polynomial controls (Schwartz, 1996). In the PDE-based OCP (Chapter 5), a combination of Forward in Time-Centred in Space (FTCS) and Backward in Time-Centred in Space (BTCS) finite difference methods was used, which apply first-order finite differences on the temporal domain and second-order finite differences on the spatial domain.

3.5.2 Control Configuration

Both the indirect and direct methods delineate an optimal control, however this control often has to be approximated. This is more often the case in solvers assuming a direct method approach, and is also a concern of the current study, since the accuracy of numerical OCP solutions are further dependent on these errors introduced when configuring an approximate control (Schwartz, 1996). However, since GA use bypasses the application of PMP, or the

Karush-Kuhn-Tucker conditions, a control form is not dictated by the problem and thus an appropriate control representation must be determined.

A user-defined encoding of a control(s) as a chromosome is then required to generate candidate optimal controls in the GA. Either, a user-designed control form must be encoded for which the GA will select the values it assumes, or if possible, a generic control should be encoded in a way that allows the GA to select the form and values that the control will take on. Since controls are extremely problem-dependent, for example, depending even on whether the OCP is ODE or PDE based, there is little precedence for the best way in which to encode controls. Due to this problem specificity, the control generation and/or encoding will be discussed in the relevant upcoming chapters, according to the OCP under consideration.

3.5.3 Objective Function Evaluation

The GA relies solely on a fitness function to determine solution quality. In all case studies considered, this fitness function was composed solely of the objective function. The objective, and thus the quadrature used to determine its value, is therefore directly responsible for promoting chromosomes encoding candidate optimal controls, thus ultimately dictating which control will be chosen as optimal. Consequently, the order of quadrature used to evaluate the objective is relevant to the current research (Bara et al., 2017).

Typically, a quadrature method of order equal to the numerical method used to approximate a solution to the dynamical system is applied to evaluate the objective (Rao, 2010). However, the order of error of the numerical methods used in the current study differed between OCPs, depending on whether the OCPs were ODE-based, PDE-based, or whether the classic OC solution was extracted from existing literature. Consequently, objective evaluation is covered in the respective chapters following, according to the methods used in each OCP.

In contrast to the GA, the objective is not explicitly used to drive the solution procedure in classic OC methods. Instead the objective is embedded into the systems of equations that is solved, and used to determine optimal adjoint, state and control variables. The value of the objective function is then only calculated once the optimal results are obtained. Consequently, the quadrature used to evaluate the objective is independent of and does not affect the optimal solution. In solutions produced using classic OC methods, the objective was thus used purely as a comparative means, in order to gauge the quality of GA solutions.

3.6 Solution Quality

As per the literature review, the effectiveness of an algorithm can be established using factors such as accuracy, or computational requirements. Establishing efficacy on the basis of computational resources can be an unreliable measure, however, as it is linked to the specific hardware within a computer and can thus change depending on the computer used (Betts, 2015). Furthermore, it is not ideal to measure complexity through computational requirements, as various algorithms applied to the same OCP can all consume different resource quantities, depending on the implementation (Betts, 2015).

The quality of an optimal solution to an OCP can be, and is often, judged according to the value of the objective function (Nezhadhosein et al., 2015). This measure of solution quality was adopted in the current research, with the accuracy of GA results assessed against classical results by comparing the respective final objective function values. The percentage difference between the best GA solution (the fittest chromosome in the final generation, out of all 30 runs) obtained in each case, and the respective classical solution was then reported.

There is considerable variability in optimal solutions obtained using classic OC methods and solvers in existing literature. Theoretical discussions were thus used to provide context with which to view optimal solutions obtained using a GA, where appropriate. In particular, the impact the control formulation and objective evaluation had on GA optimal results was examined to determine any possible ecological ramifications thereof (Barbour et al., 2016).

3.7 Summary

Amongst other factors, quadrature, control form and termination criteria, can influence OC solutions and contribute to differences observed in comparisons. To maintain comparability between methods, attempts were made to control these factors, reproducing results obtained using classic OC methods where possible. Where this was not possible, the implementation discrepancies between the classic OC methods and the GA were specified. The methodology used in this study, however, was simply to establish whether GAs provide a viable OC method in ecology. To get an indication of relative performance, a GA was applied to OCPs possessing solutions derived using classic OC methods, in Chapters 4 and 5, and then to a case study in Chapter 6 where classic OC methods became disproportionately complicated.

Chapter 4

Applications to Ordinary Differential Equation Systems

4.1 Introduction

The previous chapters established the need for and theoretical background necessary to investigate the viability of GAs as an OC method in ecological OCPs. To this end, two ODE models that have been examined by other researchers in existing literature are solved using a GA approach in the current chapter, to compare GA solutions to classic OC solutions.

A predator-prey model is examined first, presented in Section 4.2, and is solved using both a classic OC method and a GA in order to establish a basis from which in-depth observations regarding the solution methods can be made. A simple model was chosen so that dynamics of the system could more easily be identified and isolated from behaviour attributed to the GA in a transparent manner, without model complexity influencing or obscuring outcomes. Thereafter, a more complex ODE model is considered in Section 4.3, wherein an assumption pivotal to classic OC methods, namely convexity, is broken, and the resulting GA performance is investigated. Finally, concluding remarks are made in Section 4.4 to address the pertinence of the results to the aims and objectives of this study.

The focus of Chapters 4 and 5 is primarily on investigating whether a GA is capable of replicating classically-obtained OC results satisfactorily. Consequently, the emphasis in the associated comparative case studies following is on the application and outcome of applying a GA to the OCPs and not on the biological phenomena and interpretations of the systems examined. Necessary factors are discussed briefly and the interested reader is thus referred to the original texts should more information be required in this regard.

4.2 Predator-Prey Model

The general form of a predator-prey model is fairly common in OC as it is originates from the Lotka-Volterra equations (Lotka, 1925) which can be used to describe the behaviour of interacting species of predator-prey type (Murray, 2002). Adaptations to these equations further include, but are not limited to, the control of invasive plant species (Miller Neilan, 2009), plant-herbivore models (Brauer and Castillo-Chávez, 2012), or the indirect effect species have on one another through their respective interactions with their habitat (Mwakiwa et al., 2013).

The predator-prey OCP investigated in this study considers the circumstances wherein harvesting of a predator is needed to compensate for an increasing predator density driving a prey population to extinction. Using a Holling Type II functional response (Holling, 1959) and applying logistic growth to the prey population, while assuming that:

- as a specialist, the predator will die in the absence of prey,
- the only threat encountered by the prey is that of the predator,

Fourie (2018) developed an OCP using a linear harvest rate, proportional to the density of the predator population, to exert control on a predator-prey system. This OCP is next given.

4.2.1 Optimal Control Problem

To reduce the risk of prey extinction, the harvesting of predators, conducted at harvesting rate $u(t)$, was used to implement control in the system. An optimal control, $u^*(t) \in U$, corresponding to the optimal harvesting regime, was thus sought on the time interval $[0, T_f]$, where T_f denotes the final time of the interval. The admissible set of controls is then given by $U = \{u(t) : u \text{ is Lebesgue measurable}, 0 \leq u \leq u_{max} < 1\}$, where u_{max} denotes the maximum allowable rate of control that may be exerted during the time period.

The desired simultaneous increase in final prey population and decrease in final predator population, whilst reducing the associated cost of control throughout the time interval, was expressed mathematically in the form of an objective function $J(u(t))$, given in Equation (4.1), such that $J(u^*(t)) = \min_U J(u(t))$. Omitting dependence on time for ease of notation and simply denoting the prey population at time t by N_1, and the predator population by N_2, the OCP can then be stated as follows:

$$\text{minimise } J(u) = \frac{1}{2}\int_0^{T_f} Cu^2 dt - N_1(T_f) + N_2(T_f) \tag{4.1}$$

subject to:

$$\begin{aligned} \frac{dN_1}{dt} &= rN_1\left(1 - \frac{N_1}{K}\right) - \frac{gcN_1N_2}{a+N_1}, \\ \frac{dN_2}{dt} &= \frac{bdN_1N_2}{a+N_1} - mN_2 - uN_2, \end{aligned} \tag{4.2}$$

with $0 \leq u \leq u_{max} = 0.8$, and initial conditions $N_1(0) = 3000$ and $N_2(0) = 300$. Parameter descriptions and their associated values for the predator-prey OCP are given in Table 4.1.

Table 4.1: Parameter descriptions, units and assigned values, adapted from Fourie (2018).

Parameter	**Description**	**Units**	**Value**
K	Environmental carrying capacity	-	5000
r	Growth rate of prey	Per Year	0.84
a	Half saturation constant	Per unit area	2.5
b	Biomass conversion (prey to predator) rate	Per year	0.8
c	Searching efficiency of predator	Per year	0.6
d	Capture rate	Per year	0.7
g	Predation rate	Per year	0.2833
m	Natural death rate of predator	Per year	0.0625
u	Harvesting rate of predator	Per year	$0 \leq u \leq 0.8$
C	Cost of implementing harvest	Rands	100.00

The boundedness, permanence, local and global stability of the OCP has previously been established by Fourie (2018) on $\mathbb{R}^{2+} = \{(N_1, N_2) \in \mathbb{R}^2 : N_1 \geq 0; N_2 \geq 0\}$, where $N_1, N_2 \in C^1[\alpha, \beta]$ and $\alpha, \beta \in \mathbb{R}, \beta > \alpha \geq 0$. Consequently, pursuing an indirect approach, Pontryagin's Maximum Principle (PMP) was next applied to the OCP by the current author. The resulting augmented system of equations, consisting of the OCP, adjoint equations and optimality condition, was then solved using the widely used FBSM (Section 3.4.1) in the current study. The application of the indirect method to the OCP is now outlined.

4.2.2 Indirect Method and Associated Results

Defining $f_i = \frac{dN_i}{dt}$ for $i = 1, 2$, application of PMP yields the Hamiltonian of the system as

$$H = \frac{1}{2}Cu^2 + \sum_{i=1}^{2} \lambda_i f_i.$$

For $i = 1, 2$, the resulting Euler-Lagrange equations, with associated initial and transversality conditions, are then given by:

$$\begin{array}{lll} \text{State Equations:} & \dfrac{dN_i}{dt} = \dfrac{\partial H}{\partial \lambda_i}, & N_i(0) = \dfrac{30000}{10^i}, \\[2ex] \text{Adjoint Equations:} & \dfrac{d\lambda_i}{dt} = -\dfrac{\partial H}{\partial N_i}, & \lambda_i(T_f) = (-1)^i, \\[2ex] \text{Optimality Condition:} & \bar{0} = -\dfrac{\partial H}{\partial u}. & \end{array}$$

From the first order necessary conditions and existence results, also covered by Fourie (2018), the compact form of u^* can be derived as

$$u^* = min\left\{u_{max}, min\left(0, \frac{\lambda_2^* N_2^*}{C}\right)\right\},$$

where the use of a star (*) denotes the respective parameters' evaluation at an optimal state.

When solving an OCP, researchers typically consider either the accuracy of numerical methods important in quantifying solution quality (Frego, 2014; Ratković, 2016) or prioritise reducing computational cost (Rodrigues et al., 2009). As ODE systems of large dimension were not considered in this chapter, emphasis was placed on attaining higher accuracy over decreased computational cost. Based on this, the explicit fourth-order Runge-Kutta method (Section 2.2.5.5), abbreviated as R-K4, was used to solve all ODEs[1] in the current study.

To solve the predator-prey OCP using the FBSM, the time interval $[0, T_f] = [0, 5]$ was uniformly subdivided into $N = 1000$ subintervals, and R-K4 was used to generate solutions to the state, control, and adjoint equations at each of the $N + 1$ resulting nodes. This value of N is common (Lenhart and Workman, 2007), and results in a step size of $h = 0.005$ years in this OCP, which was deemed sufficiently small to ensure an acceptable balance between the level of accuracy and the computational time. The stopping criterion of the FBSM was structured to ensure that the relative error between successive iterations of all variables was less than $\delta = 0.001$ before convergence to a solution was assumed (Section 3.4.1). The *classical*

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[1] R-K4 solved the state equations in 0.042 seconds, and the augmented system of equations in 0.086 seconds.

solution produced according to these specifications is shown in Figure 4.1, where N_1^* is clearly maximised and N_2^* is minimised, as a result of applying u^* with minimum cost over $[0, T_f]$.

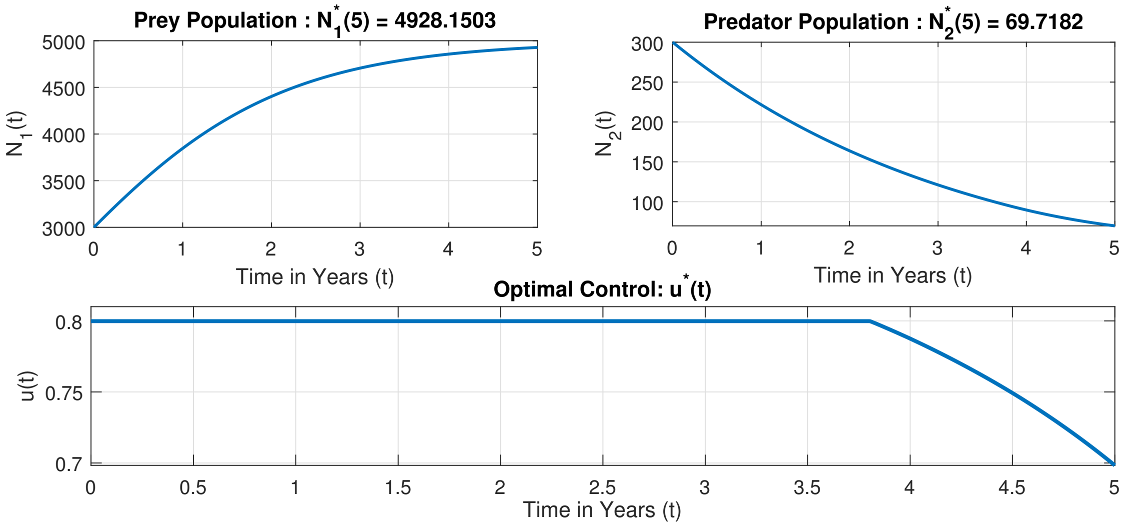

Figure 4.1: The FBSM-derived optimal solution to the predator-prey OCP

Following the argument presented by Pontryagin et al. (1962), in the absence of proof of sufficiency conditions via theorem, which would be unnecessarily complex for the scope of this study, the OCP was examined to analyse the potential global optimality of the (single) optimal control produced. Boundedness results obtained by Fourie (2018) were therefore used in conjunction with recognition of the short time frame to assume uniqueness of the optimal control, as per the findings of Jung, Lenhart and Feng (2002). Based on this assumption and the finite value obtained for the objective function (Lenhart and Workman, 2007), it was considered reasonable by the current author to conclude that a global optimum was achieved.

4.2.3 Genetic Algorithm Application and Results

To ascertain how the GA performs compared to the FBSM, which as an indirect method can guarantee an optimal solution (Lenhart and Workman, 2007), a GA was applied to the predator-prey OCP. For consistency with the FBSM, the R-K4 was applied in the GA, with an identical step size of $h = 0.005$ years, to enable a fair comparison between the methods. As there were no constraints in the model, the objective function (Equation (4.1)) was used as the GA's fitness function. The GA function in MATLAB (2018), with default parameter values (Section 3.4.2), was then used to determine an optimal control and the associated optimal solution, based on the encoded control, discussed next.

4.2.3.1 Encoding the Control as a Chromosome

To generate a control function in the GA without pre-empting its form, the time interval, $[0, T_f]$ was subdivided into n equally spaced subintervals and a control value for u generated on each subinterval. Each control value was considered constant across the length of the respective subinterval, and was encoded as a gene in the chromosome. Chromosome length thus equates to the number of subintervals, namely n, illustrated in Figure 4.2.

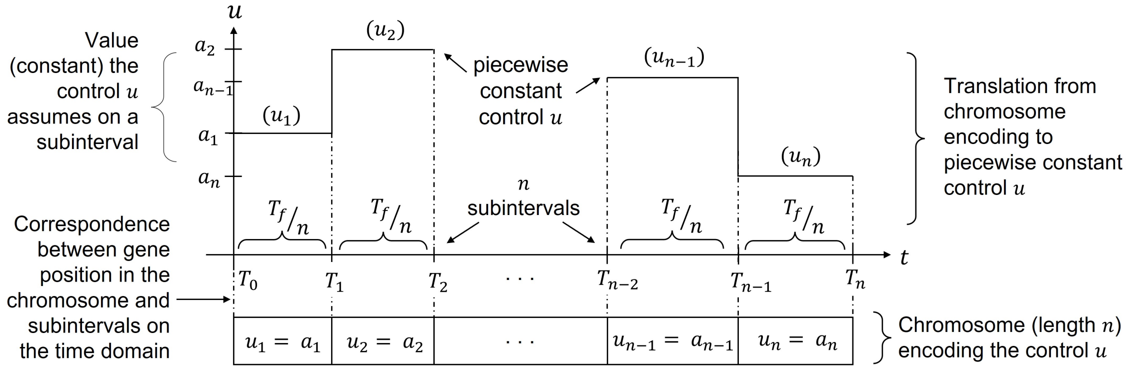

Figure 4.2: The chromosome encoding of the control(s) used in all ODE case studies

This simple implementation created a piecewise constant control, which was used for all ODE-based OCPs in the current chapter. This can reduce the accuracy of solutions, however, errors emanating from the control form can be eclipsed by the quadrature's order of error when using a fine discretisation (Schwartz, 1996). Since both high order numerical quadrature, namely R-K4, and relatively fine grids were used, the error was considered acceptable.

Although piecewise constant and piecewise linear controls are the most widely used controls (Pytlak, 1999) and are applicable to a variety of OCP formulations and solver constraints (Schwartz, 1996), the number of components used to generate the controls is not extensively dealt with in literature. In preliminary work, the chromosome length used to represent the control, u, appeared to impact the GA solution. Furthermore, several control forms were employed in the ODE case studies in the current chapter, and thus to cater for this variability, a number of different chromosome lengths were investigated.

To facilitate this, u was allowed to take on $1, 5, 25$ and 50 values respectively, denoted by u_n where $n = 1, 5, 25, 50$ corresponds to chromosome length. These lengths were chosen to divide evenly into the time intervals in both ODE-based OCPs in the current chapter, forming uniform subintervals. A maximum value of $n = 50$ was selected as increasing chromosome length beyond this point promoted suboptimality, as the capability of the GA to maintain a high level of performance was compromised by the greater complexity this incurred. This observation is in keeping with the increase in dimensionality of the search space for the GA increasing problem complexity.

4.2.3.2 Objective Evaluation

As the complement of R-K4 (Golub and Ortega, 1992), Composite Simpson's method (CS) was used to evaluate the objective functions of all ODE-based OCPs in the current study, to ensure the order of quadrature used for the objective matched that of the ODE system (Rao, 2010). Informal experimentation however, indicated that GA solutions were sensitive to the quadrature used to evaluate the fitness function (taken as the objective function). Solutions were thus also generated using a left Riemann Sum (RS) (Hughes-Hallett et al., 2013).

A RS approximates integrals by calculating the area of rectangles below a function. This allowed an exact evaluation of the objective function when used in conjunction with the GA, since the integral in the objective (Equation (4.1)) consisted solely of a piecewise constant control. Due to the pivotal nature of the objective (Section 2.2.5.2) the better accuracy of a RS in the GA, in this instance, was considered worth investigating. Furthermore, a RS was relevant in later case studies, as discussed in Section 4.3.3.2 and Section 5.4.2 respectively.

4.2.3.3 Genetic Algorithm Results

The GA was used to solve the predator-prey OCP for each combination of control form and numerical integration scheme. To adequately assess the GA's performance, the GA was run 30 times (Wang and Sobey, 2020) for each scenario considered, and the chromosome with minimum fitness across the final generations of all 30 runs was reported as the optimal solution. These results, rounded to four significant decimal places, are summarised in Table 4.2.

The FBSM-derived optimal solutions, denoted u^*_{class}, are tabulated for comparison, with optimal GA solutions denoted u^*_n, for $n = 1, 5, 25, 50$, depending on the chromosome length used. The percentage relative difference between the GA solutions and the corresponding FBSM-derived solutions, are denoted $\%\ error$. These values were calculated prior to rounding the optimal solutions. The GA solution possessing the lowest final fitness $(J(u^*))$ is given in bold, which coincided with the solution possessing the least $\%\ error$ in terms of $J(u^*)$.

Table 4.2: The GA-derived optimal solutions, as per the control form and numerical quadrature used, with the associated % *error* when compared to the FBSM-derived optimal solution.

Riemann Sum Results					
	$\mathbf{u^*_{class}}$	$\mathbf{u^*_1}$	$\mathbf{u^*_5}$	$\mathbf{u^*_{25}}$	$\mathbf{u^*_{50}}$
$\mathbf{N^*_1(5)}$	4928.1503	4928.3748	**4928.09395**	4928.1136	4927.9163
% error	0	0.004555	0.001143	0.0007444	0.004748
$\mathbf{N^*_2(5)}$	69.7182	65.9998	**69.7135**	69.6767	70.0463
% error	0	5.3335	0.006773	0.05949	0.4706
$\mathbf{J(u^*)}$	-4702.7850	-4702.5348	**-4702.7856**	-4702.7647	-4702.6527
% error	0	0.005320	**0.00001113**	0.0004316	0.002814
Composite Simpson's Results					
	$\mathbf{u^*_{class}}$	$\mathbf{u^*_1}$	$\mathbf{u^*_5}$	$\mathbf{u^*_{25}}$	$\mathbf{u^*_{50}}$
$\mathbf{N^*_1(5)}$	4928.1503	4928.3748	4928.3747	4928.2544	4928.1752
% error	0	0.004555	0.004553	0.002112	0.0005053
$\mathbf{N^*_2(5)}$	69.7182	65.9998	66.0004	66.5136	66.9315
% error	0	5.3335	5.3326	4.5965	3.9971
$\mathbf{J(u^*)}$	-4661.1725	-4662.3749	-4662.3747	-4662.1257	-4661.9445
% error	0	0.02586	0.02579	0.02045	0.01656

Overall, the GA-produced solutions corresponded closely to what was obtained using the FBSM, as can be seen by the often negligibly small error percentages. All of the GA solutions were produced in under 16 seconds; the GA taking approximately 16 times longer than the FBSM to find an optimal solution. Especially accurate solutions were obtained when using a RS to evaluate the objective in conjunction with u^*_5 or u^*_{25}, respectively. The former resembled the FBSM's objective value best (smallest % *error*), and the latter, the FBSM's optimal control best (Figure 4.4). These represented the best solutions of all that were produced when varying chromosome length (control form) and the numerical quadrature (used to evaluate the objective). These solutions are given in Figures 4.3 and 4.4 respectively.

Regardless of the numerical scheme used, the control form u_1 had the highest percentage error in the vast majority of cases. This was expected since a single-valued control is an elementary control form that cannot reasonably replicate the function produced by the FBSM. An increase in the chromosome length to $n = 5$ improved the accuracy of the GA's results across both quadrature methods. From this point onwards, the trends observed using the RS

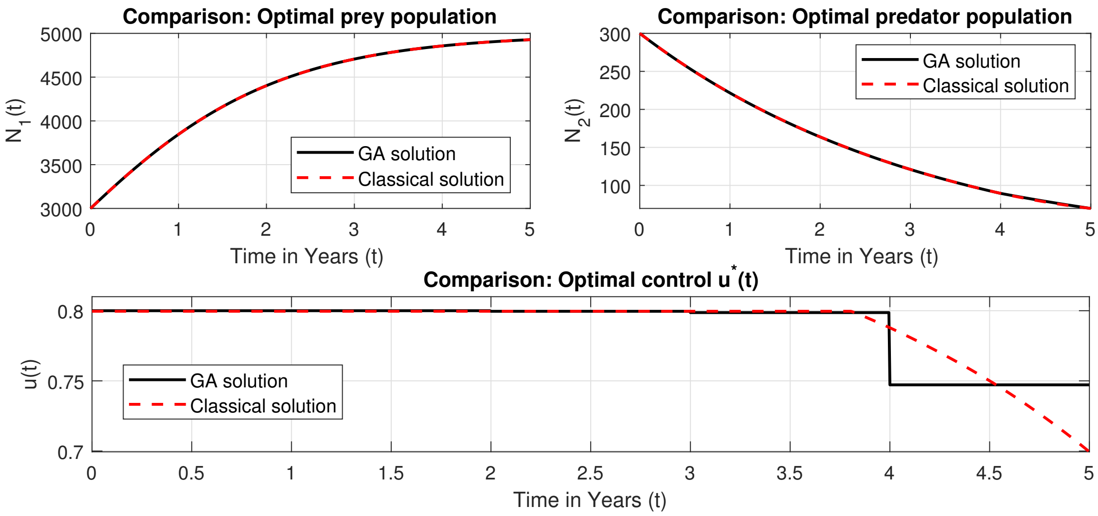

Figure 4.3: The GA-derived optimal solution to the predator-prey OCP for the optimal control u_5^* with a RS evaluation of the fitness function

and CS methods began to differ, with the RS experiencing a slight decrease in accuracy and the CS an increase, as the number of values u could assume increased. These will therefore be dealt with separately, starting with the RS case, followed by the CS.

The GA solution found using a RS and u_5^* (Figure 4.3) was distinctly better than other solutions, with negligibly, and consistently, small errors across all 30 runs of the GA. Statistics to this effect are given in Appendix A. It could also be seen that the control was beginning to mimic the form of the FBSM control, with a reduction in the harvesting rate at $t = 4$ years. An increase in the chromosome length to $n = 25$ saw a slight decrease in the accuracy of the final predator population and objective value, but an increase in accuracy of the final prey population. The control (Figure 4.4) appeared to benefit from the greater freedom and flexibility of choice an increased chromosome length allowed, resulting in it distinctly emulating the form of the FBSM's optimal control. Precision decreased once again between u_{25} and u_{50}, both in terms of final solution values and in the replicating of the FBSM control.

When using CS, the accuracy of solutions improved with increasing chromosome length, as can be seen in Table 4.2. However, the optimal control produced in each of these instances did not resemble u_{class}^*, remaining near u_{max} (maximum rate of control) throughout the time period. The repercussions of this can be seen in the reduced final predator population (N_2). There was no tapering of the harvesting rate as time increased, and no consistent control form found between GA runs. Increasing chromosome length appears to gradually remedy this, but the dissimilarity between the GA control and the FBSM control remained. The error

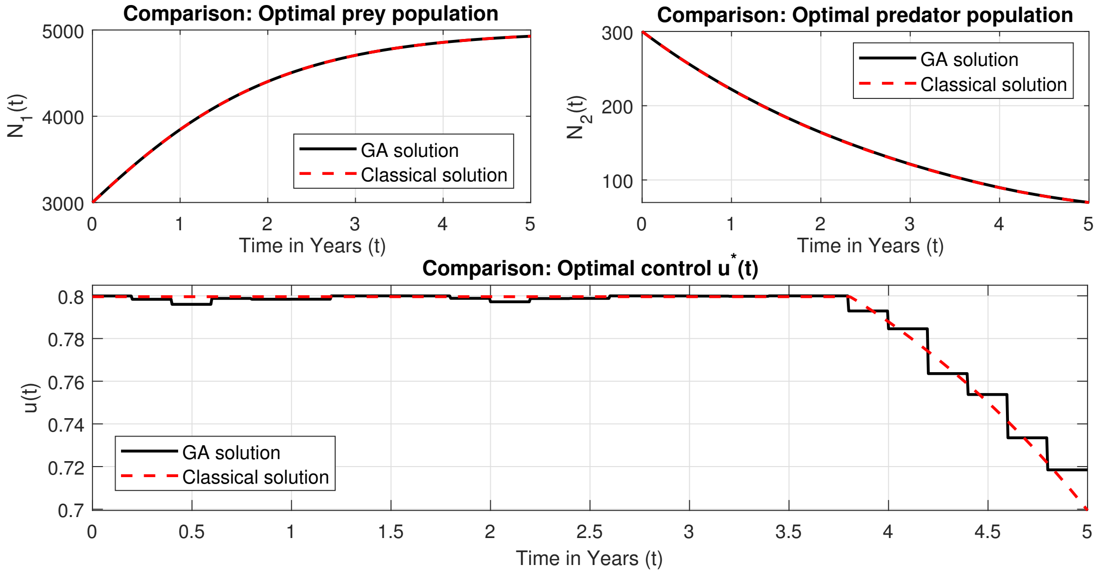

Figure 4.4: The GA-derived optimal solution to the predator-prey OCP for the optimal control u^*_{25} with a RS evaluation of the fitness function

when approximating the objective was consistently small however, regardless of the control not resembling the FBSM's control. Statistics to this effect are given in Appendix A.

Since the quadrature used deals solely with the control in this OCP, a clear correspondence between the number of values the control may assume over the time period and the accuracy of the corresponding solution is expected. However, where the CS-derived solutions experienced a pattern of improving accuracy as chromosome length increased, RS solutions saw the opposite occurring from $n = 5$ onward. It is postulated that this observation may be related to the associated methods' stability and error traits, and possible interaction thereof with technicalities within the GA, arising as a consequence of the increase in problem complexity with increasing chromosome length. It was suspected that default MATLAB parameters may need to be altered to address this, however, further investigation is deferred to future work.

4.2.4 Discussion

The GA generated optimal solutions almost identical to that of the FBSM in the predator-prey OCP, demonstrating that a GA is capable of adequately replicating classic OC results. Moreover, since a GA approach does not make use of PMP and hence the Euler-Lagrange equations, the system of equations requiring solving was substantially reduced in size. This property may become increasingly advantageous as system size increases. Furthermore, GA usage alleviates a significant amount of mathematical complexity, as the GA requires only the relevant dynamical system and some criteria by which to determine an optimum.

An assortment of chromosome lengths were utilised in determining an optimal harvesting strategy, namely $n = 1, 5, 25$ and 50. Of all the solutions produced by the GA, those found using a RS were markedly better than those produced using CS. In this particular instance, the RS calculates an exact value for the integral using a piecewise constant control in the GA. It is proposed that this is the reason for the associated more accurate results.

The quadrature used to approximate the objective played a role in solution quality, with the GA-produced control appearing sensitive to the accuracy of schemes used to determine an objective value, from which the fitness function is directly composed. Unlike the optimal control, the approximation of the objective function value was relatively unaffected by the quadrature used in the GA. The seeming dependence of the optimal control on the accuracy of numerical quadrature used to evaluate the objective is not apparent when using the FBSM.

These observations may be as a result of the order of operations differing in the respective solution approaches. In the FBSM, the objective is only evaluated once an optimal solution has been found. Consequently, the quadrature used to evaluate the objective function cannot affect the optimal control and thus the optimal solution. In contrast, the GA relies on an approximate objective value as the fitness function to generate an optimal control. Therefore, the quadrature used to determine the objective value, which is composed of the control, directly informs the GA as to which control is optimal, based on its associated fitness.

Regardless of the influence of these factors on GA performance, since one is not able to harvest continuously in practice, both classical and GA control values would be rounded and discretised when translated in reality. The GA control would therefore suffice in place of the classical, and the error observed in the GA solution would become negligible. Should a GA be applied to a problem wherein a classical solution is not readily available for comparative purposes, experimentation with the number of values the control may assume and the numerical quadrature may aid in finding a sufficient optimal solution. As can be seen in Appendix A, the user can however be reassured by the consistently good GA results.

Higher degree piecewise polynomial controls were briefly investigated in preliminary work, using built-in interpolation in MATLAB, however this resulted in the controls breaking the bounds imposed on them. Linear interpolation or a line of best fit could potentially improve solution accuracy but was not imposed in the current work, and is thus deferred to future work. An adaptive step size for the control may also act to further improve results.

The ability of a GA to achieve OC results with a degree of exactness comparable to the FBSM when applied to a simple ODE-based OCP was demonstrated in this case study. To determine whether a GA is capable of producing equally reliable results when applied to a larger system of ODEs, with the added complexity of non-convexity in one of the controls, a well-documented, dengue OCP in current literature was next investigated. The flexibility and adaptability of a GA approach was tested to see whether it could circumvent the difficulties presented by the violation of a critical assumption of classic OC methods, namely convexity.

4.3 Dengue Model

Contracting dengue is a risk borne by approximately 50% of the world's population (Schreppel and Chudej, 2018), its escalating human and economic cost establishing the infectious disease as one of the most pressing in the world today (Carvalho, da Silva and da Cunha Charret, 2019). Currently, no cure exists to combat the mosquito-borne virus, and with vaccine development still under way, methods to infer the effect of control mechanisms on the dynamics of the disease become imperative (Carvalho et al., 2019).

A wide variety of mathematical research concerned with this issue has considered potential vaccination and control strategies (Carvalho et al., 2019). One particular model, given in Equation set (4.4) of Section 4.3.1, has been used as a basis for multiple studies (e.g. Rodrigues et al., 2013, 2014; Schreppel and Chudej, 2018). Originally examined by Rodrigues et al. (2013), and subsequently by Schreppel and Chudej (2018), both studies relied on the direct methods to solve the dengue OCP. As per the nature of the current study, this model was selected as most appropriate due to the comparative capacity it presented.

Since researchers tend to favour direct methods (Biral et al., 2016), comparing a GA to two widely used direct OC methods is arguably worthwhile. Furthermore, related work by the authors from which the OCP was extracted (Rodrigues et al., 2014) provided valuable context with which to view GA results. In the related work, a variant of the dengue model used in the current study, which considered immunisation by a vaccine with waning immunity as the only control, was solved for comparative purposes using both the indirect FBSM and the direct DOT_{CVP} software (Rodrigues et al., 2014). The objective values produced by these separate methods corresponded with reasonable precision to each other, with the direct software overestimating the objective value by approximately 24%.

By eliminating the controls (setting equal to zero) in the vaccine variant of the OCP (Rodrigues et al., 2014) and in the current OCP (Equation set (4.4)), identical systems of equations are obtained. Due to the similarity of the current OCP and the vaccine variant thereof, it is proposed that the relationship between the direct and indirect methods' results may be extended to the current study and used in evaluating the performance of the GA in the comparison conducted herein. The related vaccine model (Rodrigues et al., 2014) may thus provide a link between the successful outcome in the predator-prey OCP (Section 4.2.3), when comparing a GA to the FBSM, and an extension of the comparison to direct methods.

The variability of results reported using existing classic techniques should arguably be factored in when ascertaining the accuracy of a GA approach. This benchmark variation, along with results seen in Section 4.2, could then potentially aid in generalising the capability of a GA to replicate classic OC solutions, should reasonable correspondence between solutions obtained using a GA (Section 4.3.3) and that of the direct results (Section 4.3.2) be seen. The OCP formulation of the dengue model is now given.

4.3.1 Optimal Control Problem

Dengue exhibits unusual behaviour in its transmission mechanism, with both humans and mosquitoes acting as infectious agents (Carvalho et al., 2019). A susceptible human (S_h) can become infected through the bite of an infectious female *Aedes aegypti* mosquito (I_m) and similarly infectious humans (I_h) can transmit the virus to susceptible mosquitoes (S_m). Only humans can recover (Carvalho et al., 2019). Thus, six mutually exclusive compartments were used to describe the propagation of the disease in a SIR-ASI model by Rodrigues et al. (2013), with humans, denoted by the subscript h, separated into S_h, I_h and Recovered (R_h) classes, and mosquitoes assigned to the Aquatic Phase (A_m), comprised of mosquitoes in the egg, larva and pupa life stages, S_m or I_m classes, with subscript m denoting a mosquito host.

Three control strategies were considered to combat the vector-borne virus in the various stages. Adulticides (c_m) were used to target the S_m and I_m classes and a combination of larvicides (c_A) and mechanical control (α) used on the A_m phase. Complications arise with the use of the mechanical control, due to the non-convexity it introduces into the OCP. The repercussion thereof is that only a suboptimal extremal solution was found for the associated control (Schreppel and Chudej, 2018). Descriptions of the parameters used in the dengue OCP, given in Equation set (4.4), and their accompanying values are given in Table 4.3.

Table 4.3: Parameter descriptions, units and assigned values, adapted from Rodrigues et al. (2013) and Schreppel and Chudej (2018).

Symbol	**Description**	**Units**	**Value**
$S_h(0)$	Number of initial susceptible humans	-	479990
$I_h(0)$	Number of initial infected humans	-	10
$R_h(0)$	Number of initial recovered humans	-	0
$A_m(0)$	Initial number of aquatic phase mosquitoes	-	1440000
$S_m(0)$	Initial number of susceptible mosquitoes	-	1440000
$I_m(0)$	Initial number of infected mosquitoes	-	0
N_h	Total human population	-	480000
$1/\mu_h$	Average lifespan of humans	Days	75×365
β_{hm}	Disease transmission probability: I_h to mosquitoes	Per bite	0.375
β_{mh}	Disease transmission probability: I_m to humans	Per bite	0.375
B	Average number of bites by a mosquito	Per day	0.8
$1/\eta_h$	Duration of infection	Days	3
$1/\mu_m$	Average lifespan of adult mosquito	Days	10
μ_A	Natural mortality of larvae	Per day	0.25
η_A	Mosquito larvae to adult maturation rate	Per day	0.08
ρ	Number of eggs at each deposit per mosquito	Per day	6
m	Number of female mosquitoes per human	Per human	3
k	Total number of larvae per human	Per human	3
γ	Normalised weight related to the cost associated with application of a control measure	-	0.25
c_m	Proportion of adulticides applied	-	$0 \leq c_m \leq 1$
c_A	Proportion of larvicides applied	-	$0 \leq c_A \leq 1$
α	Proportion of mechanical control applied	-	$0.001 \leq \alpha \leq 1$

Using the transformations specified by Schreppel and Chudej (2018), namely

$$s_h = \frac{S_h}{N_h},\ i_h = \frac{I_h}{N_h},\ r_h = \frac{R_h}{N_h},\ a_m = \frac{A_m}{kN_h},\ s_m = \frac{S_m}{mN_h} \text{ and } i_m = \frac{I_m}{mN_h},$$

where $N_h = S_h + I_h + R_h$ is assumed constant, the system of Rodrigues et al. (2013) was normalised in the current study, and is given by Equation set (4.4). The environmental and economic costs associated with applying the controls were taken into account by weighting the factors optimised in the objective function with weight γ. Only equal weights were formally considered by both Rodrigues et al. (2013) and Schreppel and Chudej (2018), and were thus used in the current study. Once again, dependence on time is omitted for ease of notation. The OCP can then be stated as:

$$\text{minimise } J(c_A, c_m, \alpha) = \int_0^{T_f} \left(\gamma i_h^2 + \gamma c_m^2 + \gamma c_A^2 + \gamma (1-\alpha)^2\right) dt \tag{4.3}$$

subject to:

$$\begin{aligned}
\frac{ds_h}{dt} &= \mu_h - (B\beta_{mh} i_m m + \mu_h) s_h, \\
\frac{di_h}{dt} &= B\beta_{mh} m i_m s_h - (\eta_h + \mu_h) i_h, \\
\frac{dr_h}{dt} &= \eta_h i_h - \mu_h r_h, \\
\frac{da_m}{dt} &= \rho \frac{m}{k} \left(1 - \frac{a_m}{\alpha}\right) (s_m + i_m) - a_m (\eta_A + \mu_A + c_A), \\
\frac{ds_m}{dt} &= \frac{k}{m} \eta_A a_m - s_m (B\beta_{hm} i_h + \mu_m + c_m), \\
\frac{di_m}{dt} &= B\beta_{hm} i_h s_m - (\mu_m + c_m) i_m,
\end{aligned} \tag{4.4}$$

with $0 \leq c_m \leq 1$, $0 \leq c_A \leq 1$, $0 < \alpha_{min} = 0.001 \leq \alpha \leq 1$ and normalised initial conditions $s_h(0) = 0.9999$ [2], $i_h(0) = 0.0001$, $r_h(0) = 0$, $a_m(0) = 1$, $s_m(0) = 1$ and $i_m(0) = 0$.

4.3.2 Classic Optimal Control Approach and Results in Literature

The dengue OCP was transcribed using direct methodology into a non-linear programming problem (NLP) and DOT_{CVP} and *IPOPT* software used to obtain optimal results by Rodrigues et al. (2013) and Schreppel and Chudej (2018) respectively. Despite both pursuing a direct approach, different objective function values and peak proportions of I_h (denoted i_h in the current study) were obtained in these two separate studies.

The approach of each of these authors is presented in Sections 4.3.2.1 and 4.3.2.2 respectively, followed by a commentary on the methods employed and the potential effect on the results, as per literature regarding these factors. This critique will serve as a basis to substantiate the arguments put forward for use of particular methods in the GA approach that differ from those of Schreppel and Chudej (2018) and Rodrigues et al. (2013).

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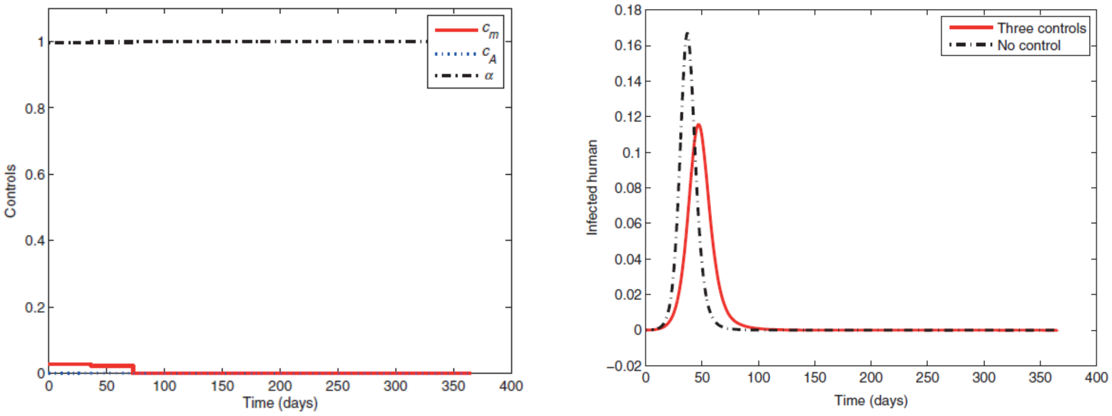
[2] The current author obtained $s_h(0) = 0.999979$, but for consistency with the previous authors, truncated this value to correspond to that used by Rodrigues et al. (2013) and Schreppel and Chudej (2018).

4.3.2.1 DOT_{CVP} Method

Rodrigues et al. (2013) used DOT_{CVP} software to solve the OCP, neglecting to mention software inputs such as step sizes or the methods used in producing the solution. An objective function value of 0.06691425 was obtained, with the optimal controls and resulting proportion of I_h due to normalisation (i_h), as found by Rodrigues et al. (2013), given in Figure 4.5.



(a) Optimal controls

(b) Proportion of I_h

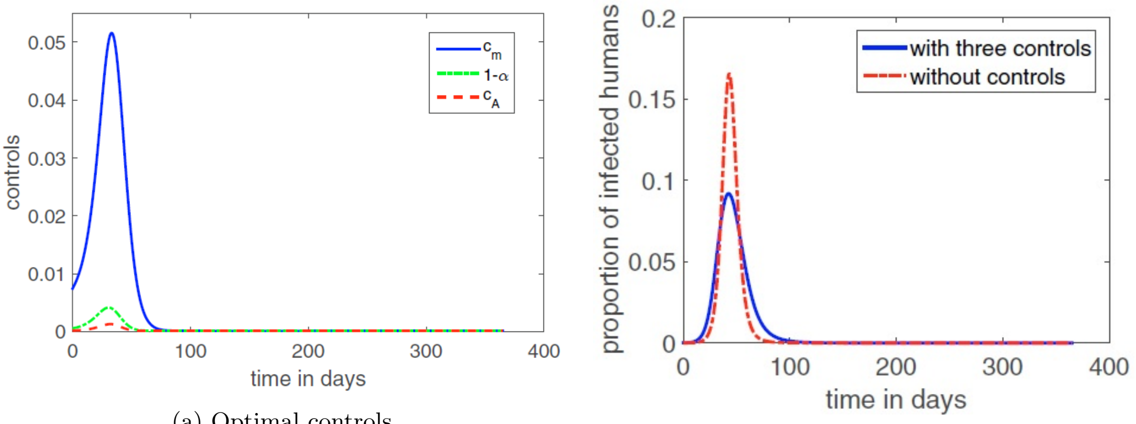
Figure 4.5: The optimal DOT_{CVP} solution to the dengue OCP. Copyright ©2013 Taylor & Francis. Reprinted with permission from original publication: "Bioeconomic perspectives to an optimal control dengue model" by H. S. Rodrigues, M. T. T. Monteiro and D. F. M. Torres. (2013). *International Journal of Computer Mathematics* **90**(10): 2126-2136

Since it is unclear which settings were used to produce the results of Rodrigues et al. (2013), those of Schreppel and Chudej (2018) will be used in the discussions following and in conducting comparisons with a GA. DOT_{CVP} and GA solutions will, however, be compared.

4.3.2.2 *IPOPT* Solver

Schreppel and Chudej (2018) used the interior-point solver *IPOPT* (Wächter and Biegler, 2006) to solve the dengue OCP, requiring discretisation of both the states and controls. A uniform mesh was used with a constant time step of $h = 0.365$ days. The Implicit Euler method ($O(h)$ accuracy) was used to approximate a solution to the dynamical system, and the rectangular method used to approximate the objective, resulting in an objective value of 0.0592. This was contrasted to the value of 0.0669 acquired by Rodrigues et al. (2013). The optimal controls and the resulting proportions of I_h obtained are given in Figure 4.6.

The non-convexity present in the use of the mechanical control α was addressed in the



(a) Optimal controls

(b) Proportion of I_h

Figure 4.6: The optimal *IPOPT* solution to the dengue OCP. Copyright ©2018 International Federation of Automatic Control (IFAC). Reprinted with permission from original publication: "Numerical optimal control applied to an epidemiological model", by C. Schreppel and K. Chudej. (2018). *IFAC-PapersOnLine* **51**(2): 1-6

work by Schreppel and Chudej (2018), as per recommendations to exercise caution when transcribing an OCP displaying non-convexity in the controls (Vanderbei, 2001). To determine the influence the non-convexity had on the solutions, an *a posteriori* analysis using the necessary conditions of PMP was conducted, following the approach of Dussault (2014), in order to analyse the optimality of the solutions. These considerations were not taken into account by Rodrigues et al. (2013).

Analysis of the controls using the necessary conditions of PMP found that both c_m^* and c_A^* coincided with their analytical counterparts. No analytical solution could be found for α^*, however, as irregularity in the Hamiltonian and violation of the necessary conditions led to contradictory behaviour when using the solver. Thus, α^* was considered suboptimal.

Schreppel and Chudej (2018) also noted in passing that inconsistent discretisation[3] may exist between the respective studies, however the possible effect that this and the low accuracy methods employed had on the veracity of the solutions, was not covered. Similarly, no reference to the error control related to the numerical approximations used was made; a key consideration of solver use (Schwartz, 1996).

Although it would appear that the reduced objective value achieved by Schreppel and Chudej (2018) constitutes a better solution than that obtained by Rodrigues et al. (2013), care must be taken before making this inference, as it is dependent on the accuracy of the

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[3] Schreppel and Chudej (2018) appear to describe what is termed numerical integration in the current study as **discretisation**.

numerical schemes used (Frego, 2014; Nezhadhosein et al., 2015). The Implicit Euler method ($O(h)$) provides a crude approximate solution to a system of ODEs (Burden and Faires, 2011), and may bear responsibility for the lower peak of i_h in Figure 4.6b compared to Figure 4.5b. Similarly, the rectangular method ($O(h)$) conducts a single function evaluation over the interval of interest, giving an equally rudimentary estimate of an integral (Stengel, 1994).

The comparatively better *IPOPT* results should therefore be regarded cautiously, as they may be attributed to the use of methods with lesser orders of accuracy. There is, however, ambiguity in the terminology used. Numerical integration of an ODE system and the objective typically have matching orders of error (Rao, 2010). To ensure that the magnitude of $O(h)$ was consistent for the approximate solutions to the objective and the ODE system, it is thus probable that a composite approach to applying the rectangular method was used, which would resemble a RS[4]. An equivalent discretisation of $h = 0.365$ days would then be used for the objective and ODEs, rather than using $h = 365$ days to evaluate the objective.

4.3.2.3 Discussion of Direct Results

Considerably different optimal solutions to the dengue OCP were reported by the two solvers employed. Since both solvers employed a direct approach, these discrepancies could arguably be attributed to numerical implementation (Dal Bianco et al., 2019). Amongst other factors, such as control form, it is thus important that the precision of the numerical schemes be examined in conjunction with an evaluation of the numerical results (Ratković, 2016).

Limited information regarding the control formulation was provided. In Figure 4.5a, it appears that each control assumes only a few distinct values, in keeping with the piecewise constant controls typical of DOT_{CVP} software (Rodrigues et al., 2014). In contrast, smooth control functions were obtained by Schreppel and Chudej (2018), seen in Figure 4.6a. These differences may have been influential in producing the different optimal solutions found.

Values assigned to objective functions by various solvers have been found to underestimate their true value, in analyses done of the respective solver performances against benchmark problems in literature (Frego, 2014). Integration techniques of order greater than two may rectify this and, in the absence of an analytical solution with which to make a comparison,

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[4] Similar notation used by Dussault (2014) seems to suggest that the discretisation is performed on a subinterval of the domain. Mention of the objective being composed of the sum of discretised pieces further substantiates this conclusion.

a detailed analysis is recommended to ascertain whether optimality has been achieved (Dussault, 2014). In light of this, related work was referred to in order to obtain context when interpreting results found by Rodrigues et al. (2013) and Schreppel and Chudej (2018).

Whilst information regarding the numerical schemes was not provided by Rodrigues et al. (2013) concerning the solution produced, earlier work by the same authors (Rodrigues et al., 2009, 2010) concluded that there was no advantage in using more accurate numerical integration methods, nor in increasing the discretisation resolution. This argument was reiterated by Vanderbei (2001), an influential source in the work of Schreppel and Chudej (2018).

An opposing view is held by the author of the current study, who assumes the position that the quality of the solution produced should be a key factor in any such comparison. The Implicit Euler method is an elementary technique used for illustrative purposes with insufficient accuracy to warrant its use in practice (Burden and Faires, 2011). Use thereof may have therefore had an adverse effect on the accuracy of the results obtained.

Software such as *IPOPT* is able to locate local optima of OCPs, but in the presence of issues like non-convexity, the stationary point to which the algorithm converges is dependent on factors like initialisation and method choice (Wächter, 2009). Moreover, the use of first-order methods in OCPs can be unsuccessful (Polak, 1993). Where indirect methods may even admit analytical solutions and achieve global optimality, direct methods, although powerful, are in a sense a substitute, producing less accurate (Subchan and Żbikowski, 2009), suboptimal solutions (Frego, 2014). Where possible, the loss in degree of optimality by transcription using the direct method should not be further exacerbated by use of low order accuracy numerical methods, which act to compound the error introduced by using simplistic approximations.

The R-K4 strikes an acceptable balance between precision and computational intensity (Stengel, 1994), only requiring a step size four times that of Euler's Method, with the same number of evaluations, to produce superior results (Burden and Faires, 2011). In addition, decreasing step size ($h \to 0$) facilitates a rapid decline in error, with the associated local truncation error reducing drastically ($O(h^4)$) as opposed to the Euler Method ($O(h)$) (Burden and Faires, 2011). A finer discretisation would however increase the dimension of the system being solved. These factors were taken into consideration when pursuing the GA approach.

The direct approach, pursued by Rodrigues et al. (2013) and Schreppel and Chudej (2018), utilises optimisation to obtain a solution to an OCP (Section 2.2.3.3). Extensive comparisons between EAs and classical optimisation techniques have found that whilst the latter may outperform the former under specific mathematically advantageous formulations, the reverse may occur when typical assumptions are broken (Engelbrecht, 2007). Since convexity is a critical requirement of classic OC approaches, the indifference of the GA to this condition further advocates its potential in OC, should sufficiently accurate results be obtained.

4.3.3 Genetic Algorithm Application and Results

As per the literature reviewed and the preceding discussion, only the R-K4 was considered in compiling results using the GA, the chief motivation being the superior accuracy of the method in comparison to the alternative schemes already used in solving the dengue OCP. The sustained consistency and global truncation errors thereof when applied in OC, also serves to justify its use (Schwartz, 1996). A discretisation step size of $h = 0.365$ days was again employed in all numerical methods and as before, the default GA parameter values in MATLAB (2018) were used (Section 3.4.2). Once again, the objective function of the OCP (Equation (4.3)) was used as the fitness function in the GA.

4.3.3.1 Encoding the Control in a Chromosome

As per Figure 4.2, the controls c_A, c_m and α, were generated by uniformly subdividing the time interval and allocating a constant value to each control on each of the resulting equally spaced subintervals, forming piecewise constant controls. Acknowledging the possibility that the number of values encoded in the control may be a problem-specific consideration, to maintain consistency throughout the entirety of this chapter, identical control lengths to the predator-prey OCP were considered. The controls were all encoded in a single chromosome of length $3n$, where $n = 1, 5, 25, 50$, denotes the number of values generated for each control.

4.3.3.2 Objective Evaluation

To maintain the order of error incurred in producing a solution, CS was used to evaluate the objective. Although a RS does not provide an exact evaluation in this instance (as the integral does not consist solely of a piecewise constant function), use thereof was still considered worthwhile since it would strongly resemble the composite application of the rectangular method previously suspected (Section 4.3.2.2). This helped preserve consistency between the

ODE case studies in the current chapter, and with the solution of Schreppel and Chudej (2018). As before, results were therefore generated using both of these quadrature schemes.

4.3.3.3 Genetic Algorithm Results

The GA was used to solve the OCP for each of the control forms and quadrature schemes considered. The resulting objective values obtained for the optimal controls, denoted $J(c_A^*, c_m^*, \alpha^*)$, are tabulated in Table 4.4, rounded to four significant decimal places. The GA was run 30 times for each combination, and the solution with the minimum fitness overall, in each case, was reported. The percentage relative difference between the GA and direct methods' results are given according to the software used as % *DOT*$_{CVP}$ and % *IPOPT* respectively. Statistics regarding the GA performance across all 30 runs are given in Appendix A.

Table 4.4: The GA-derived optimal objective values, as per the numerical quadrature and chromosome length n used.

Riemann Sum Results			
n	$\mathbf{J(c_A^*, c_m^*, \alpha^*)}$	**% DOT$_{\mathbf{CVP}}$**	**% IPOPT**
1	0.07894	17.9784	33.3520
5	**0.06697**	**0.08199**	13.1235
25	0.06049	9.6028	2.1767
50	0.06087	9.03228	2.8216

Composite Simpson's Results			
n	$\mathbf{J(c_A^*, c_m^*, \alpha^*)}$	**% DOT$_{\mathbf{CVP}}$**	**% IPOPT**
1	0.07902	18.0964	33.4854
5	0.06702	0.1508	13.2013
25	**0.06046**	9.6441	**2.1301**
50	0.06075	9.2156	2.6144

Unlike the predator-prey OCP, minor differences were seen between results acquired using CS and RS in the dengue OCP. Both were seen to consistently produce optimal controls resembling those found using the direct methods. In particular, a chromosome length of 15, corresponding to five piecewise constant components in each control ($n = 5$), emulated the *DOT*$_{CVP}$ solution superbly. This solution is bolded in Table 4.4 and given in Figure 4.7.

In this GA solution, the peak of i_h^* was almost identical to that of the *DOT*$_{CVP}$ software (Figure 4.5b), occurring at approximately 50 days in both solution approaches. Likewise, the

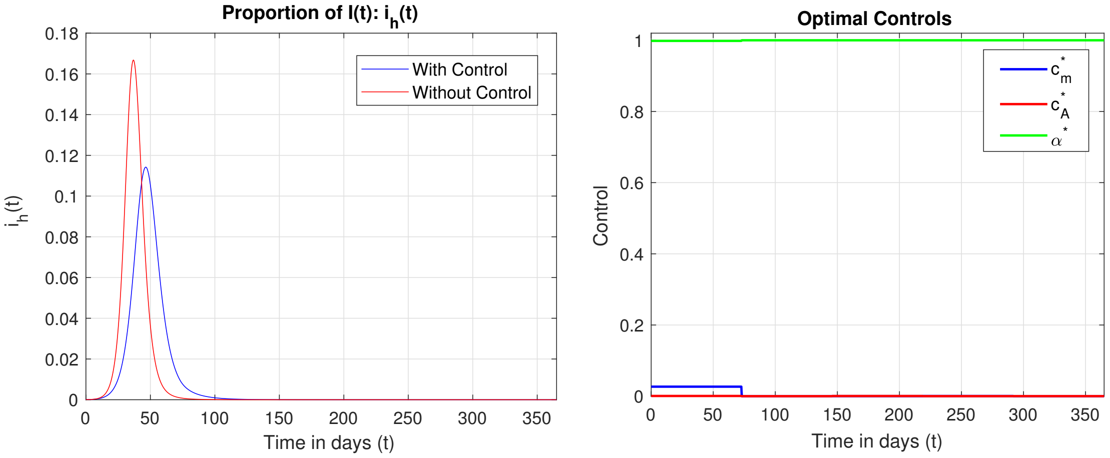

Figure 4.7: The GA-derived optimal solution to the dengue OCP, corresponding to the solution given for $n = 5$ and a RS evaluation of the fitness function in Table 4.4

optimal controls appeared very similar, with c_m^* clearly decreasing to zero at approximately 75 days in both solutions. Inspection of the graph produced using DOT_{CVP} software in Figure 4.5, leads to the assumption that approximately three distinct values were adopted when constructing the piecewise constant control that was produced. The similarity between the DOT_{CVP} optimal control and that of the five-valued piecewise constant control in the GA approach may have been instrumental in obtaining extremely similar results.

In a similar manner, the controls produced using $n = 25$ components in the GA corresponded well to the *IPOPT* software solution. This result, bolded in Table 4.4, is shown in Figure 4.8, where $1 - \alpha^*$ is plotted for consistency with the *IPOPT* solution, in order to more easily compare the results. Once again, the peak i_h^* found using the GA closely resembled the peak of approximately 0.09 found using *IPOPT* software (Figure 4.6), however, in this instance, the GA solution reached this peak slightly later than the direct method's solution. The maximum values reached by each of the controls using the GA also replicated that of the direct method well, however beyond 100 days, the direct-produced controls tapered off to zero whilst the GA controls oscillated in the interval $[0, 0.004]$. Differences in graph scale and the non-smoothness of the GA controls, complicated a thorough comparison, but a clear resemblance between the *IPOPT* solution and that of the GA can be observed.

Fairly inaccurate results were obtained when using only a single value for each control, but as in the predator-prey case study, this can be justified as too simplistic a control form, and not a fault of the GA performance. Increasing the number of components in each control from $n = 1$ to $n = 5$, decreased the error of the GA in replicating both of the direct methods'

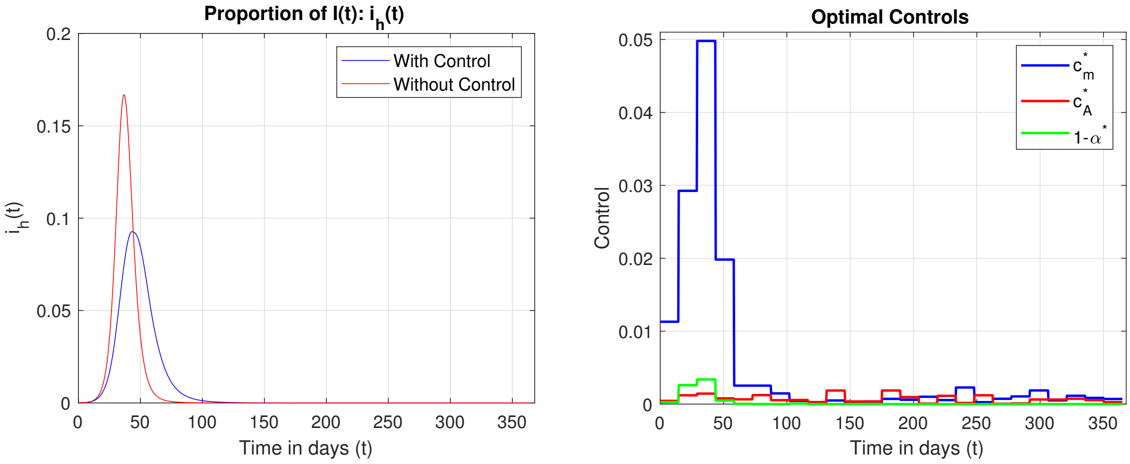

Figure 4.8: The GA-derived optimal solution to the dengue OCP, corresponding to the solution given for $n = 25$ and a CS evaluation of the fitness function in Table 4.4

results. This was anticipated, as the controls produced in the direct approaches assumed more than one value, and thus in order to replicate these results, the GA too should be allowed to select more than one value for each control.

A subsequent increase from $n = 5$ to $n = 25$ resulted in increased error when comparing the GA to the DOT_{CVP} software and a decreased error when comparing the GA to *IPOPT* software. This may be explained by the number of components of each control far exceeding that employed by the DOT_{CVP} software. Thus, the more dissimilar the controls became, the more the GA results diverged from those of the DOT_{CVP} software. This may too explain the resulting decrease in error between the GA and *IPOPT* software, since increasing the number of components in the GA controls, enabled the form of the GA-generated control to better mimic the continuous form of the *IPOPT* software (Figure 4.6).

As the chromosome length was increased, the form of the controls generated using the GA increasingly resembled the form produced using *IPOPT* rather than DOT_{CVP}. Simultaneously, the peak proportion of I_h was reduced, analogously to the progression of the solution from Rodrigues et al. (2013) to the re-solving by Schreppel and Chudej (2018). This reiterates the extent of the influence changes in implementation can exert on an OCP. The diminished proportion I_h (i_h) may have contributed to decreasing the value of the objective observed in the decreased error seen for DOT_{CVP} between $n = 25$ and $n = 50$ in Table 4.4.

The GA-produced controls began displaying erratic behaviour at $n = 50$, with pronounced oscillatory behaviour occurring from $t = 100$ days onwards. This could explain the increased error between the smooth optimal controls of the *IPOPT* software and the noisy characteristics of the GA controls from $n = 25$ to $n = 50$. As in the predator-prey OCP, the complexity induced by longer chromosome lengths in the GA appeared to concurrently reduce the accuracy of the algorithm compared to classic OC schemes, although this was less pronounced in the dengue OCP. Implementing an adaptive step size in the GA controls may remedy the behaviour observed, as larger step sizes could be used in areas of inactivity to dampen the oscillations. This oscillatory behaviour is, however, not unique to a GA approach and is quite commonly observed in classical approaches (Section 2.2.5.5). It may therefore have presented in the GA solution as a result of the higher-order numerical methods used (Vanderbei, 2001).

4.3.4 Discussion

The GA was able to adequately reproduce both results obtained using direct methods for the dengue OCP. Discounting the instance wherein only a single value was used for each control, the GA solutions differed by approximately half the amount that was observed between indirect and direct implementations in a related dengue OCP by Rodrigues et al. (2014). The error of the GA results was thus taken as falling within an acceptable range for the OCP.

Previously, caution was advised, as per the literature, on the dependence of results on the numerical scheme employed. This was emphasised by the discrepancies in the solutions produced by the respective solvers, both of which adhered to a conventional direct approach. In this case study however, the GA was shown to be capable of reproducing both of the classically-obtained solutions to a sufficient accuracy.

Differences in objective values could not concretely be attributed to numerical methods or variations in control form, and were likely a combination of both factors. The low order integration methods used by Schreppel and Chudej (2018) (Section 4.3.2.2) could reasonably have underestimated the true objective value, as could the oscillating behaviour of the GA controls have contributed towards overestimating the objective. However, since only negligible differences were seen between applications of CS and RS, it is probable that the form of the control contributed more weightily to the different objective function values obtained.

Changing the control configuration in the GA had a definitive effect on the solution produced, altering both the proportion of infected humans and the optimal controls. It could, however, be argued that the form of control chosen for the GA and the numerical quadrature employed had no more impact on the performance of the GA in producing optimal results than it had on existing classic OC methods. Moreover, all variation in classical results could be generated using a single GA, by altering only the chromosome length used.

As before, the theoretical complexity which encumbers the direct approach was absent when applying a GA. Furthermore, transformation to a NLP and the associated proof of equivalence to the original OCP (Ratković, 2016) was avoided when using a GA, as were the addition of Karush-Kuhn-Tucker conditions. This significantly decreases the number of equations in the system requiring solving. It would thus seem reasonable to conclude that the GA was adept at yielding solutions equivalent to those of the direct methods and possibly reducing complexity associated with finding an optimal solution to the dengue OCP.

4.4 Concluding Remarks

In support of the primary aim of the study (Section 1.3), two ODE-based OCPs were investigated using a GA approach in a comparative capacity with classic OC methods. Models of increasing complexity were chosen to showcase GA performance under varying circumstances. Comparing the effectiveness of a GA approach to classic OC techniques when solving OCPs led to a number of interesting observations in line with the objectives of the study.

Importantly, GA-produced solutions were on par with both the global optimum guaranteeing FBSM and the widely applied, powerful software available for the direct methods. This reinforced the proposition that GAs are capable of adequately replicating classic OC results. Additionally, the fulfilling of mathematical conditions associated with classic OC methods, and the subsequent impact on the solution procedure, was avoided. This included the deriving and solving of the Euler-Lagrange equations when using PMP, and the Karush-Kuhn-Tucker conditions associated with direct methods. This simultaneously bypassed the theoretical background needed to employ these methods and substantially reduced the size of the system of equations requiring solving, to approximately half that of classic OC methods.

The dimensionality of the system solved is a critical factor in many classical solution procedures, with accuracy often the first casualty as higher order methods are forfeited to enable computation in a reasonable amount of time for large systems. Since the GA utilises a considerably smaller system, it may be possible to use numerical methods of better accuracy when employing a GA approach compared to a classical approach.

The GA produced results analogous to classic OC methods in both case studies considered in this chapter, whilst solving a radically simplified version of the OCP. However, there were various drawbacks associated with pursuing a GA approach. The most prominent thereof was the sensitivity of the GA to the numerical methods and control configuration used. In the predator-prey OCP, the numerical integration scheme had a noticeable effect on the objective function value, whereas the form of the control had less of an effect. The reverse was seen in the dengue OCP, where the control form appeared to have a significant effect on results whereas the numerical quadrature altered the objective value to a lesser extent. This may have been due to comparing the GA results to two separate solvers that utilised different methods in their approaches. Furthermore, the finer discretisation used in the predator-prey OCP compared to the dengue OCP may bear responsibility for the variable impact of the control representation on the respective OCPs (Section 2.2.5.6).

Nonetheless, both these factors had relative importance in the applications considered and are thus both relevant considerations when adopting a GA approach. Both the predator-prey and dengue OCPs may too benefit from the use of an adaptive step size in the control formulation when solving the OCP, with a refinement of discretisation in the area where the bulk of activity is seen. This would exploit the resources in these regions where they are most needed, and may address the disparities seen between the GA and classical solutions.

The successful applications of GAs to OCPs in this chapter addressed in part the primary aim and associated objectives of the study, when considering ODE systems, with and without complexities. Results appeared to support the hypothesis that GAs may increase the ease of applying OC in ecology while producing satisfactory results. These promising results served as motivation for extending the comparisons to explore the applicability of GAs to more complex problems, such as PDE-based OCPs (Section 3.2.1). PDEs have also been advocated as more realistic in ecology in the literature reviewed (Section 2.2.5.3). Consequently, a PDE-based OCP will be considered in the chapter following.

Chapter 5

Application to a Partial Differential Equation System

5.1 Introduction

Spatio-temporal dynamics can be incorporated in ecological models through the use of PDEs, which can act to increase realism and improve the predictive capability of a model. The computational and theoretical requirements involved in solving and subsequently analysing a PDE-formulated OCP, however, increase substantially. Consequently, the viability of a GA approach under the more complex circumstances of a PDE-based OCP is next investigated.

Globally, rabies poses a serious healthcare concern (Wheeler and Waller, 2008), accruing both economic and human cost with a case-fatality higher than any other infectious disease (Rupprecht et al., 2020). Since the 1990s, the wildlife-borne *Rhabdoviridae lyssavirus* (hereafter referred to as *rabies*) has been responsible for over 90% of all reported rabid animal cases in the US (Pedersen et al., 2018). Transmitted via the saliva of an infected animal through direct contact, genetically distinct virus strains carried by omnivorous mammals such as bats, foxes, skunks or raccoons, are capable of cross-species infection (Wheeler and Waller, 2008).

Raccoons (*Procyon lotor*) account for the majority of rabid wildlife cases (Gordon et al., 2004). Consequently, an OCP (Section 5.3) relating specifically to rabies transmission among raccoons (Miller Neilan, 2009) was extracted from existing literature, and is solved using both a classic OC method (Section 5.4) and a GA (Section 5.5) in the current chapter. This serves to investigate the primary research aim (Section 1.3) in a PDE-based OCP.

5.2 Raccoon Reservoirs of Rabies

With an *epizootic*[1] stretching back over 50 years, raccoons have had one of the largest rabies outbreaks historically recorded (Childs et al., 2000). Colonisation of both rural and urban areas alike (Gilbert et al., 2018) has led to a continuous spatial distribution of raccoon populations across the US (Pedersen et al., 2018). This, and translocation of infected raccoons (Slate et al., 2005), have facilitated the spread of rabies, posing a transmission risk to domestic animals and increased human exposure (Gilbert et al., 2018; Pedersen et al., 2018).

5.2.1 Vaccination Strategies

With little to no natural immunity (Childs et al., 2000), immunisation through vaccination is vital to containing rabies spread amongst raccoons (Pedersen et al., 2018) as culling is not a viable method of containment (Jenkins, Perry and Winkler, 1988). Vaccine-laced baits, typically made with fish meal and oil enclosing a vaccine chamber (Miller Neilan, 2009), serve as the primary form of control (Gilbert et al., 2018). Packaged as pellets when distributed by hand, or in an oily-coated packaging when distributed by aircraft, baits must be consumed by raccoons prior to any bait deterioration for antibodies to be developed (Miller Neilan, 2009).

The effectiveness of oral rabies vaccination strategies (ORVS) in containing rabies spread is dependent on factors such as the bait used, as well as temporal, spatial and environmental factors (Slate et al., 2005). Temporal (time dependent) disease and raccoon population dynamics are correlated with transmission to secondary species (Gordon et al., 2004), whilst spatial and environmental factors influence rabies spread. Rivers or mountains for example, can act as natural barriers to transmission (Wheeler and Waller, 2008) and infections can fluctuate based on changing population density due to spatial factors (Childs et al., 2000).

The cost of ORVS further poses a barrier to rabies elimination. Air-dropping baits, for instance, generates significant expenses (Slate et al., 2005) and high bait densities are required to attain the large percentage uptake by raccoons (Sattler et al., 2009) necessary for raccoon populations to acquire herd-immunity and thereby eliminate rabies (Gilbert et al., 2018). OC may aid in determining containment strategies while maintaining cost-effectiveness, however, effective models are required.

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[1] The analogue of an epidemic disease outbreak within an animal population

5.2.2 Modelling Rabies

The impact of landscape on rabies transmission, termed *landscape epidemiology* (Wheeler and Waller, 2008), is crucial when modelling patterns of disease spread (Smith, Lucey, Waller, Childs and Real, 2002). Rivers, for example, slow rabies spread substantially and can produce a containment effect comparable with a *cordon sanitaire*[2] (Smith et al., 2002). Furthermore, analysis of observed data has found that including rivers and long-distance translocation (LDT) in models is critical to model fit (Miller Neilan, 2009; Smith et al., 2002).

Several approaches have been used to model the spatial dynamics of rabies, the most popular of which makes use of reaction-diffusion PDEs (Smith et al., 2002). This allows the inclusion of environmental heterogeneity, which is critical in predicting the irregular wavefront of disease transmission in management strategies (Smith et al., 2002; Wheeler and Waller, 2008). Translocation may too contribute to rabies spread, and both local translocation and LDT can interfere with vaccination strategies designed to contain rabid populations through the creation of immune buffer zones using vaccine-laden baits (Slate et al., 2005).

Assisted by natural semi-permeable barriers such as the Appalachian mountain range (Wheeler and Waller, 2008), ORVS have limited the westward spread of rabies in the US (Gilbert et al., 2018) by creating buffer zones (Slate et al., 2005). Rabies elimination however, has not occurred. To contain the irregular wavefront of rabies spread, control strategies incorporating both landscape features and LDT are needed. Thus, an OCP modelling vaccine placement, given a domain of spatial heterogeneity and the LDT of an infectious raccoon, was formulated by Miller Neilan (2009) and subsequently examined in the current study.

5.3 Optimal Control Problem

To determine an optimal vaccination strategy to contain rabies spread on a heterogeneous spatial domain $\Omega \subset \mathbb{R}^2$, Miller Neilan (2009) developed an OCP with raccoons classified as susceptible ($S(x, y, t)$) if not exposed to rabies, infectious ($I(x, y, t)$) if able to transmit rabies, and immune when vaccinated ($R(x, y, t)$). The S-I-R model of rabies transmission was expressed as a system of coupled, parabolic PDEs, incorporating diffusion in both the x and y spatial dimensions, with no-flux boundary conditions (Miller Neilan, 2009). That is, it was

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[2] A designated quarantine zone, or cordoned-off, sanitary area around the outbreak of an infectious disease

assumed that there is no movement of raccoons across the boundary of Ω, denoted $\partial\Omega$.

For a fixed number of weeks $T > 0$, an optimal vaccination strategy $v^* = v^*(x, y, t) \in V$ at $(x, y) \in \Omega$ on week $t \in [0, T]$, was sought in order to minimise both the total number of infectious raccoons, and the cost of vaccination. Let $V = \{v \in L_\infty(Q) \,|\, v : Q \to [0, V_{max}]\}$ be the set of admissible controls, where $V_{max} \in \mathbb{R}^+$ denotes the maximum bait density per km^2, and $Q = \Omega \times [0, T]$ where the space $L_\infty(Q)$ is the set of all measurable and Lebesque integrable functions. Then, omitting dependence on space and time, for ease of notation, for S, I, R and v only, the OCP can be stated as:

$$\underset{V}{\text{minimise}}\ J(v) = \int_Q \left(I + cv^2\right) dQ \tag{5.1}$$

subject to:

$$\begin{aligned}
\frac{\partial S}{\partial t} &= a_{11}(x,y)\,\frac{\partial^2 S}{\partial x^2} + a_{22}(x,y)\,\frac{\partial^2 S}{\partial y^2} + b(t)(S+R) - \mu_1 S - \beta SI - avS,\\
\frac{\partial I}{\partial t} &= a_{11}(x,y)\,\frac{\partial^2 I}{\partial x^2} + a_{22}(x,y)\,\frac{\partial^2 I}{\partial y^2} + \beta SI - \mu_2 I,\\
\frac{\partial R}{\partial t} &= a_{11}(x,y)\,\frac{\partial^2 R}{\partial x^2} + a_{22}(x,y)\,\frac{\partial^2 R}{\partial y^2} - \mu_1 R + avS,
\end{aligned} \tag{5.2}$$

with initial conditions $S(x, y, 0) = S_0(x, y)$, $I(x, y, 0) = I_0(x, y)$ and $R(x, y, 0) = R_0(x, y)$ $\forall\ (x, y) \in \Omega$, and boundary conditions, $\frac{\partial S}{\partial x} = \frac{\partial I}{\partial x} = \frac{\partial R}{\partial x} = 0$ and $\frac{\partial S}{\partial y} = \frac{\partial I}{\partial y} = \frac{\partial R}{\partial y} = 0$ on $\partial\Omega \times (0, T)$. Constant parameters of the OCP, specific to rabies transmission in raccoon populations, are given in Table 5.1, and non-constant parameters, in Section 5.4.1.

Table 5.1: Constant parameters with their associated units and values (Miller Neilan, 2009).

Parameter	**Description**	**Units**	**Value**
μ_1	Natural death rate	Per week	0.026
μ_2	Death rate of I	Per week	0.490
β	Rabies transmission rate	(Raccoons/km^2·week)$^{-1}$	0.03
a	Vaccine uptake rate	(Vaccine · week)$^{-1}$	0.01
c	Cost balancing coefficient	(Raccoons/km^2)/vaccine^2	0.1
T	Vaccination period	Weeks	20

Not all implementation factors were given explicitly in previous work (Miller Neilan, 2009; Miller Neilan and Lenhart, 2011), and thus the OCP was re-solved using a classic OC approach in the current study, the results of which are next reported.

5.4 Indirect Method Approach and Associated Results

Suppose $(S^*, I^*, R^*) = (S, I, R)(v^*)$ are the optimal state variables corresponding to the optimal control v^*. Then there exists adjoint variables λ_1, λ_2 and λ_3 with adjoint equations:

$$\begin{aligned}
\frac{\partial \lambda_1}{\partial t} &= -a_{11}(x,y)\frac{\partial^2 \lambda_1}{\partial x^2} - a_{22}(x,y)\frac{\partial^2 \lambda_1}{\partial y^2} - b(t)\lambda_1 + \mu_1\lambda_1 + \beta I^*\lambda_1 + av^*\lambda_1 - \beta I^*\lambda_2 - av^*\lambda_3, \\
\frac{\partial \lambda_2}{\partial t} &= -a_{11}(x,y)\frac{\partial^2 \lambda_2}{\partial x^2} - a_{22}(x,y)\frac{\partial^2 \lambda_2}{\partial y^2} + \beta S^*\lambda_1 - \beta S^*\lambda_2 + \mu_2\lambda_2 - 1, \\
\frac{\partial \lambda_3}{\partial t} &= -a_{11}(x,y)\frac{\partial^2 \lambda_3}{\partial x^2} - a_{22}(x,y)\frac{\partial^2 \lambda_3}{\partial y^2} + \mu_1\lambda_3 - b(t)\lambda_1, \qquad (5.3)
\end{aligned}$$

with transversality conditions $\lambda_k(x, y, T) = 0$ and boundary conditions $\frac{\partial \lambda_k}{\partial x} = \frac{\partial \lambda_k}{\partial y} = 0$ on $\partial\Omega \times (0, T)$ for $k = 1, 2, 3$. From the optimality condition, v^* can be derived as

$$v^* = \min\left(\left(\frac{(\lambda_1 - \lambda_3)\,aS^*}{2c}\right)^+, V_{max}\right) \qquad (5.4)$$

where the notation $x^+ = \max(x, 0)$. The existence and uniqueness of the optimal control, for sufficiently small T, was proven in previous work (Miller Neilan, 2009; Miller Neilan and Lenhart, 2011), along with proof of the existence of solutions to the system of state equations.

5.4.1 Heterogeneous Domain and Associated Parameter Initialisation

Both rabies spread and raccoon population densities are dependent on environmental factors. Urban populations, for example, flourish compared to their rural relatives, with densities up to 20-times that of rural populations (Miller Neilan, 2009). Additionally, decreased rabies transmission is associated with lightly forested areas and no transmission with densely forested areas separated by rivers (Miller Neilan, 2009). A heterogeneous domain was thus constructed by Miller Neilan (2009), composed of a river Ω_R, light forest cover Ω_F, and urban areas, Ω_U.

A diagram of the 30 km × 20 km rectangular domain Ω, constructed and applied in the current study, is given in Figure 5.1. Initially, all infectious raccoons were concentrated in $\Omega_I \subset \Omega_U$; the initial site of infection. Infections originating from Ω_I will thus be referred to as the Ω_I wave. Ω_R was considered to lie in both Ω_U and Ω_F, that is $(\Omega_R \cap \Omega_F) \neq \emptyset$ and $(\Omega_R \cap \Omega_U) \neq \emptyset$. According to their location in Ω, and further classified as S, I or R, the initial number of raccoons per km^2 (Miller Neilan, 2009) are given by:

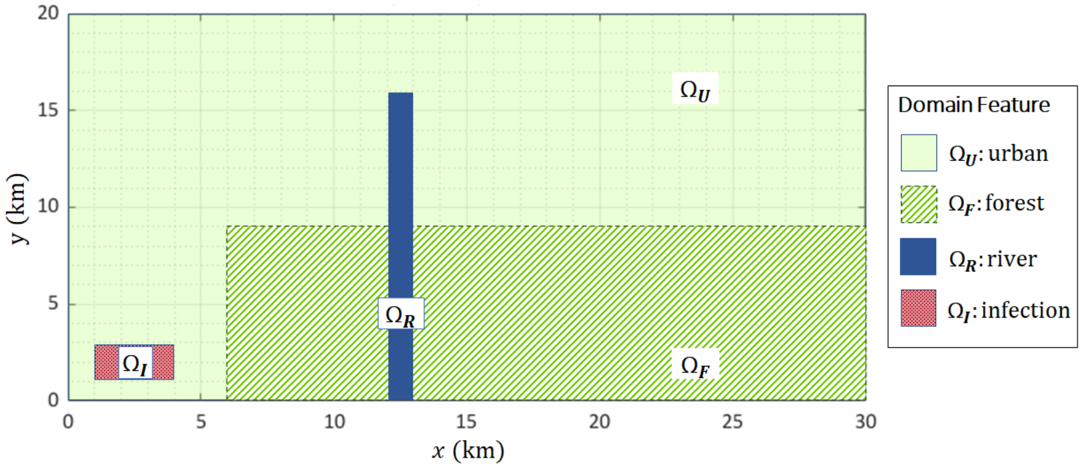

Figure 5.1: The heterogeneous spatial domain Ω used in the raccoon-rabies OCP

$$S_0(x,y) = \begin{cases} 0 & \text{if } (x,y) \in \Omega_R \\ 10 & \text{if } (x,y) \in \Omega_F \\ 30 & \text{elsewhere} \end{cases} ; \quad I_0(x,y) = \begin{cases} 2 & \text{if } (x,y) \in \Omega_I \\ 0 & \text{elsewhere} \end{cases} ; \quad R_0(x,y) = 0 \,\forall\, (x,y) \in \Omega.$$

Allowing for the irregular rabies wavefront caused by changing raccoon movement in response to the heterogeneity of Ω, spatially dependent diffusion rates (Miller Neilan, 2009) are given in km^2/week by:

$$a_{11}(x,y) = \begin{cases} 0.5 & \text{if } (x,y) \in \Omega_U \\ 0.2 & \text{if } (x,y) \in \Omega_F \\ 0.05 & \text{if } (x,y) \in \Omega_R \end{cases} \quad \text{and} \quad a_{22}(x,y) = \begin{cases} 0.2 & \text{if } (x,y) \in \Omega_F \\ 0.5 & \text{elsewhere.} \end{cases}$$

Since raccoons only give birth during an approximately 14-week period in springtime, a time dependent birth rate of $b(t) = 0.096$ per week for $t \in [13, 28)$ was used (Miller Neilan, 2009).

5.4.2 Optimal Vaccination Strategy

Vaccination strategies take time to develop and thus control is rarely imposed as soon as rabies appears in a raccoon population. Furthermore, rabies may also spread, undetected, for a period of time. To maintain realism, it was thus assumed that rabies spreads on Ω for 20 weeks according to the S-I-R model in Equation set (5.2), with the initial conditions in Section 5.4.1, prior to implementing OC. Furthermore, during week 20, the LDT of an infectious raccoon occurs at $(x,y) = (27,15)$ and thus $I(27,15,20)$ is set to $I(27,15,20)+1$.

The OCP was then solved using the FBSM (Section 3.4.1), with $\delta = 0.001$, from week 21 through to 41, or from $t = 1$ until $t = 20$ in the vaccination strategy. Consequently, raccoon densities at week 20 (without control) were used as the initial conditions ($t = 0$) in the OCP. To maintain well-posedness with the boundary conditions, the FTCS and BTCS finite difference methods (Section 3.5.1) were used to solve the state equations (Equation set (5.2)) and adjoint equations (Equation set (5.3)) respectively. A grid of $\Delta x = \Delta y = 1$ km was applied in the current study, with $\Delta t = 0.05$ weeks to ensure stability. A value of $V_{max} = 75$ baits/km^2 (Sattler et al., 2009) was used, as Miller Neilan (2009) did not specify V_{max}.

The optimal solution at week $t = 1$ of the vaccination strategy is given in Figure 5.2. Initially, v^* placed the highest bait density on the LDT focus, with lesser quantities in the immediate surrounding area. A lower bait density was placed directly in the diffusive path of the infection wave emanating from Ω_I, and a low density on the remainder of Ω_U. Overall, v^* placed the largest bait densities on weeks $t = 1, 2$ and 3, after which the bait density was gradually reduced. Correspondingly, infections increased slowly from week $t = 1$ to $t = 3$.

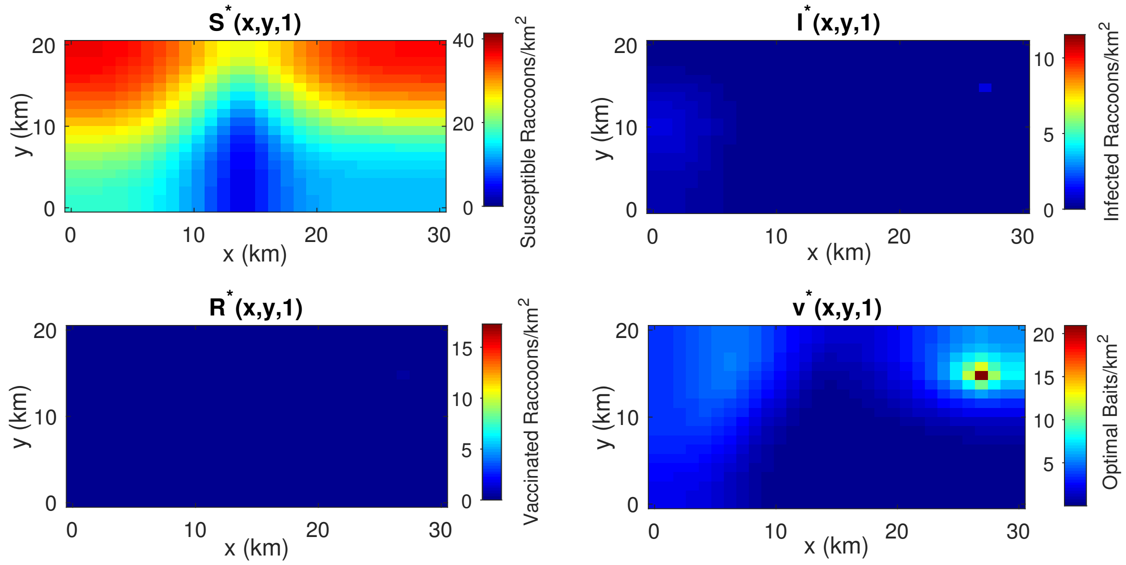

Figure 5.2: The FBSM-derived optimal solution at week 1 of the vaccination strategy, with the LDT of an infectious raccoon appearing in the top right of Ω

Infections doubled every two weeks from $t = 4$ until $t = 7$, but stabilised between $t = 9$ and $t = 10$, reaching a peak of about 11 infectious raccoons/km^2. Infections then began decreasing, linearly, from $t = 11$ (Figure 5.3) onwards. Baits were continually placed above-right of the Ω_I wave and to the left of the LDT wave, anticipating raccoon movement to ensure baits were consumed prior to the arrival of raccoons to an uninfected area.

From $t = 12$, the LDT wave began to grow at a higher rate than the Ω_I wave, overtaking

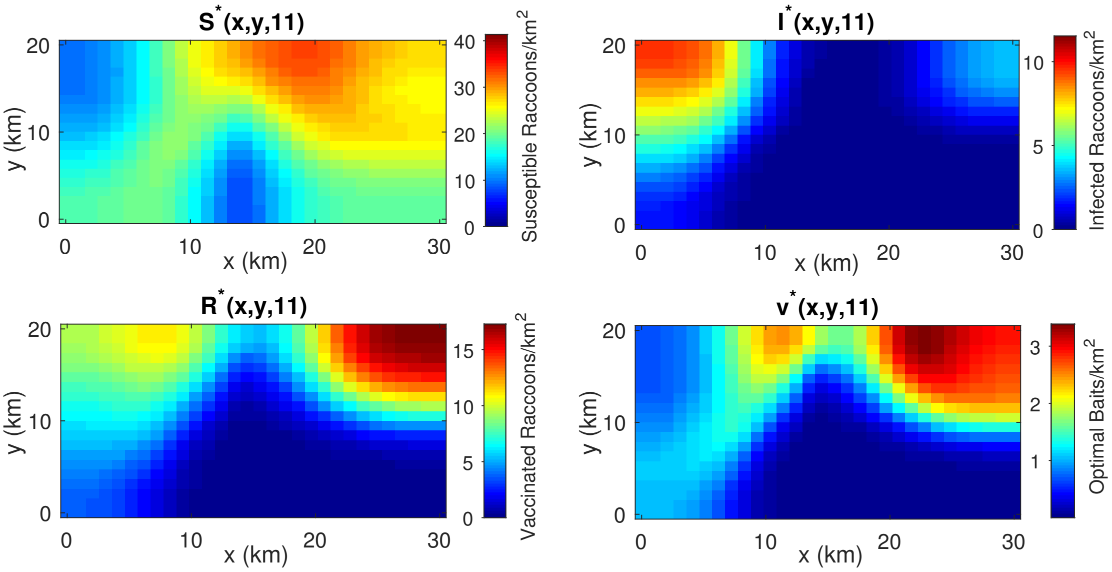

Figure 5.3: The FBSM-derived optimal solution at week 11 of the vaccination strategy

Ω_I as the main source of infection at $t = 15$. The Ω_I wave, having diffused upwards and over Ω_R, merged with the leftward spreading LDT wave at approximately $t = 18$. Baits were once again distributed ahead of the Ω_I and LDT waves, merging at the top right of Ω_R between $t = 12$ and $t = 13$, preceding the merging of infectious waves. Infections/km^2 however, continued decreasing, albeit at a decreasing rate. From $t = 15$ onwards, the maximum bait density dropped below one, decreasing to zero by $t = 20$, at which time infections had dropped below 2/km^2. The final vaccination week, $t = 20$, can be seen in Figure 5.4.

From the onset of control, large bait quantities were continually placed at and concentrically outwards and to the left of the LDT, stretching towards the eventual path of the Ω_I wave. Lower densities were also distributed in front of the Ω_I wave. Apart from the small number of baits placed where the Ω_I wave path crossed the top, left corner of Ω_F, no baits were placed in Ω_F or Ω_R over the entire time period. Although S raccoons reside in Ω_F, neither I nor R raccoons transitioned to Ω_F. The relatively low bait density along the borders of Ω_R and Ω_F, in combination with the inhibited movement in Ω_R and Ω_F, appeared to create a buffer zone, preventing the infectious waves from entering Ω_F to the right of Ω_R.

Objective function evaluation was not covered in the PDE-based OCPs reviewed (Section 2.2.5.5). Since CS consumes significant computational time to approximate triple integrals and exceeds the FTCS method's order of error, a RS was used to approximate the objective on Q, producing a value of $J(v^*) = 14501.5695$, to four significant decimal places.

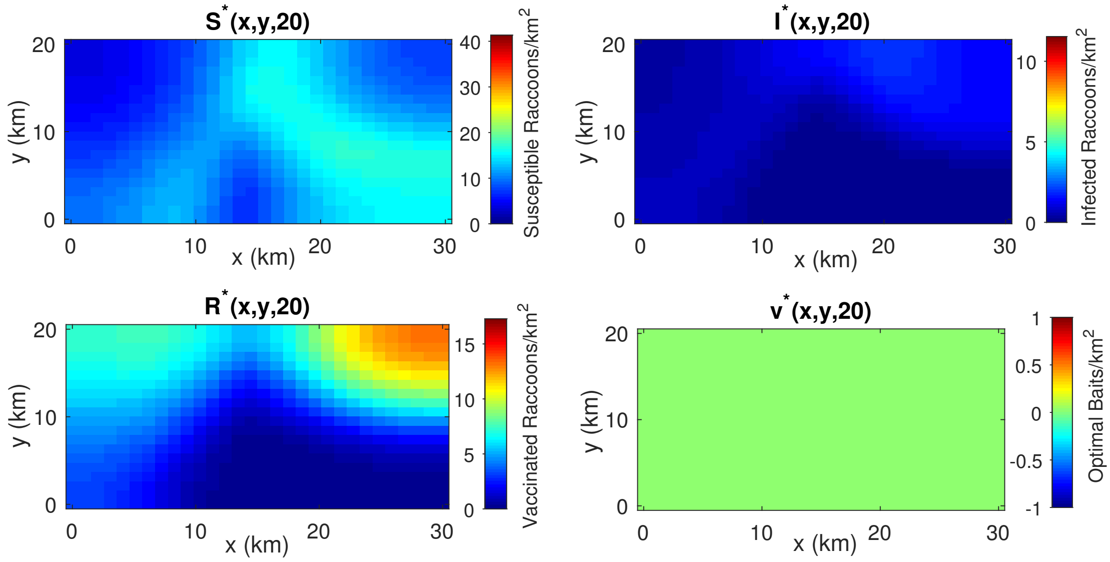

Figure 5.4: The FBSM-derived optimal solution at week 20 of the vaccination strategy

5.5 Genetic Algorithm Application and Results

In keeping with the indirect method approach, the FTCS method was used to solve the S-I-R model of the OCP in the GA, and a RS was used to evaluate the objective function. A spatial discretisation of $\Delta x = \Delta y = 1$ km was again employed to generate solutions, with a time step of $\Delta t = 0.05$ weeks. As before, the objective function was used as the fitness function in the GA, and the OCP was solved using default GA parameter values in MATLAB (2018).

5.5.1 Control Construction and Subsequent Encoding

The least subjective way of implementing control in the GA would be to simply allow the GA to select a bait density for every spatial node in time. This would ensure that the GA could select both the control form and the values used to populate the control form. With the chosen discretisation of $\Delta x = \Delta y = 1$ km and $\Delta t = 0.05$ weeks, a chromosome length of 240000 would be required to encode each of these values (600 spatial at 400 temporal nodes), which was completely intractable. Consequently, decreasing the computational cost became an important consideration in the PDE problem using a GA approach.

Even if control values were only generated at intermediate spatial and temporal nodes, analogously to the relatively generic, piecewise constant approach pursued in Chapter 4, a chromosome length exceeding 1000 would be required, which was beyond the scope of this study. Consequently, various assumptions had to be made to shorten chromosome length, which, while endeavouring to remain as realistic as possible, inevitably became artificial. No precedent could be found as to how to best accomplish this, and thus a more creative approach had to be adopted in order to adapt the control formulation by restricting its form.

In an attempt to construct an unbiased control form that would have minimal influence on the optimal strategy, while simultaneously reducing computational complexity, ORVS were reviewed. Typically, ORVS air-drop baits in parallel flight lines (Pedersen et al., 2018). Aerial distribution is, seemingly, conducted once during an ORVS, and distribution by vehicle, or on foot, is used in urban areas when there is a risk of property damage (Sattler et al., 2009).

Inspired by these ORVS factors, the control was formulated as a PDE (the form was not selected by the GA itself) and the GA was used to populate this pre-empted form. The diffusion terms $D_1(x, y, t)$ and $D_2(x, y, t)$ were used to model bait distribution by foot or vehicle in the PDE, in order to obtain bait densities at each time increment. To avoid bait deterioration, placement should occur near raccoon populations. Bait distribution was thus modelled at a rate proportional to raccoon movement (described by $a_{11}(x, y)$ and $a_{22}(x, y)$ in Section 5.4.1), with the speed of bait distribution able to exceed raccoon movement. A term, $k(t)$, was included in the PDE to ensure that bait density could be reduced during the vaccination strategy. A GA was then used to generate optimal parameters for the PDE:

$$\frac{\partial v}{\partial t} = D_1\left(x, y, t\right) v_{xx} + D_2\left(x, y, t\right) v_{yy} - k(t)v. \tag{5.5}$$

To accomplish this, the GA generated 20 proportionality terms, 10 of which were diffusion coefficients, denoted d_i, and the remaining 10, reduction terms, denoted k_i for $i = 1, 2, \ldots, 10$. Each $d_i \in [0, 4]$ was allocated to two consecutive weeks in the vaccination period to form a time dependent diffusion term $d(t)$ for $t \in [1, 20]$. Spatio-temporal diffusion rates were then formed by assigning $D_1(x, y, t) = d(t) \times a_{11}(x, y)$ and $D_2(x, y, t) = d(t) \times a_{22}(x, y)$, with $D_1(x, y, t) = 0$ if $(x, y) \in \Omega_R$, as baits are not placed in water bodies (Sattler et al., 2009).

A similar process was used to develop a time dependent reduction term $k(t)$, however, this was allocated from $t = 2$ onwards, with $k(1) = 0$ on week 1. This facilitated a different combination of diffusion and reduction rates to be used in each week of the vaccination strategy, allowing the GA optimal strategy to vary, if desired, during each week. The overlapping fashion in which diffusion and reduction terms were allocated is illustrated in Figure 5.5.

To initialise bait distribution $v(x, y, 0) = v_0(x, y)$, an initial bait density was generated

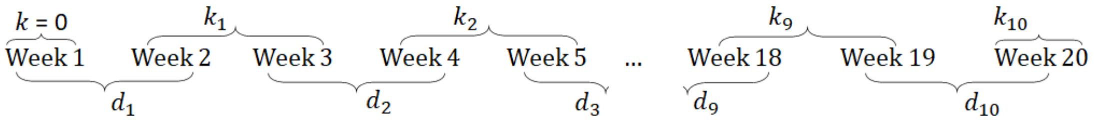

Figure 5.5: Alternating allocation of diffusion and reduction terms in the GA control

by the GA for each of the 20 y and 30 x coordinates in Ω, namely $\{y_1, y_2, \ldots, y_{20}\}$ and $\{x_1, x_2, \ldots, x_{30}\}$, where $x_i, y_j \in [0, \sqrt{75}]$ for $i \in [1, 30]$ and $j \in [1, 20]$. These bait quantities were assigned in 1 km intervals to the x and y spatial dimensions respectively, forming perpendicular lines with $v_0(i, y) = x_i$ for $i \in [1, 30]$ and $v_0(x, j) = y_j$ for $j \in [1, 20]$. At the intersection of two lines, bait quantities were multiplied[3]. This ensured that every discretisation node in the FTCS method had an associated initial value in the interval $[0, V_{\max} = 75]$, given by $v_0(i, j) = x_i y_j$ for each $i \in [1, 30]$ and $j \in [1, 20]$. Initial bait densities, diffusion and reduction terms were encoded in a chromosome of length 70, as shown in Figure 5.6.

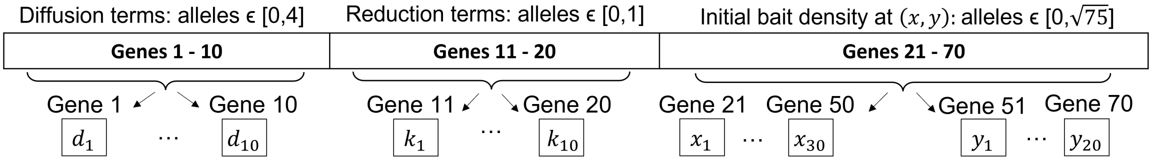

Figure 5.6: Chromosome encoding used in the raccoon-rabies OCP

In this way, an individual value could be assigned to the 600 spatial nodes using only 50 initial values encoded in the chromosome. This predisposes the control strategy to commence at $t = 0$, and thus assumes that an optimal strategy should immediately distribute baits. Air-dropping initial baits in parallel flight lines and subsequently distributing baits by foot or vehicle, according to the solution to Equation (5.5), is however in accordance with typical ORVS. Since baits are only air-dropped once, the cost of the strategy is also decreased.

5.5.2 Genetic Algorithm Results

The GA was run 30 times and the solution with minimum fitness out of all 30 final generations was once again selected as the optimal solution. The GA-derived optimal solution, obtained on Q, had an objective value of $J(v^*) = 14804.6047$, to four significant decimal places; a mere 2.08967% greater than the FBSM's objective value of $J(v^*) = 14501.5695$. The first week ($t = 1$) of the optimal vaccination strategy found by the GA is shown in Figure 5.7.

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[3] Quantities could also be added, however this would increase complexity as a constraint would need to be instituted so that $v_0(i, j) = x_i + y_j \leq 75$ since x_i and y_j would then have to be generated in the interval $[0, 75]$.

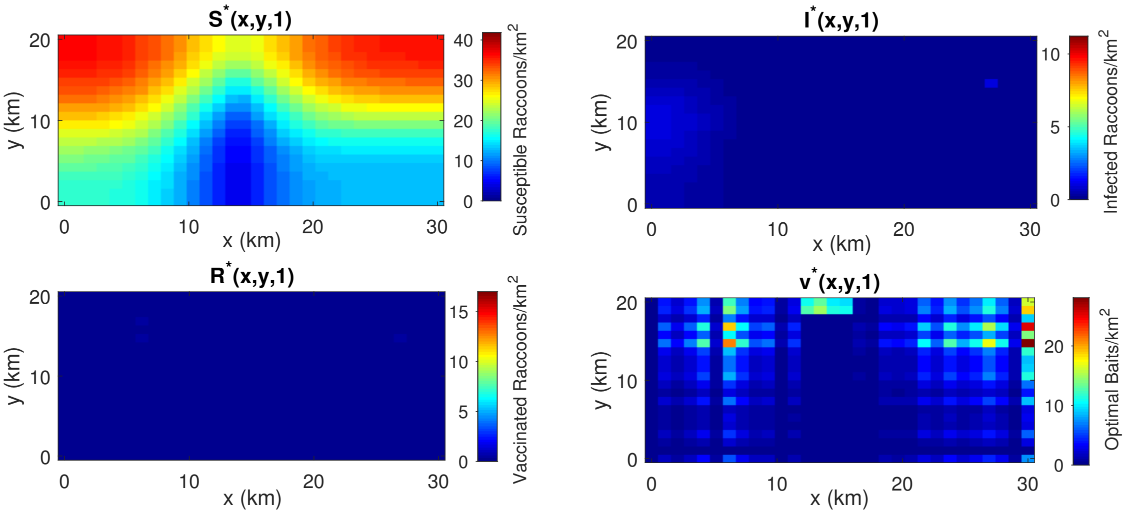

Figure 5.7: The GA-derived optimal solution at week 1 of the vaccination strategy

Analogous to the FBSM's control, the GA placed the highest concentration of baits near the LDT, albeit at a higher density (28 baits/km^2) than the classical control (21 baits/km^2). Baits were again distributed on and around the LDT, with the largest quantity to the right of the LDT. The GA placed a greater quantity of baits above the Ω_I wave than the FBSM's control and, deviating from the FBSM's control, created a bait distribution focus above Ω_R. This focus, however, became obsolete by $t = 3$. Low bait quantities were also distributed across Ω_F. Overall, the pattern of bait densities resembled the pattern seen for $S(x, y, 1)$.

Once again, the largest bait quantities were placed during $t = 1, 2,$ and 3. During this time, I was almost identical in the FBSM and GA solutions. Similarly to the FBSM solution, from $t = 3$ until $t = 7$, infections doubled every two weeks, peaking at approximately 11 infectious raccoons/km^2 between $t = 9$ and $t = 10$; achieving an almost identical peak to the classic solution. The maximum number of baits/km^2 remained at 6 from $t = 3$ until $t = 7$, after which it was gradually reduced to 4 baits/km^2 at $t = 10$. Infections then began a gradual descent, decreasing at a decreasing rate from $t = 11$ onwards, shown in Figure 5.8.

From $t = 12$, the LDT wave again grew at a faster rate than the Ω_I wave, overtaking Ω_I as the main source of infection at $t = 14$, prior to the $t = 15$ anticipated in the FBSM strategy. Bait distribution continued decreasing, dropping below a density of 1/km^2 around $t = 14$; one week earlier than the FBSM's control. Bait densities continued slowly decreasing until $t = 16$, after which the peak bait quantity halved in each successive week, reaching less than 0.0088/km^2 at $t = 20$. At this time, infections were below 2.3/km^2. The final week $t = 20$ of the GA vaccination strategy is shown in Figure 5.9.

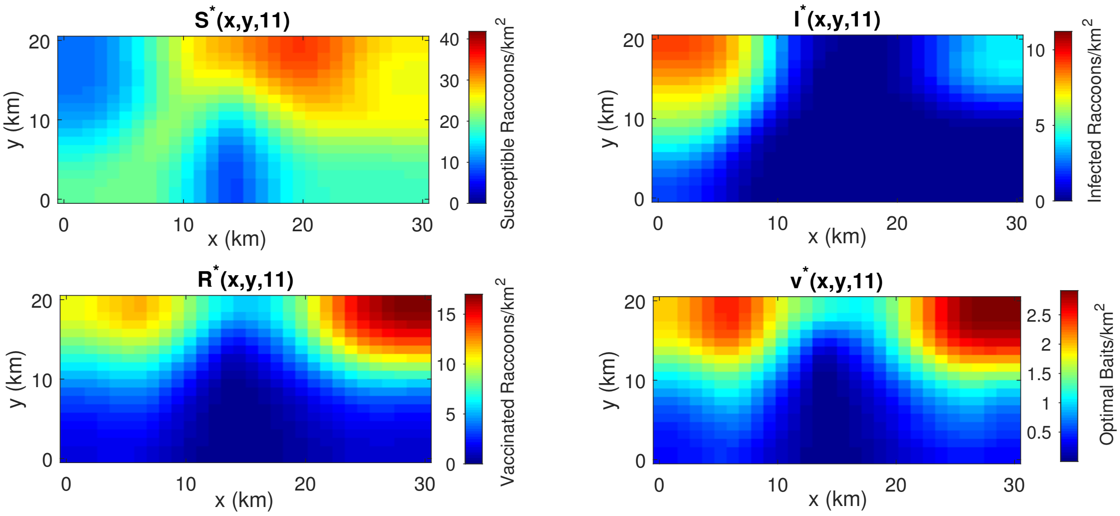

Figure 5.8: The GA-derived optimal solution at week 11 of the vaccination strategy

Unlike the FBSM's control, bait placement in the GA solution did not precede the movement of I, but remained concentrated in zones around where they were initially distributed, throughout the vaccination strategy. Baits were also placed in Ω_F, which while dissimilar to the FBSM's control, were in such minor quantities (less than 1/km^2) that it would likely be negligible in practice. Lastly, in contrast to the classical solution, all areas of the domain Ω, except Ω_R, had baits placed in them at some point during the GA's OC strategy.

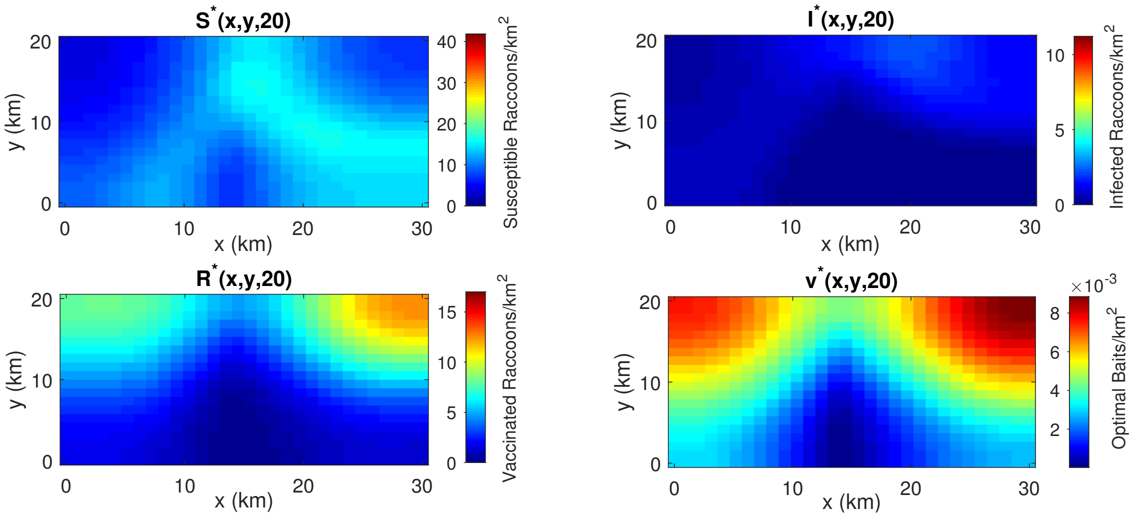

Figure 5.9: The GA-derived optimal solution at week 20 of the vaccination strategy

For comparative purposes, the FBSM-produced optimal bait distribution and resulting population of infectious raccoons are shown alongside the corresponding GA-produced optimal solution in Figure 5.10, at two intermediate weeks in the optimal vaccination strategy.

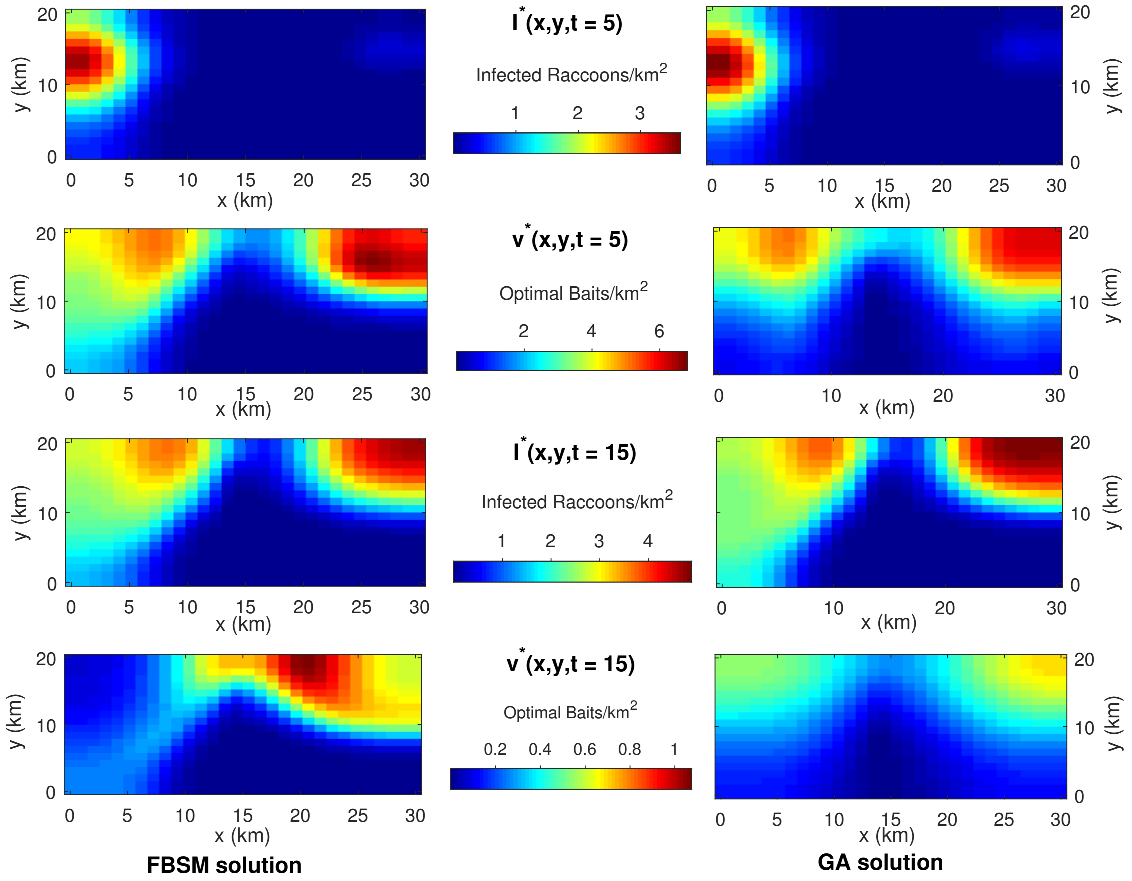

Figure 5.10: Comparison between the optimal solutions to the raccoon-rabies OCP, found by the FBSM and GA respectively, at weeks $t = 5$ and $t = 15$

Overall, GA results were consistent across all 30 runs, with an average percentage relative difference (error) of 2.4194% between the GA-derived optimal solution and the FBSM's optimal solutions. Moreover, the average error had a variance of 0.03478 and a standard deviation of 0.1865. GA performance is further discussed next.

5.5.3 Discussion

Although the GA initialised bait distribution in a similar manner to the FBSM-derived control, the optimal vaccination strategies differed considerably. Since the GA control was reliant on the form encoded from the onset of the GA, different assumptions may produce vaccination strategies more in keeping with classic OC methods. An alternative control formulation can be seen in Appendix B, where terms proportional to the population classes were used.

The GA approach followed in the current study had a number of associated advantages. First and foremost, a significant amount of non-trivial mathematical theory was avoided. The

GA also produced a simpler strategy to implement in practice than the FBSM, continually placing baits in the same area, which did not require the distribution of baits in specific density patterns. Furthermore, the differences between the final population classes generated using the GA's control (Section 5.5.2) and those obtained using the FBSM's control (Section 5.4.2) were relatively minor.

A number of limitations were attached to the GA application. Primarily, the GA took substantially longer than the FBSM to generate an optimal control; taking 4-5 hours to converge to an optimal solution as opposed to the FBSM converging in under 5 minutes[4]. The running time is partially reliant on chromosome length, and thus the encoding of the control would have played a role in the time it took the GA to generate an optimal solution.

Additionally, the diffusive approach to vaccination in the GA meant that throughout the vaccination period, baits were distributed in zones. This prevented bait distribution from following or preceding I and/or S movement. Experimentation with diffusion rates larger than that chosen in Section 5.5.1, did not allow the bait distribution patterns to change as radically as the added dependence on population classes in Appendix B, for example, does.

A sufficiently accurate optimal control was obtained using a GA, which while not identical to the FBSM-control, generated final population classes strongly resembling the FBSM-solution. Disadvantages of the GA approach however, included the time taken to produce an optimal control (compared to the FBSM), and the deriving of a control form. The GA approach may thus benefit from further investigation regarding the formulation of a control that would not influence the form of the optimal vaccination strategy generated.

5.6 Concluding Remarks

To conclude the comparative component of this research and further address the primary aim and associated objectives (Section 1.3), a GA was applied to an OCP formulated using PDEs. The capability of a GA to adjust to the increased complexity associated with PDE applications in OCP, demonstrated by classic OC methods, was examined in the current chapter, in order to further address the research question and primary aim.

Both the classical FBSM and a GA were applied to the OCP in this chapter. The more prominent disadvantages of each approach occurred at different stages in solving the OCP.

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[4] The GA began converging within 15 minutes, dropping below a 5% error (relative to the FBSM solution) in under 18 minutes, with the balance of time allocated to refining the solution to meet termination criteria.

The FBSM approach experienced the most complexity in the theoretical stages, namely in the derivation of an optimal control and the associated proofs, which was once again avoided in the GA approach. From there, the computational component was relatively straightforward, whereas the most notable disadvantage of the GA was the computational time taken to generate a solution. Similarly to the dengue OCP (Section 4.3.3.3), the final solution was heavily dependent on the control form, as can be seen in Appendix B, where a different control form is used. The control formulation is thus an influential factor in a GA approach.

The time taken to generate solutions using a GA increased appreciably from what was seen in the ODE cases, and further far exceeded that of the FBSM. GA implementation was also more complex when applied to a PDE-based OCP than ODE-based OCPs due to the increase in dimension inducing considerably greater difficulty when encoding a control, predominantly due to computational resource limitations. This led to a less automated process in constructing a control for the GA, which was more subject to researcher preference.

Overall, the GA produced satisfactory, near-optimal results, bypassing a significant amount of mathematical theory in the process. This served to support the hypothesis that a GA is a viable OC method alternative, which may increase the ease of applying OC in ecology while producing satisfactory results. This finding is however, likely both problem dependent, and dependent on researcher preference, as computational time is considered over accuracy by many researchers as an important indicator of method capability (Section 2.2.5.5).

In both ODE and PDE case studies, the GA appeared to generate optimal solutions resembling classical solutions derived using complex mathematics. The GA thus demonstrated the capability of achieving what is conventionally deemed an optimal solution. However theoretically optimal solutions are not always optimal in practice, since the optimal solution of an ecological model describing an abstraction of a system, is not necessarily the optimum of the ecological system itself (Barbour et al., 2016).

Aside from implementation features that can affect GA performance, the ecological model itself is critical to obtaining truly optimal solutions. The simultaneous intricacy and enormity of ecological systems is difficult for any method to adequately capture. GAs, uninhibited by restrictions of mathematical techniques, could potentially help improve realism by utilising more unconventional OC models, to which the optimal solution may better concur with the optimal solution to the real-world system itself. This notion was investigated in Chapter 6, in which a case study was developed to address the second research aim (Section 1.3).

Chapter 6

Application to an Unconventional Optimal Control Problem

6.1 Introduction

The impact of humans on ecological systems is resulting in an ever increasing risk of ecological collapse as habitat destruction, resource overharvesting, soil erosion, chemical toxicity, and pollution, threaten the biosphere upon which humankind depends (Salomon, 2019). Among the casualties of this human impact are wild bee populations (Hymenoptera: Apidae), whose declines have been necessitated by habitat loss (Pufal, Steffan-Dewenter and Klein, 2017).

The destruction of natural habitat is primarily driven by agricultural expansion (Murray, Kuhlmann and Potts, 2009) and intensification (prevalence of mono-cultures and escalating chemical use), resulting in bee habitat declines and alterations (Hemberger, Frappa, Witynski and Gratton, 2020). As a result, wild bee populations are declining which in turn affects crop yields, as many plants are tailored specifically to bee pollination (Goulson, 2010), creating a demand for improved agricultural design to address these issues (Landis, 2017).

Providing nesting and floral resources at appropriate locations in a landscape can increase wild bee abundance (Bennett, Gensler and Cahill, 2014) and thus the modification of agricultural land has been proposed to prevent further declines (Pufal et al., 2017). Although habitat provision promotes bee population growth (Murray et al., 2009), the placement and overall landscape configuration is crucial to the success of schemes, with optimal strategies to achieve such yet to be derived (Holland, Smith, Storkey, Lutman and Aebischer, 2015).

OC has been used to control ecological systems in order to accomplish human goals, and more recently, maintain the functions of ecosystems to ensure their sustainability for future generations (Bolton, 2019). Ecological systems are not always well-described using models, however, and thus mathematically-optimal solutions are not always optimal in practice (Loehle, 2006). Meta-heuristic algorithms like the GA, however, have advanced the capabilities of optimisation in complex systems through their pliability in problem formulation (Barbour et al., 2016), and could thus act as an alternative to classic OC methods.

The viability of a GA as an OC method was assessed in the previous chapters by comparing its performance to that of classic OC methods in ecological OCPs. These comparisons demonstrated that GAs are capable of producing comparable results to classic OC methods, thus proving GAs to be a reliable and accurate OC method. In line with the second research aim (Section 1.3), an unconventional OCP is thus developed in Section 6.3 to address wild bee conservation goals as realistically as possible, regardless of the mathematical consequences. Arguably, the resulting OCP cannot be solved using conventional methods (motivated in Appendix C), and is thus solved using a GA approach in Section 6.4.

This serves to investigate whether a GA can maintain its performance when applied to an OCP that arguably cannot be solved using classic OC methods. In order to both develop an OCP and assess GA results (presented in Section 6.5) in the absence of a comparison with classic schemes, ecological background to the problem is next given. The GA approach follows, and, lastly, concluding remarks are made in Section 6.6.

6.2 Agricultural Ecosystems

Globally, agricultural intensification is being adopted to support the rapidly growing food and fuel requirements of an ever increasing human population (Landis, 2017). Already, almost 40% of ice-free land has been appropriated for agriculture, with agricultural intensification now the leading cause of habitat loss worldwide, creating landscapes dominated by agricultural ecosystems (agroecosystems) (Murray et al., 2009). Habitat loss can reduce the *resilience* of a species, which can result in catastrophic collapse if overextended (Bolton, 2019); calling the sustainability of these practices into question (Landis, 2017).

Agroecosystem design is based on the concept of engineering resilience, where resilient systems are characterised by stability and permanence (Bolton, 2019). This has resulted in the homogenisation of agriculture (simplification of complex/heterogeneous landscapes) (Landis, 2017). Historically, ecological modelling reflects this focus, examining systems at equilibrium and their ability and speed in returning to such a state after a perturbation (Holling, 1973).

Ecosystems are not usually in equilibria (Bolton, 2019) however, and resource exploitation accompanying economic and population growth, drives ecosystems away from equilibrium states (Holling, 1973). Thus, whilst crop yields have temporarily benefited from this approach, ecosystems have suffered substantial biodiversity loss, leading to, perhaps most significantly, the degradation of *ecosystem services*[1] (Landis, 2017), which humans are dependent on for life itself (Bolton, 2019).

Homogeneous landscapes tend to have increased stability but decreased resilience, emphasising the subtle dissonance between engineering resilience, based on equilibrium states or stability, and ecological resilience (Bolton, 2019), which measures the persistence of a system, or its ability to tolerate perturbations and non-equilibrium conditions and retain critical functions through the maintenance of structures and relationships (Holling, 1973).

Since ecological systems can simultaneously be both resilient and appear unstable due to large fluctuations in their state (Holling, 1973), resilience is better fostered through adaptive management, which recognises the limits of human understanding of ecological systems and thus policies are regularly updated to account for their effects on natural systems (Salomon, 2019). The OC of complex systems can thus no longer be expected to provide a conclusive optimal solution, but should rather be used to investigate various alternatives (Barbour et al., 2016) and the effects thereof; characteristics suited to the use of EAs in OC.

6.2.1 Pollinators and Pollination Services

Modern agriculture prioritises human management ease by increasingly homogenising heterogeneous landscapes, resulting in a loss of plant diversity and natural habitat (Delaplane and Mayer, 2000); edging the ecosystems bees depend upon, closer to their ecological resilience thresholds (Bolton, 2019). Worldwide, both wild and managed bee populations are declining (Murray et al., 2009), with further severe shortages forecast (Goulson, 2010). With about 33% of food crops dependent on wild pollinators, and ecosystem services valued at about US$33 trillion a year (Salomon, 2019), conservation becomes imperative (Landis, 2017).

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[1] Oxygen generation, water purification, pollination, and soil maintenance, amongst others (Bolton, 2019).

Many crops are reliant on external pollinators, and even crops capable of self-pollination experience significant yield improvements when externally pollinated (Delaplane and Mayer, 2000). Few pollinators besides the honeybee have been successfully cultured commercially, and as the primary[2] commercial pollinator (Bänsch, Tscharntke, Ratnieks, Härtel and Westphal, 2020), honeybee declines could signify future food insecurity (Timberlake, 2019), heralding the conservation of wild bees as an insurance policy (Delaplane and Mayer, 2000).

While the simple act of timing pesticide application can reduce the toxicity bees are exposed to in crops, promoting bee conservation, habitat alteration alone accounts for a third of all changes seen in bee populations (Murray et al., 2009). Altering agroecosystem design to conserve wild bees may thus aid in prolonging the resilience of bee species and their service provision (Landis, 2017). This approach is also relatively cost effective, as land that would otherwise remain unused, including ditches or field margins, can be converted into appropriate habitat at little expense other than land provision (Delaplane and Mayer, 2000).

Biodiversity initiatives and financial incentives exist across Europe and the UK, to foster conservation by farmers, however most are not specific to bees (Murray et al., 2009). OC can be used to determine habitat layout to conserve wild bees under threat, however an understanding of their behaviour, nesting and floral resources is required (Pufal et al., 2017), which can be species-specific. This would serve to consolidate conservation goals and economic considerations, promoting increased wild bee populations and crop yields (Goulson, 2010).

6.2.1.1 Wild Bee Pollinators: Bumble and Solitary Bee Species

Unlike their social counterparts, solitary bees are specialist bees (Delaplane and Mayer, 2000), which makes them crucial pollinators in minor-flowering crops during their seasonal life cycle, as they do not abandon foraging in the low floral cover of minor-flowering crops in favour of the high floral cover of mass-flowering crops (Bänsch et al., 2020). In studies examining the amount and composition of habitat allocated to bee conservation however, in excess of 90% of wild bees are bumblebees (Holland et al., 2015). Similarly, the vast majority of bees observed in minor-flowering crops are bumblebees (Bänsch et al., 2020).

As social bees, bumblebees generally outnumber other native pollinators like the solitary bee in both natural and man-made habitats (Goulson, 2010). As a result, bumblebees have

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[2] Bees gather pollen for brood production and therefore forage at higher rates than other pollinators like butterflies, who forage only for their own energetic requirements (Goulson, 2010).

been widely studied compared to other wild pollinators, and thus detailed information of their life history, dispersal ranges, dietary preferences, as well as the effects of specific landscape interventions on bumblebees, is known (Timberlake, 2019).

Equipped with longer tongues, greater tolerance for unfavourable weather, and the ability to *sonicate*[3], bumblebees outperform honeybees as pollinators in many crops, including tomatoes and apples (Delaplane and Mayer, 2000). Undeterred by wind, rain, and subzero temperatures, bumblebees visit and pollinate a greater proportion of flowers per bee than honeybees, while foraging for 24 hours a day (Goulson, 2010). Bumblebees also have higher visitation rates per minute and transport larger pollen loads (Delaplane and Mayer, 2000). This, coupled with the better studied dynamics of bumblebees, led to the development of an OCP focusing on the bumblebee within the current study.

Alternative wild bee taxa, like solitary bees, are likely to benefit from the conservation measures considered, as bumblebees are generalists and therefore their characteristics embody attributes of other wild bees (Timberlake, 2019). This has been verified by increases in overall wild bee abundance following habitat interventions (Holland et al., 2015). Consequently, bumblebee dynamics will be assumed true for solitary bees in the work following and the use of the term *bee* will refer to non-honey, wild bees, unless stated otherwise.

6.2.1.2 Habitat-Based Interventions

Bumblebees can be cultivated to provide pollination services commercially or by providing habitat comprised of appropriate nesting and foraging resources. Due to the high cost of a commercial approach, commercial colonies are better suited to intensive farming, such as in glasshouses, and thus a habitat-based approach is typically more affordable (Delaplane and Mayer, 2000) and has greater long term benefits for general conservation, including plant and animal richness and diversity (Korpela, Hyvönen, Lindgren and Kuussaari, 2013).

Although the overall amount of bee habitat within bumblebee dispersal ranges in agroecosystems impacts on bee abundance (Holland et al., 2015), conservationists typically advocate plantings along field borders as a means of counteracting declining wild bee populations (Lowe, Groves and Gratton, 2021). This simultaneously encourages wild bees to forage within crops and contributes to bee conservation (Häussler, Sahlin, Baey, Smith and Clough, 2017)

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[3] Certain flowers only release pollen when a buzz-pollinator such as a bumble or solitary bee (Delaplane and Mayer, 2000), vibrates the flower's anthers at a specific frequency (Goulson, 2010).

while requiring small, often unused, areas of land for conservation (Lowe et al., 2021).

With less land and investment commitment required, field margins have been shown to have a strongly significant effect on pollinator abundance and diversity compared to controls, in both Europe and the US (Lowe et al., 2021). These so-called edge habitats are favoured by bumblebees, providing wind protection and water retention, which acts to decrease energy expenditure (Bennett et al., 2014). Both grass margins and flower strips improve bee *fitness* (a proxy for reproductive capability) and thus colony reproductive success, while also increasing early and late-season pollination (Häussler et al., 2017). Sowing wild-flower strips however, largely independent of their shape, size, and in many instances, placement:

- rapidly increases pollinator diversity, services and abundance (Korpela et al., 2013),
- provides triple the benefit of grass margins (Häussler et al., 2017),
- incurs increased growth in bumble and solitary bee populations as floral cover improves with maturity (Lowe et al., 2021).

However, the increase in bee abundance, diversity and pollination services observed in wildflower strips and margin plantings (Korpela et al., 2013) is not always replicated within crop fields themselves, with bee visitation to crops often remaining unchanged, but not adversely affected or lessened (Lowe et al., 2021).

In order to accommodate the population growth expected from greater floral availability, habitat interventions should also provide adequate nesting habitat (Häussler et al., 2017). Both bumble and solitary bee foundress queens prefer linear borders like fence-lines, hedgerows and margins (O'Connor, Park and Goulson, 2017), or bare, sunny ground, in undisturbed patches, as nesting sites, as these conditions encourage colony development (Delaplane and Mayer, 2000). Artificial nest boxes in proximity to good floral coverage, can also be used to entice queens to nest at predetermined locations (Goulson, 2010).

The experimental scale required to understand the response of bee populations to habitat changes limits inferences that can be made from this process. Modelling can therefore be used to improve understanding of the system and facilitate management actions (Murray et al., 2009). In order to develop successful management strategies, models of bee populations are first needed to encapsulate bee behaviour and adequately model their response to landscape alterations (Olsson, Bolin, Smith and Lonsdorf, 2015), an overview of which is now given.

6.2.2 Modelling Bumblebee Behaviour

Ecological models commonly assume animal behaviour to be subject to laws of diffusion, accounting only for random movement with no cognitive ability or decision making (Svirezhev, 2008). The unsuitability of such an approach is apparent when modelling bees, whose colony behaviour has inspired complex, modern optimisation algorithms (Jawad et al., 2021), yet this same behaviour is often not reflected in models of bee populations themselves.

Colony activity ultimately revolves around gyne (virgin queen) production in mid to late summer, the success of which is reliant on season-long floral availability, as the greater their nutritious intake, the higher their fitness and the more gynes are produced (Delaplane and Mayer, 2000). Bumblebee colonies thus synchronise their activity with floral availability so as to maximise their fitness (Murray et al., 2009). The annual colony life cycle, shown in Figure 6.1, begins with a solitary phase wherein the foundress queen (mated queen) produces a brood during spring and incubates the larvae until workers emerge in early summer and take over foraging, commencing the social phase of the cycle (Timberlake, 2019).

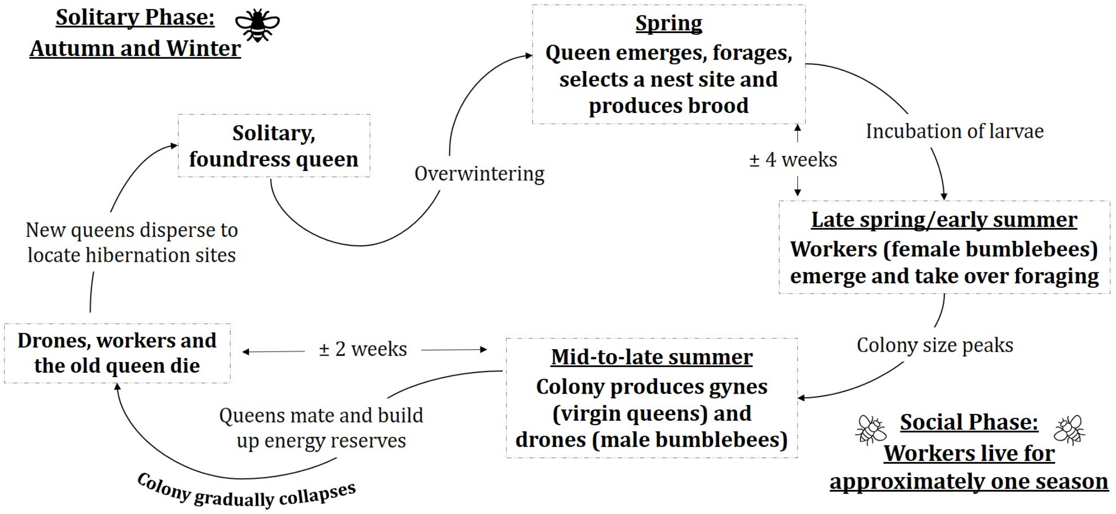

Figure 6.1: The annual life cycle of a bumblebee colony, adapted from Delaplane and Mayer (2000); Suzuki, Kawaguchi, Munidasa and Toquenaga (2009) and Timberlake (2019)

Emerging at low floral densities, bumblebee workers (females) reach their peak foraging workforce in mid-summer, at peak floral availability, and begin declining shortly thereafter as floral density declines (Holland et al., 2015). The colony then begins to produce reproductive individuals (drones/males and gynes) rather than workers (Delaplane and Mayer, 2000). Late-season floral resources benefit colony reproduction for the following year (Holland et al., 2015), aiding the new queens to build up energy reserves for hibernation, and subsequently, establish a new colony as a foundress (Suzuki et al., 2009).

Representing bee dispersal as a diffusive process rather than behaviour-based decisions may bear responsibility for contradictions between model predictions and empirical evidence, which demonstrates that both local and neighbouring floral coverage determines foraging behaviour (Olsson et al., 2015). Consequently, bee conservation would benefit from the inclusion of bee behavioural ecology (Bennett et al., 2014). Häussler et al. (2017) thus argues that it is necessary for models to be based on optimal foraging theory in order to create realistic predictions of both pollination and population dynamics. This would serve to improve current statistical approaches and management decisions (Häussler et al., 2017).

6.2.3 Optimal Foraging Theory

Optimal foraging theory is based on the marginal value theorem, which describes how foragers will behave in an environment of patchy resources so as to best exploit patch quality (Goulson, 2010). Optimal foraging theory thus supposes that foragers optimise their foraging practices to both minimise their energetic cost, and maximise their gain from patches (Delaplane and Mayer, 2000). This has been found to accurately describe worker bumblebee behaviour, who:

- forage to the exclusion of any other activity (Goulson, 2010),
- weigh up distance and floral quality in patch choice (Delaplane and Mayer, 2000),
- use systematic searches to determine an optimal foraging strategy to exploit the patchiness of floral resources at both a landscape and single plant level (Timberlake, 2019).

Model predictions therefore typically converge to observed data as patch size decreases, and are only minimally suboptimal in large patches (Goulson, 2010).

As central-place foragers, a bumblebee colony inhabits a fixed nesting site, which workers return to in between foraging trips (Suzuki et al., 2009). Like honeybees, bumblebees gravitate towards the patches of best floral quality through a process involving both individual and colony level decisions (Delaplane and Mayer, 2000). Habitat configuration thus critically affects bee fitness (Lonsdorf et al., 2009), with large dispersal ranges increasing energetic requirements and decreasing foraging efficiency, which ultimately reduces food provision to nests and therefore inhibits colony reproduction and development (Suzuki et al., 2009).

While bumblebees select foraging patches in a manner that maximises their fitness, the positioning of the nest critically affects foraging efficiency and colony growth (Suzuki et al., 2009), leading to the concept of central-place foraging theory (CPFT) (Olsson et al., 2015). This can help predict behaviour in the presence of variable floral cover, typical of mass-flowering crops, and thus be used to develop management strategies (Häussler et al., 2017).

Prior to Olsson et al. (2015), CPFT had been used to model acceptable foraging distances and loads, but not habitat use. However, both habitat arrangement and composition impact on patch choice by foraging bees (Bennett et al., 2014), with the optimisation thereof for wild bees, yet to be addressed (Pufal et al., 2017). Consequently, an OCP was developed in the current study, based on a CPFT model by Olsson et al. (2015), to maximise colony growth by controlling the placement of bee habitat within an agricultural area.

6.3 Optimal Control Problem

The majority of bee optimisation problems consider only economic or agricultural goals rather than conservation (e.g. Brosi, Armsworth and Daily, 2008; Gavina, Rabajante and Cervancia, 2014; Narjes and Lippert, 2019). Near-optimal layout of floral strips has been simulated for conservation purposes (e.g. Häussler et al., 2017), but neither OCT nor explicit optimisation were used. Before establishing bee habitat in agroecosystems however, an optimal management scheme should be developed, by means of an OCP, to determine the contribution thereof towards conserving declining bee populations (Klatt, Nilsson and Smith, 2020). This allows important factors, like the native bee taxa, to be taken into consideration to ensure that species-appropriate resources are provided at the relevant spatial scale (Murray et al., 2009).

The location of nesting and foraging resources, for example, affects foraging efficiency and colony development (Suzuki et al., 2009). A control, $B_{habitat}$, was therefore developed in the current study to represent the set of all patches in a two-dimensional domain C that should be dedicated to conservation habitat. $B_{habitat}$ further determines the optimal combination and location of patches used for nesting (B_{nest}), foraging (B_{floral}), and hedgerows (B_{hedge}) to ultimately increase bee fitness and consequently population growth by the end of a breeding season of length T, subject to bumblebee behaviour, which was described by CPFT.

Using CPFT, bumblebee fitness (G_N) relates the energy gained (E_N) while foraging in N patches within an environment to reproductive capacity, given that the bumblebee survives, with probability P_N, until a reproductive event (Olsson, Brown and Helf, 2008). This can be written as $G_N = P_N F_N$ where $F_N = E_N^x$, for $0 \leq x < 1$, is the expected energy contribution towards fitness (Olsson and Bolin, 2014). Amongst other factors, energy gains and predation risk are affected by the time spent foraging in some patch i (t_i), the time taken to reach patch i (τ_i) at flight speed v, and the time spent in the nest, given by h_N (Olsson and Bolin, 2014).

Additionally, bumblebees weigh up the floral quality of patches (A) within an environment with distance from the nest (Olsson and Bolin, 2014). Suppose the domain C can be divided into a grid of N patches, numbered $1, 2, \ldots, N$, where each patch has a location given by the coordinates $(x, y) \in C$, and a floral quality $A(x, y, z)$ for $(x, y, z) \in C \times [0, T]$. This can also be written as A_i for $i = 1, 2, \ldots, N$ at each time $z \in [0, T]$. Both notations will be used interchangeably throughout the chapter for both notational ease, and clarity, depending on the context. Then the set of all patches in the domain is given by $C = \{A_1, A_2, \ldots, A_N\}$.

A proportion of A_i, where $i = 1, 2, \ldots, N$, is lost to each bumblebee visit, resulting in competition for floral resources (Joseph et al., 2020). This has not been taken into account in previous CPFT models[4]. Interspecific competition was thus incorporated in the current OCP by depleting floral resources after bee visitation. Intraspecific competition (within colonies) was not included, and neither pollination nor competition by non-bee pollinators was accounted for in the OCP, as is typically assumed (Häussler et al., 2017).

The optimal control $B^*_{habitat}$ was then sought to determine the number and location of bumblebee colonies and habitat placed in C, as well as the optimal set of foraging patches required to maximise bee fitness, while minimising the area of habitat placed within crop fields ($C_{field} \subset C$). Since each colony inhabits a fixed nesting site, the number of colonies in C is equal to the number of nests in C, denoted J. For each nest j, where $j = 1, 2, \ldots, J$, the corresponding colony must then select an optimal set consisting of N_j^* patches, denoted S_j^*.

The optimal set of all foraging patches for all J nests is given by $S^* = \{S_1^*, S_2^*, \ldots, S_J^*\}$, which consists of a total of $N^* = \sum_{j=1}^{J} N_j^*$ patches. For ease of notation in the summations and subscripts following, patches in S^* were renumbered to correspond to the order in which they appeared in S^*, since the position of a patch in S^* is imperative to the OC strategy[5]. For example, if $S^* = \{A_{48}, A_{102}, A_{22}\}$, patches would be referred to by patch $i = 1, 2, 3$, with patch 1 denoting A_{48}, patch $2 \equiv A_{102}$ and patch $3 \equiv A_{22}$.

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[4] Including Häussler et al. (2017); Olsson and Bolin (2014); Olsson et al. (2015) and Lonsdorf et al. (2009).

[5] For example, A_N could be selected first based on floral quality versus distance.

The OCP can then be stated as, find N^*, S^* and $B^*_{habitat}$ in order to:

$$\text{maximise } G_N \text{ and minimise the land area of } (B_{habitat} \cap C_{field}) \tag{6.1}$$

subject to:

$$P_N = \exp\left\{-\left(\mu\sum_{i=1}^{N} t_i + \delta\mu h + \epsilon\mu\sum_{i=1}^{N}\tau_i\right)\right\}, \tag{6.2}$$

$$E_N = NL - c\sum_{i=1}^{N}(t_i + \beta\tau_i) - \alpha c h_N, \tag{6.3}$$

$$h_N = T - \sum_{i=1}^{N}(t_i + \tau_i) \geq 0, \tag{6.4}$$

$$\tau_0 = \tau_{max} + \frac{\omega}{A_i} \geq \tau_i \geq 0, \tag{6.5}$$

$$0 \leq (\text{Area of } B_{habitat}) \leq 0.06 \times (\text{Area of } C), \tag{6.6}$$

$$\emptyset = B_{hedge} \cap C_{field}, \tag{6.7}$$

for each patch $i = 1, 2, \ldots N$. Drawing on the depletion of floral quality by honeybees (Joseph et al., 2020), after all visits to patch i by colony (nest) j, and for each $j = 1, 2, \ldots, J$,

$$A_i = r(K_i - (1-d)^V A_i) + (1-d)^V A_i, \tag{6.8}$$

where $i \in S^*_j$ denotes the optimal set of patches for nest j. Thus, A_i is depleted proportionally to the total number of visits V by colony j, from its initial quality $K(x, y) = A(x, y, 0)$, where $(x, y) \in C$, prior to any foraging, and is renewed at rate r after all visits by nest j.

The contribution of patch i to the optimal set of patches (S^*) is described by the marginal fitness of patch i, namely $\Delta_i = G_{N^*} - G_{N^*-i}$ (Olsson and Bolin, 2014). Consequently, the nullcline of Δ_i (Olsson and Bolin, 2014), given by $\tau_0 = \tau_{max} + \frac{\omega}{A_i}$, constrains the maximum allowable travel time to and from a patch of quality A_i, where ω scales travel time and patch quality (Olsson et al., 2015) according to the systematic search technique of worker bumblebees (Goulson, 2010). The nullcline, bounded from above by τ_{max} ($\lim_{A_i\to\infty}(\tau_{max} + \frac{\omega}{A_i}) = \tau_{max}$), can thus be used to determine the optimum amount of time a bee spends in a patch.

The variables τ_{max} and ω are therefore dependent on the solution that maximises fitness, found by solving $\Delta = 0$ (contribution of all selected patches). Estimates of τ_{max} and ω can be obtained iteratively by assuming that there exists a patch of quality A_0, that takes τ_0 time units to reach, which can be added to the optimal set of patches S^* such that $\Delta = 0$ (Olsson and Bolin, 2014). At this patch, the foragers' fitness must satisfy $G_{N^*} = G_0$ and thus τ_{max}

and ω can be approximated by

$$\hat{\tau}_{max} = \frac{E_{N^*} - L}{E'} - \frac{xPW_1}{P'} \tag{6.9}$$

$$\hat{\omega} = \left(\frac{xPW_1}{P'} - \frac{xPW_2}{P'} - \frac{\dot{E}}{E'} \right) L \tag{6.10}$$

until $\hat{\tau}_{max} \to \tau_{max}$ and $\hat{\omega} \to \omega$, where W_1 and W_2 are Lambert W functions[6] defined by

$$W_1 = \text{Lambert W} \left(\frac{E_{N^*} P'}{E' P x} \exp \left\{ \frac{(E_{N^*} - L) P'}{E' P x} \right\} \right) \tag{6.11}$$

$$W_2 = \text{Lambert W} \left(\frac{E_{N^*} P'}{E' P x} \exp \left\{ \frac{(E_{N^*} - L) P'}{E' P x} - \frac{\dot{E} P' - E' \dot{P}}{E' P x} \right\} \right), \tag{6.12}$$

with $E' = \frac{dE}{d\tau} = c(\alpha - \beta)$, $\dot{E} = \frac{dE}{dt} = c(\alpha - 1)$, $\frac{P'}{P} = \frac{dP/d\tau}{P} = \mu(\delta - \epsilon)$ and $\frac{\dot{P}}{P} = \frac{dP/dt}{P} = \mu(\delta - 1)$. Parameter descriptions and values are given in Table 6.1. Equations (6.2)–(6.5) and (6.9)–(6.12) were taken either directly, or adapted from Olsson and Bolin (2014). A motivation for the atypical nature and corresponding complexity, or possible inability, of solving the OCP using classic OC methods can be found in Appendix C.

Table 6.1: Parameter values with arbitrary time (tu) and energy (eu) units (to balance foraging and travel times), obtained from Olsson et al. (2015), unless otherwise specified.

Symbol	**Description**	**Value**	**Units**
T	Length of the bumblebee breeding season	250	tu
v	Flight speed of a bumblebee	1	km/tu
β	Metabolic rate multiplier when flying	1.1	-
ϵ	Predation rate multiplier when flying	1.1	-
L	Load (pollen/nectar) carrying capacity	4	eu
c	Metabolic rate when foraging	4	eu/tu
μ	Predation rate when foraging	0.002	tu^{-1}
α	Metabolic rate multiplier when in nest	0	-
δ	Predation rate multiplier when in nest	0.1	-
x	Diminishing energy return	0.75	-
d	Proportion of floral quality lost per visit to pixel (calculated based on Joseph et al. (2020))	$\frac{47}{35000}$	-
r	Floral renewal rate (Joseph et al., 2020)	0.7	-

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[6] Supposing $we^w = a$ is a transcendental equation, then the Lambert W function is used to obtain the implicit solution $w = \text{Lambert W}(a)$ (Olsson and Bolin, 2014)

6.4 Genetic Algorithm Approach

To solve the OCP using the GA function in MATLAB, with default parameter values, a fitness function (f) was constructed from the objective in order to simultaneously maximise bee fitness and minimise the area of bee habitat placed in crop fields. Taking on the form

$$\text{maximise } f = G_N \ - [\text{Number of elements in } \ (B_{habitat} \cap C_{field})],$$

f was maximised in the GA to determine $S,^{*}$ N^{*} and $B^{*}_{habitat}$. By minimising the number of patches placed in crops, the area of bee habitat in crops was automatically minimised.

Bumblebee fitness was calculated using code from Olsson et al. (2015). With the exception of the functions *csHS* and *taucurve*, the code was altered substantially to cater for changes to the model, including the addition of floral depletion, constraints, controls, objectives, and a GA approach, which impacted the mechanisms of the model. For example, depleting floral quality meant that each colony could select a different number and combination of patches to forage in, and thus N^{*} was optimised for each nest over the breeding season of length T.

Following the encroachment of agricultural land into natural habitat, wild bees reside primarily in agroecosystems, with habitat intersecting with farmland fringes (Murray et al., 2009). The success of bee conservation within agroecosystems thus depends on its uptake within the agricultural community. The less inconvenient and more cost effective a strategy, the more likely it is to be adopted by farmers (Klatt et al., 2020). Consequently, the domain upon which the OCP was implemented was structured to incorporate these factors.

6.4.1 Domain Construction: Layout and Discretisation

Due to the variety of locations appearing in literature (e.g. the UK, US and Sweden), farmlands differ considerably. Simple landscapes are both easier to model and present the greatest threat to wild bee declines (Landis, 2017) and thus improving bee abundance there is critical. A simple landscape, while artificial, can also be adjusted to reflect an actual location.

Consequently, a relatively simple domain C was constructed, containing four separate crop fields and their internal margins (denoted $C_{field} \subset C$) and a 10 m border around the entire domain ($\Omega \subset C$) composed of a 5 m wide domain boundary $\partial\Omega$ and the 5 m crop field margins running along the inside of the boundary, given by $\Omega \backslash \partial\Omega$. This is shown in Figure 6.2, for the reasons next outlined. Habitat is to be primarily implemented on $\Omega = \{\Omega_1, \Omega_2, \Omega_3, \Omega_4\}$, where Ω_i refers to the border along the edge of C numbered i, as it is preferable to place as little habitat as possible in C_{field}, and if so, within C_{field}'s internal margins.

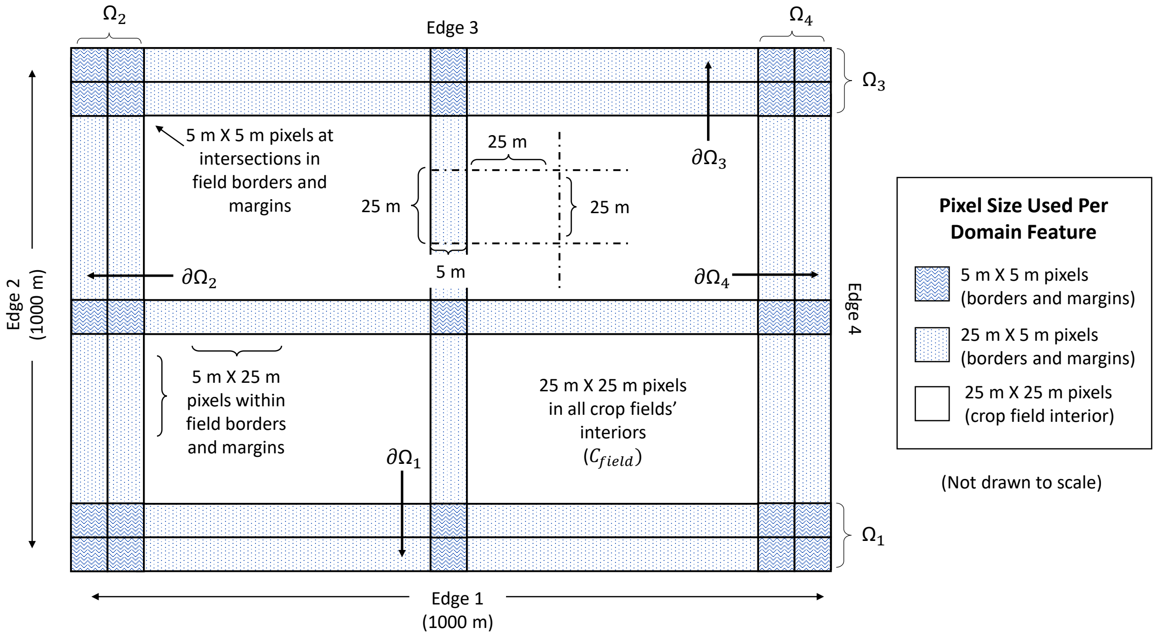


Figure 6.2: An unscaled diagram of the subdivision of C into foraging pixels

The majority of bumblebee species forage within a 1 km radius, with the dispersal ranges of most species lying between 750 and 775 m (Murray et al., 2009). C was thus simulated as 1 km^2, which is also in keeping with field studies that are usually conducted over 100 hectares (equivalent to 1 km^2) (Holland et al., 2015). Furthermore, solitary bees have much shorter flight ranges (Gathmann and Tscharntke, 2002), well within these dimensions.

Bumblebees favour hedgerows, fence-lines, margins and field boundaries, with these edge habitats capable of supporting triple the wild bee density of any other habitat (Holland et al., 2015). The proportion of edge habitat to total agricultural land decreases with increasing land size however, resulting in a lack of nesting resources, thereby restricting bumblebee colony growth and crop pollination (Goulson, 2010). Consequently, doubling typical margin widths from 2.4 m to 4.8 m significantly improves nesting potential (Häussler et al., 2017) by decreasing the amount of disturbance experienced at nest sites (Delaplane and Mayer, 2000).

Similarly, artificial nest boxes are colonised more readily in undisturbed areas (Goulson, 2010) such as wider margins, provided these margins are not herbicide treated or ploughed, but are instead dedicated to conservation purposes (Delaplane and Mayer, 2000). Field margins and borders in the domain C were therefore modelled as 5 m, which enabled a simpler landscape subdivision than 4.8 m. This is typically the most acceptable strategy to landowners as the borders and margins are most often unused and thus less agricultural land is removed from crop production (Lowe et al., 2021).

Lastly, bee foraging patches (or parcels) are usually 25 m by 25 m, and thus this grid size is typically used as a landscape unit measure in bee models (Häussler et al., 2017; Suzuki et al., 2009), referred to as a pixel. To model both crop fields and margins however, the land was divided into various pixel sizes, with crop fields modelled as 25 × 25 m, field margins as 5 × 25 m, and intersections between borders and margins as 5 × 5 m. These dimensions allowed for a simple, albeit non-uniform, subdivision of the landscape into 44 × 44 pixels.

6.4.2 Composition and Design of Controlled Habitat

As central place foragers, bees return to the nest to feed offspring between foraging trips (Lonsdorf et al., 2009) and thus nest placement should ensure access to foraging resources within typical dispersal ranges (Olsson et al., 2015). Consequently, the optimal placement of nesting (B^*_{nest}) and floral (B^*_{floral}) resources contributes to bee fitness and thus conservation. Moreover, hedgerows (B^*_{hedge}) provide habitat suitable for nesting, foraging, and general biodiversity, and thus act to increase the resilience of agroecosystems (Landis, 2017).

While there are a number of habitat interventions in literature, the controls in Table 6.2 were designed to incorporate the conservation measures expected to deliver the most benefit, for the reasons next outlined. There is, however, little precedence for bee habitat patch size in farmland, with patches ranging from as little as $16\,\mathrm{m}^2$ to $50\,000\mathrm{m}^2$ (Lowe et al., 2021), and both strips and blocks sown (Holland et al., 2015). Nonetheless, analyses of pollinator plantings have found that patch size does not affect either the abundance or diversity of bumblebee species observed in patches (Lowe et al., 2021). Patch sizes in the controls were therefore kept relatively small as the accuracy of CPFT models is increased under such circumstances (Goulson, 2010). B_{hedge} dimensions were based on Klatt et al. (2020).

Similarly, bumblebee responses to wild-flower strips are independent of the design, such as length or breadth, and robust to characteristics such as floral composition, thus fostering their flexibility as a conservation measure (Korpela et al., 2013). Floral strips also provide greater benefit to bumblebees than grass strips, and deliver an overwhelming proportion of the benefit when in combination with grass strips (Häussler et al., 2017). With land a limited resource, a combination of floral resources should therefore be sown so as to provide continuous floral

Table 6.2: Properties of the control variables making up $B_{habitat}$.

Control	**Description**	**Size (m)**
B_{hedge}	Provides both good floral quality and nesting, with nest sites every two pixels on average (1 nest per 250 m^2)	5×1000
B_{nest}	Artificial nest erected with supporting habitat, e.g. a grass buffer strip, established in a patch around the nest to ensure the nest remains undisturbed	$5{\times}5, 5{\times}25$, or 25×25
B_{floral}	High floral quality patch (usually clover or wild-flowers), suited to both the local bee taxa and agroecosystem properties, e.g. climate and soil, that provides continuous floral availability throughout the colony life cycle	$5{\times}5, 5{\times}25$, or 25×25

availability for the duration of the colony life cycle (Hemberger et al., 2020) as bumblebees need access to pollen in the vicinity of nests during breeding season (Klatt et al., 2020). Floral composition can further be varied to suit characteristics of the agricultural land, such as soil type, and optimised for the dominant local wild bee taxa (Korpela et al., 2013).

In addition, the allocation of nesting habitat should take into account both species-specific foraging ranges and the availability of nest construction materials (Murray et al., 2009). Alternatively, artificial nest boxes can be provided, positioned where they can remain long-term as relocation results in bumblebee stress with workers unable to locate the nest and queens abandoning the nest or reverting to foraging (Delaplane and Mayer, 2000).

Lastly, hedgerows provide important habitat corridors for bumblebees, being conducive to nesting, navigation (Osborne et al., 2008), and generating more foraging resources per unit area for the majority of the year than any other farm habitat (Timberlake, 2019). Hedgerow placement is restricted to borders as it would be impractical within crop land and thus deter farmers from adopting conservation incentives. Greater benefits to both bee diversity and conservation are obtained, however, when habitat is implemented along field edges or margins, as this creates connectivity between habitats (Korpela et al., 2013).

Not only do hedgerows with good foliage coverage support double the bumblebees of low quality habitat, but this value is transferred into surrounding crop fields (Garratt, Senapathi, Coston, Mortimer and Potts, 2017). A nest site was thus modelled every two pixels (5×50 m) in B_{hedge}; exceeding the minimum observed distance of 2 m between colonies (Harder, 1986). This coincides with observations of bees establishing double the nest densities in linear features compared to non-linear features (Osborne et al., 2008). Planting hedgerows along edges in agroecosystems, which proportionally have few linear features (Goulson, 2010), thus produces conservation benefits far exceeding the loss of crop land (Osborne et al., 2008).

6.4.3 Encoding the Control as a Chromosome

Before determining the number and location of B_{nest} erected, B_{floral} sown and B_{hedge} established, if any, within the domain, $B_{habitat}$ was subjected to various constraints in order to construct a chromosome of fixed length. This approach had associated advantages, for example, inequality constraints involving habitat allocations (Equation (6.6)) were built into the chromosome encoding, thereby avoiding having to implement penalty terms (Section 2.6.1).

Let the allele corresponding to gene i in the chromosome of length $n = 55$ be denoted g_i, for $i = 1, 2, \ldots n$. Then, each chromosome was structured so that the value, or habitat type, the control assumes was encoded in genes $1 - 21$, and the pixel where a patch is placed, in genes $22 - 55$. This correspondence between control and its encoding in the chromosome is illustrated in Figure 6.3, followed by explanations for the encoding constructed.

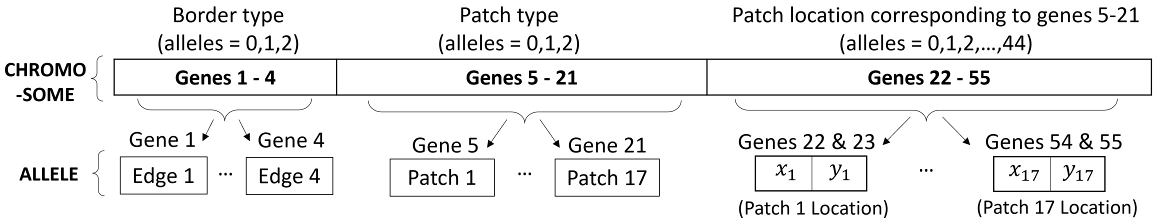


Figure 6.3: Chromosome encoding of the habitat controls in the bumblebee OCP

The minimum area of conservation habitat in policy typically equates to approximately 1.5% of farmland, with farmers generally setting the maximum acceptable allocation at 6% (Holland et al., 2015). Since the pre-allocated land in C, consisting of widened borders and margins corresponds to 4.9375% of the modelled area, and B_{hedge} should ideally be placed along edges, genes $1 - 4$ were used to dictate whether a hedgerow ($g_i = 1$) or floral-hedgerow combination ($g_i = 2$) would be placed on edges $1 - 4$, or whether the designated area would revert to crop usage ($g_i = 0$), with corresponding edge and gene positions for $i \in [1, 4]$.

The remaining 1.0625% of conservation habitat equates to 17 additional patches of pixel size 25 m × 25 m. To encode each of these patches, along with coordinates for their placement, an additional 51 genes were required. The 17 additional patches were therefore encoded in genes $5 - 21$, where the allele value denotes the habitat type placed. Namely, $g_i = 1$ referred to a B_{nest}, $g_i = 2$ to a B_{floral} patch and $g_i = 0$ to nothing. The alternating (x, y) coordinates corresponding to the location of each patch, were then encoded in genes $22 - 55$.

6.4.4 Initial Floral Quality

The initial floral quality of C, given by K, is dependent on both crop quality and $B^*_{habitat}$. Consequently, a translation from the chromosome encoding to the associated control intervention in the OCP is given in Table 6.3. A floral quality, scaled arbitrarily between 0 and 25, was then assigned to each control variable, as can be seen in Figure 6.4a. Since B_{floral} provides the highest floral quality, $K_i = 25$ when patch $i \in B^*_{floral}$. Similarly, B^*_{hedge} provides good foraging and nesting, and thus $K_i = 18$ when patch $i \in B^*_{hedge}$. B^*_{nest} however, has low floral quality, and thus $K_i = 5$ when patch $i \in B^*_{nest}$.

Table 6.3: Translation from chromosome encoding to $B^*_{habitat}$ in C.

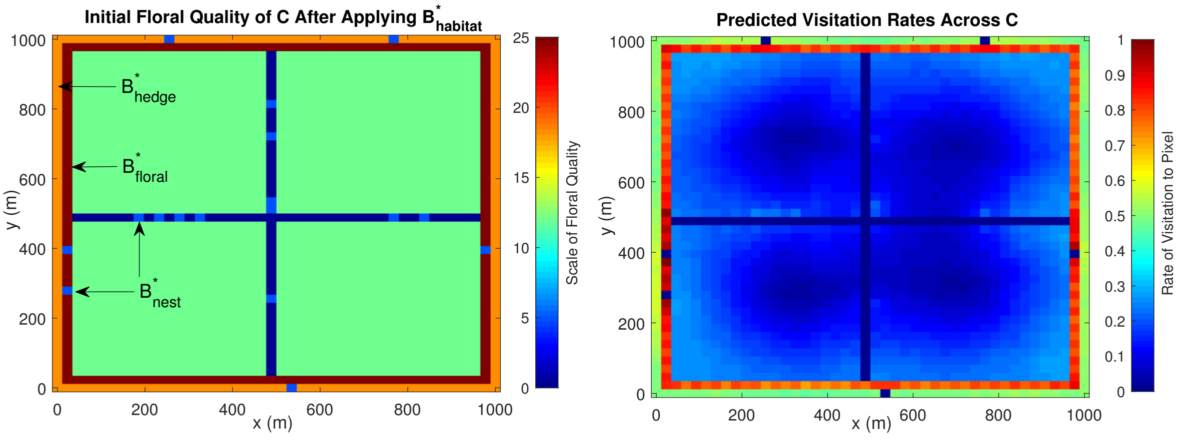
	Habitat type specified by allele $\mathbf{g_i}$, for $\mathbf{i = 1, \ldots, 21}$		
	$\mathbf{g_i = 0}$	$\mathbf{g_i = 1}$	$\mathbf{g_i = 2}$
If $i \in [1, 4]$ $\mathbf{\Omega(x, y, 0)} =$	$\Omega_i(x, y, 0)$ $\forall\ (x, y) \in \Omega_i$	B_{hedge} $\forall\ (x, y) \in \partial\Omega_i$	$B_{floral}\ \forall\ (x, y) \in \Omega \backslash \partial\Omega_i$ $B_{hedge}\ \forall\ (x, y) \in \partial\Omega_i$
else if $i \in [5, 21]$ $\mathbf{C_{field}(x, y, 0)} =$	$C_{field}(x, y, 0)$	B_{nest}	B_{floral}
	where $(x, y) = (\mathrm{g}_{(2i+12)}, \mathrm{g}_{(2i+13)})$ is the pixel location		

To determine an optimal layout of conservation habitat, crops were simulated as possessing medium floral quality, namely $K_i = 12.5$ when $i \in C_{field}$. This floral quality was chosen as it can reasonably represent either a minor or a mass-flowering crop, depending on when in the crop-blooming season the strategy is implemented. In minor-flowering crops, this relatively low floral quality would be seen at the peak of floral availability, whereas in mass-flowering crops, a medium floral quality would be observed in the late-season

In both instances, floral resources act as the limiting factor in colony reproduction and thus additional foraging and nesting habitat would be required to sustain colony development and reproduction. Furthermore, many minor-flowering crops depend on wild bees to produce sufficient yields, and up to three quarters of bees observed in these crops are wild bees (Bänsch et al., 2020). Consequently, the GA was run 30 times using this initial floral quality, and the chromosome with maximum fitness (maximisation OCP) out of all 30 final generations was selected as the optimal solution. These GA results are presented next.

6.5 Genetic Algorithm Results and Discussion

The GA-generated optimal control, $B^*_{habitat}$, placed a combination of hedgerows and floral strips around the entire domain, using all pre-allocated land, as shown in Figure 6.4a. These habitats provided the highest floral quality in C, addressing the lack of floral resources presented by the crop. No other floral resources were placed in C, with $B^*_{habitat}$ instead dictating that all remaining habitat should be nesting sites. The majority of nest sites were placed along internal field margins, and none within C_{field}. The nest sites expected to be established in hedgerows by bees can be located by observing the nest fitnesses in Figure 6.5a.



(a) Initial floral quality K of C

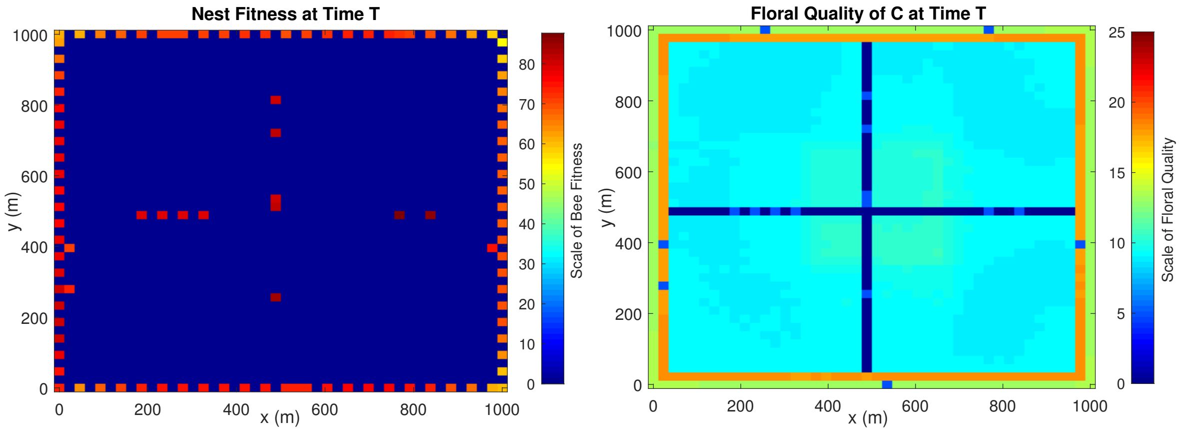
(b) Bee visitation rates

Figure 6.4: The GA-derived initial floral quality of C, after the placement of $B^*_{habitat}$, and the corresponding predicted visitation rates to landscape pixels

A total of 4.0975% of C was allocated to bee habitat by the optimal control which is well within the allocation considered acceptable to farmers. Since hedgerows were positioned on every edge and all control patches selected as nests, the total number of nests in C corresponds to 1.04 per ha which coincides with observed values (O'Connor et al., 2017). Only 17 of these nests are artificial nest boxes placed by the farmer, which was considered reasonable.

Based on the optimal arrangement of bee resources, predicted visitation rates to pixels within C are given in Figure 6.4b, which gives an indication of crop pollination (Häussler et al., 2017). Floral strips can be seen to encourage the greatest foraging rates, particularly in close vicinity to nests. Minor foraging takes place in crops, which is concentrated in the outermost corners and decreases towards the interior of each crop field with distance from both nests and floral resources. This can be expected in landscapes with relatively low floral quality, where bumblebees will instead be drawn to floral patches (Korpela et al., 2013).

The effects of floral depletion and competition can be seen in the differing nest fitnesses given in Figure 6.5a. Greater crowding and therefore more competition for resources in the corners of the domain resulted in lower nest fitnesses, whereas the relatively isolated nests, around $(x, y) = \{(500, 200); (800, 500)\}$, have much higher fitnesses, even though further from the best floral quality. Furthermore, at time T, floral quality can be seen to have depleted quite substantially in Figure 6.5b, owing to the high visitation rates. The pattern of depletion differs slightly from that of visitation rates since floral quality was only depleted after all visits by an entire colony and not after each visit, as is mapped by visitation rates.



(a) Colony nest fitness

(b) Floral quality at T

Figure 6.5: The expected fitness of each colony's nest, based on the predicted foraging patterns, and floral quality after foraging throughout the breeding season of length T

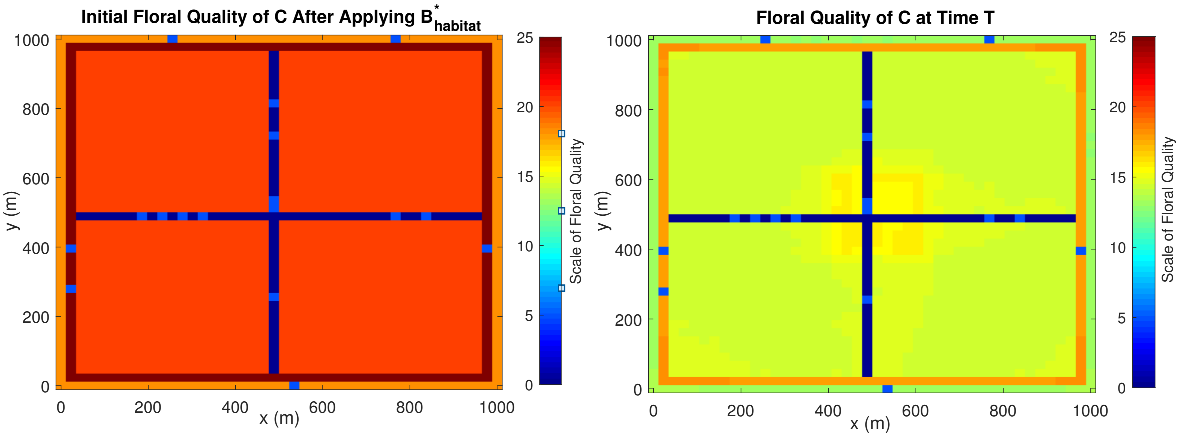
In accordance with bumblebee observations, some competition can be seen between B^*_{floral} and crop fields, with bumblebees visiting B^*_{floral} at higher rates, demonstrating the trade-off between patch quality and distance from the nest. This apparent competition, however, can be expected to decrease soon after habitat establishment as bumblebee populations increase as a result of the additional nest and floral resources (Häussler et al., 2017).

Overall, GA results corresponded with bumblebee behaviour, management interventions, and strategies acceptable to farmers, with nest fitness appearing to depend on habitat layout. Wild bee abundance can be expected to increase with the habitat instituted by $B^*_{habitat}$ (Holland et al., 2015; Timberlake, 2019), benefiting from both the increased connectivity resulting from B^*_{hedge} (Korpela et al., 2013), and the increased heterogeneity of C (Pufal et al., 2017). Since the GA was shown to produce near-optima in Chapters 4 and 5, it was assumed that the conservation strategy generated by the GA in the current chapter was at least near-optimal and maximised bee fitness in a crop of medium floral quality. The optimal (maximum) GA solution[7] had a fitness function value of $f = 7368.05259$ to four significant decimal places.

6.5.1 The Impact of Changing Floral Quality on the Optimal Solution

The GA solutions in Section 6.5 correspond to either a minor-flowering crop at peak bloom, or a mass-flowering crop in the late-season, at the end of bumblebee seasonal activity. Supposing the latter were true, then $B^*_{habitat}$ was determined when the crop had passed its peak bloom and floral quality was in decline. Consequently, during the mass-flowering crop's peak blooming events in the years following, the floral quality of crops would be much higher.

Both the spatial and temporal availability of floral resources in agroecosystems impact bee fitness (Hemberger et al., 2020). Mass-flowering crops create pulses in foraging resources (Lowe et al., 2021), and thus boost colony growth during peak floral availability, but fail to provide sufficient resources in the late season when resources are diverted to reproduction (Häussler et al., 2017). While keeping the optimal layout of $B^*_{habitat}$ determined previously constant, the impact of higher crop quality was thus investigated by assigning $K(x, y, 0) = 20\,\forall\,(x, y) \in C_{field}$. The resulting floral quality of C can be seen in Figure 6.6a.



(a) Initial floral quality K

(b) Floral quality at T

Figure 6.6: The initial floral quality of C during a mass-flowering event, after establishment of $B^*_{habitat}$, and the subsequent quality after foraging for time T

To ensure the optimal controls were left unchanged, that is, neither their location, type, nor quality was altered, $B^*_{habitat}$ was inputted in the GA, and predicted bumblebee visitation

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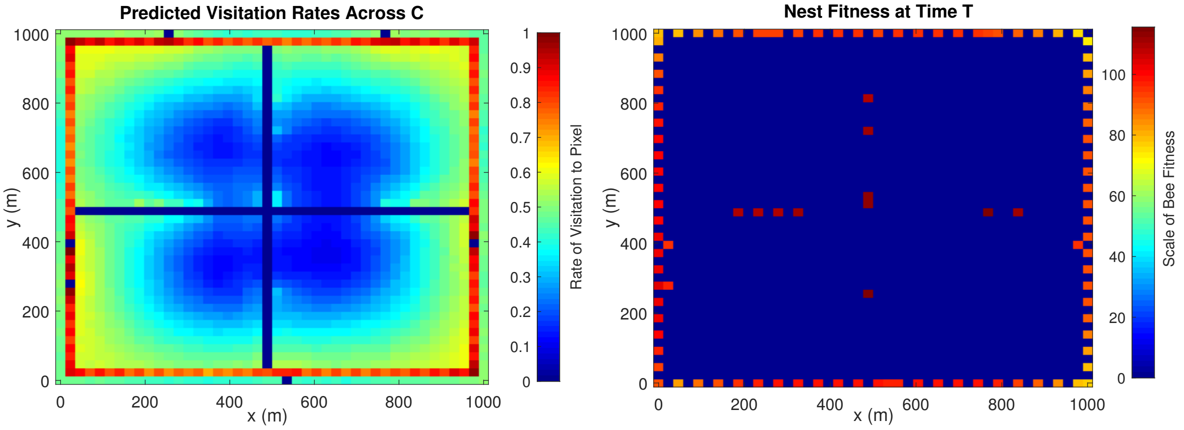
[7] The average of the 30 GA fitness function values was $f = 7236.1988$, with a standard deviation of 65.4561.

(Figure 6.7a), nest fitness (Figure 6.7b) and subsequent floral depletion (Figure 6.6b) were generated when accounting for higher floral quality in crop fields. Although nest fitness increased when crops were assigned a higher initial floral quality, similar, albeit more clearly defined, trends can be observed in the predicted visitation rates shown in Figure 6.7a, and floral depletion (Figure 6.6b) compared to the late-season (Figures 6.4b and 6.5b).



(a) Bee visitation rates

(b) Nest fitnesses

Figure 6.7: Predicted visitation rates to pixels within the landscape and the corresponding fitness of each nest in the early season of a mass-flowering event

Naturally, constantly high floral availability benefits colonies more than high, but pulsed, availability, however worker mortality and drone production are relatively consistent under either of these conditions and in some cases, bumblebees are able to store excess resources during periods of high availability (Hemberger et al., 2020). Similarly, the benefits of late-season resources in mass-flowering crops to solitary bees, accumulate throughout consecutive years (Pufal et al., 2017). Consequently, the GA's habitat interventions can be expected to benefit bumblebee fitness and thus reproduction, regardless of the crop quality.

6.6 Concluding Remarks

An OCP was formulated to address the conservation of wild bees using habitat interventions in agroecosystems in the current chapter. A GA was then used to obtain an optimal strategy that would maximise bee fitness at the end of a breeding season. This served to investigate the second research aim (Section 1.3), namely to examine the performance of an EA in a realistic ecological OCP, where classic OC methods are excessively complex, or inapplicable.

The results generated by the GA were in alignment with interventions shown to improve colony fitness in practice, while also producing a strategy that is likely to be acceptable to landowners. Furthermore, based on the designated conservation habitat placed within the agricultural area, bee fitness, and thus reproduction, can be expected to improve in either mass or minor-flowering crops. Since the GA performed sufficiently in previous chapters, the realism of the results further served to justify the validity of the GA solution.

Various assumptions, including the layout of crop fields and the chromosome encoding, may have impacted the solution and could thus be improved upon in future work. For example, a more complex domain with less floral scarcity could be simulated, or the OCP applied to a real landscape. The chromosome encoding could also be adjusted to allow for a greater variety of layout options, such as the length of hedgerows or floral strips along edges.

Similarly, the assumption that competition is only interspecific between bee colonies could be addressed in future work by improving the model of bee behaviour. The assumption that bee colonies can simply be placed at nest sites or that colonies will translocate to nest sites, could also be more carefully considered. The complexity involved in addressing such, however, may not be justified, as results appeared reasonable in the current, less complex, model.

With climate change expected to increase the already disproportionate climatic influence on bees, more radical habitat changes may be needed, for example, encouraging organic farming which can support up to eight times more bees and triple the species diversity of conventional agriculture (Murray et al., 2009). Similarly, research is needed to model the impact of pesticides, grazing, and climate change on bees, and interventions to mitigate these factors or mediate bee responses (Hanberry et al., 2021).

GAs may provide a means to address these, and other, ecological research gaps, having been shown to provide a viable, alternative way in which to implement OC in ecological OCPs throughout the entirety of this study, suitable in ordinary, complex, or atypical OCPs. Furthermore capable of generating realistic management strategies, GA strategies can also easily be altered to accommodate the increasing importance of adaptive management practices. As demonstrated in this research, GA-use in ecological OCPs could therefore contribute towards addressing many of the ecological challenges facing society. The investigation in this study sought to examine this under-explored potential, key findings of which are summarised in Chapter 7, along with limitations and future research directions.

Chapter 7

Conclusions and Future Work

7.1 Introduction

Ecological systems are inherently difficult to control. Consequently, classic OC methods often require complex mathematical knowledge to produce useful solutions. Inspired by ecological systems themselves, the flexible EAs may provide an alternative to classic OC methods in ecology. Despite the undeniable success of EAs in an OC capacity in many disciplines, the potential of EAs in ecological OC remains under-explored, with EAs seldom applied to ecological OCPs. Motivated by the desire for methods to better manage ecological systems, this research proposed to investigate the viability of an EA approach as an alternative to classic OC methods in ecological OCPs; formalised as the research question in Section 1.2.

The conclusions drawn from this investigation are presented in the current chapter. Firstly, the research is summarised in Section 7.2, where it is argued that a GA is a viable alternative to classic OC methods. Key findings and contributions to existing knowledge are then given in Section 7.3, followed by limitations and future work recommendations in Section 7.4. Lastly, concluding remarks are made in Section 7.5.

7.2 Research Summary and Conclusions

To comprehensively examine the research question and thereby establish the viability of an EA approach to ecological OCPs, two research aims (Section 1.3) were investigated. Four case studies pertaining to current ecological issues were nominated to facilitate the research aims, and were presented in order of increasing complexity. The first three case studies served as a basis for comparison between an EA and classic OC methods; forming the comparative component of the research. Existing OCPs were selected in this respect. The final case study was developed and formulated as an OCP in the exploratory component of the research.

The primary aim of this study sought to determine whether an EA is capable of achieving sufficient accuracy (compared to classic OC methods) when applied to ecological OCPs. To investigate this, related literature was reviewed in Chapter 2 and appropriate case studies, classic OC methods and an EA were identified. Comparisons were then conducted in Chapters 4 and 5, where results obtained using an EA were compared to results found using classic OC methods according to the methodology established in Chapter 3. Increasing complexity was incorporated with each successive case study.

To begin with, a relatively simple predator-prey OCP was solved using the FBSM in Section 4.2. Next, a dengue OCP that has previously been solved using a variety of classical approaches was examined in Section 4.3, due to both the comparative capacity it represented, and the increasing complexity incurred by the presence of non-convexity. Lastly, a PDE-based raccoon-rabies OCP, representing the importance of including spatio-temporal dynamics, was solved using the FBSM in Section 5.4.

To maintain tractability of the study, only a single EA was applied, with a GA chosen as most suitable. To get a comprehensive picture of the GA's performance as an OC method, the GA was run 30 times for each OCP formulation considered. Even at its worst, the GA produced accurate solutions, comparable to the corresponding classic OC method(s). Summarising statistics, not presented in totality in-text, are supplied in Appendix A to substantiate this observation. The results obtained in the comparative chapters addressed the primary aim, demonstrating that a GA is capable of accurately replicating classical OC solutions. Results further supported the hypothesis (Section 1.2) that a GA increases the ease of applying OC by avoiding a substantial amount of mathematical theory associated with the classic OC methods with which the GA was compared, while maintaining accuracy.

Results, however, indicated that both the control formulation and encoding, as well as the quadrature used to evaluate fitness/objective functions affected the accuracy of GA solutions. The relative impact was dependent on the OCP under consideration and was related to the complexity of the OCP, the OCP formulation and the corresponding computational requirements. In the ODE case studies, the accuracy of the control was dependent on the accuracy of the quadrature used. This was to be expected, as the fitness (objective) function in the GA determines the optimality of each candidate optimal control. Hence, the more accurate the assessment of the control by the quadrature, the more accurate the control, and consequently, the more accurate the optimal solution. All optimal strategies found by the GA, however, appeared reasonable and either conformed with, or were considered sufficiently accurate compared to the corresponding classic OC method.

Although the accuracy of GA results deteriorated slightly with increasing case study complexity, it was deemed reasonable to conclude that the comparative chapters established a GA as a viable alternative to classic methods in ecological OCPs; thereby supporting the research question. The GA results also appeared to support the hypothesised increased ease associated with applying OC using a GA in ecology, whilst producing satisfactory results.

Due to the promising results obtained in the comparative chapters and the consequent fulfilling of the primary research aim, the secondary aim (Section 1.3) was then investigated in Chapter 6. This consisted of the exploratory component of the research which sought to determine how the EA (namely a GA) would perform in an unconventional OCP framework, to which classic OC methods could arguably not be applied. Since no comparison was available in the exploratory component, more ecological detail was given to guide the OCP formulation and subsequently assess the optimal solutions produced and, ultimately, substantiate results.

The final case study was formulated to simultaneously address the pertinence of wild bee conservation in agroecosystems and the second research aim. Consequently, the OCP formulation prioritised ecological considerations over mathematical considerations, resulting in an unconventional OCP that would be exceptionally difficult, or even unsolvable, classically. The resulting GA-based OCP formulation was intuitive and logically straightforward, but exceedingly complex to solve within a classical framework, and was solved using only a GA.

The resulting near-optimal solution not only satisfied all problem constraints but was also in accordance with current management strategies found to be successful in practice, appearing both realistic and implementable, thereby supporting the feasibility of results. Moreover, the optimal solution was robust to variation in crop qualities. This acted to further support the research question and hypothesis.

Based on recommendations to examine any possible ecological repercussions that either the objective or control formulation may have (Barbour et al., 2016), these two factors were examined in all case studies. As is often the case in solvers, the accuracy and performance of the GA relied on both the order of quadrature used and the choice of control representation. Each OCP was susceptible to and responded to each of these factors differently.

In the ODE-based OCPs, a simple and general control encoding was possible which avoided restricting the control form. This was considerably more complex to accomplish in the PDE-based OCP, primarily due to computational constraints. Nonetheless, differences between the GA and FBSM-derived controls in the PDE problem had little impact on either the optimal solution or the objective value. The control form can also easily be altered in a GA approach, which could improve the correspondence between the GA and FBSM controls.

There were also no apparent adverse ecological implications emanating from the control forms applied. The GA control strategy in the raccoon-rabies OCP (Section 5.5) for example, while different to the FBSM, produced final population classes almost identical to the FBSM's solution (Section 5.4.2), and is thus unlikely to have any unforeseen adverse effects. Moreover, the transitioning of optimal solutions to a realistic setting, which requires rounding, would make the differences observed between GA and classical solutions obsolete. Similarly, the bumblebee OCP (Section 6.5) is in keeping with realistic practices.

A wide variety of classic OC schemes exist and with them a variety of so-called optimal results. Different schemes commonly produce different optima and yet all are termed optimal, having been found using classic OC methods. A GA performed on par with these methods in this study, thus proving to be a viable alternative to classic OC methods. As a representative EA, the GA performance thus acts to advocate an EA approach to ecological OCPs.

7.3 Key Findings and Contributions to Existing Work

When comparing a GA to a classic OC algorithm, the numerical methods and discretisation used should ideally be kept constant by the researcher to ensure that the only implementation factor that differs in the comparison is the algorithm itself. Under these circumstances, the major difference between the approaches is the derivation of the control(s). Implementation factors, however, are not always explicitly stated by researchers.

Excepting the dengue OCP, classical results were therefore reproduced within this study so as to conduct as thorough a comparison as possible[1]. Where this was not possible, implementation differences may have impacted observations and reduced their generalisability.

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[1] The GA and FBSM had different stopping criteria in keeping with the differences in algorithm approach. A larger stopping criterion, however, could improve GA efficiency and should thus be examined in future work.

This study, however, endeavoured merely to establish whether or not an EA approach is a viable alternative to classic OC methods, key findings of which were as follows:

1. A GA is capable of producing accurate solutions, on par with the classical, global optimum guaranteeing FBSM, and comparable to the direct methods.
2. A GA approach bypasses non-trivial mathematical theory, arguably increasing the ease of applying OC to ecological OCPs. Additionally, a GA approach considers a much smaller system of equations - approximately half the size of its classical counterpart.
3. Numerical integration methods play a role in the accuracy of optimal solutions produced by the GA. This is, however, true of classic OC methods as well.
4. The control formulation impacts GA performance.
5. The GA takes much longer (computational time) than the FBSM to generate an optimal solution, particularly in a PDE-based OCP, but is still reasonably quick in ODE-based OCPs. This scales up considerably with increasing problem complexity.

Consistent with the fundamental differences between an EA and a classical approach, the primary concern of the GA approach is the formulation and subsequent encoding of a control. By avoiding mathematical theory, the theoretical optimal control is forfeited and an appropriate control form must be determined. Typically, the user must design and encode as general a control as possible (without biasing the optimal solution) which can become a disadvantage of the GA approach. A general control could be formulated in a relatively straightforward manner in the ODE-based OCPs, as there was dependence on only a single variable, but the general control formulation did not translate well to the PDE-based OCP.

Nevertheless, accurate results were obtained while avoiding disadvantages associated with classic OC methods, such as extensive mathematics. While in some cases it may be excessively complex to derive an optimal control using classic OC methods, a set of mathematical rules exist whereby an optimal control can be obtained, whereas this is subject to user-preference in the GA. This can, however, be an advantage in unconventional OCPs since a GA allows the user to adapt the control to problem type, as demonstrated in the final case study.

The viability of an EA approach as an alternative to classic OC methods in ecological OCPs has, to the best of the author's knowledge, not been previously investigated. While it is widely acknowledged that an optimal solution is not guaranteed by EAs like the GA, comparisons are seldom used as a means of ascertaining the extent of GA accuracy ecology. As demonstrated in this study, from simple to complex, ODE to PDE, caveat-based to exploratory, a GA approach is capable of adequately replicating OC results found using typical conventional techniques; both when applying the FBSM (capable of obtaining global optima) and two prominent solvers that have been widely applied to a broad range of OCPs.

Moreover, the differences observed between GA and classical results were less than those observed between classical schemes in literature. There is also more leeway in a GA versus a classical approach to ecological OCPs, as GAs are not constrained by the assumptions necessary to classic OC methods. Consequently, a GA can be applied to OCPs that cannot be solved using classic OC methods, and could therefore contribute to increasing OCP realism. By investigating the feasibility of an EA as an OC method in ecology, the research thus addressed, in part, a research gap, and acts to motivate further investigation in this regard.

7.4 Limitations and Future Work

Various limitations were imposed to maintain tractability in the current study. More influential limitations of this study included examining only a single EA, and conducting the dengue OCP comparison using alternative numerical methods in the GA (non-identical implementation factors) to those used by previous authors. To further improve the GA approach, additional limitations of the current study could be addressed, including determining:

- whether alternative control formulations would improve solution accuracy, and
- the impact that default GA parameters in MATLAB may have had on solutions.

All limitations however, could be addressed relatively easily in future work.

Interpolation, for example, may assist in circumventing some of the challenges experienced in control formulation, and possibly reduce chromosome length by requiring fewer control values to be generated by the GA when constructing a control. Similarly, an adaptive discretisation could be used, particularly in the control formulation, or as is commonly done in EA approaches, complex problems could be solved coarsely at first, and then refined according to results. Deviating from default GA parameters however, which ensure a standard algorithm is available to non-specialists, may incur additional, unnecessary complexity.

To improve the generalisability of results, a GA could be applied to OCPs based on different ecological model types, like stochastic models, which could serve to improve realism.

Investigating alternative EAs would also advance the investigation of the current study, as only a GA was examined. GAs could, potentially, be better-suited than other EAs, and may have provided a skewed representation, as could alternative EAs like differential evolution (Yang, 2014) have outperformed GAs. The investigation could also be extended to include more advanced computational methods like artificial neural networks (Engelbrecht, 2007). Similarly, a GA approach could also be compared to alternative classic OC methods.

Perhaps most importantly, the ecological effects of model assumptions and control strategies designed using an EA approach could be examined in future work. This would assist in determining not only the posited realism of an EA approach, but also whether EAs are a viable management tool, and if resulting strategies are indeed easily refined.

7.5 Concluding Remarks

OCT is ideally placed to address the increasing number of ecological issues faced by society today, as are EAs equipped to circumvent challenges associated with conventional methods used to solve these OCPs. The combination of these two powerful techniques has seldom been investigated in an ecological capacity; a deficit this research endeavoured to address.

Comparisons between an EA and classic OC methods found that the EA approach avoided complexities associated with classic OC schemes while producing comparable, near-optimal solutions. These near-optima may have equal standing with classical optimal solutions in reality as classical solutions are typically approximated to enable actual application. The OCP formulation also appeared to affect GA performance, with the computational time taken to solve the PDE-based OCP scaling up substantially from the ODE-based counterparts.

The EA was further found to produce a feasible and robust near-optimal solution when applied to an unconventional OCP. This supported the viability of an EA approach as an alternative to classic OC methods, as the EA allowed ecological factors to be taken into account more easily than in conventional methods, which may result in an OCP that better reflects reality. An EA approach is not standardised, however, as is the case when using OCT, and can therefore be user-biased.

Ultimately, OCT is a comprehensive field with many highly successful schemes. In addition to classic OC methods, this research proposes that an EA approach is worth consideration. Many OCPs, however, may be more appropriately, and accurately, solved using classic

OC methods and advanced mathematics. This work does not intend to discount the use of classic OC techniques. This research does, however, posit that OC schemes could be problem dependent, and that an EA may be better-suited to certain OCP formulations.

Like any OC approach, both ecological and mathematical knowledge is required to produce useful solutions using an EA approach. Nonetheless, and as demonstrated by the GA in the current study, an EA approach can provide modellers with an OC technique that is not obscured in complex mathematical theory and which avoids substantial mathematics relating to OCT. This may increase the ease associated with determining management strategies and their ecological impact. Strategies can also more easily be altered in an EA approach once their effects are noted, or in the presence of changing environments or management goals.

OC should not, however, be "a plug-and-play exercise" (Subchan and Żbikowski, 2009, pg. 163). Similarly, controlling ecological systems is not simply a matter formulating and solving an ecological OCP, as any developments made can have lasting, and often life-changing repercussions (Sontag, 2004). Consequently, it is important that control strategies are monitored throughout the duration of application to ensure alterations are made if and when necessary, according to their impact. Similarly, ecological considerations should inform mathematical strategies, and not the reverse. This was the primary motivation for pursuing an EA approach in the current study. An EA approach however, is not immune to this same phenomenon.

Nonetheless, an EA approach to ecological OCPs appears to be a viable and worthwhile addition to OC methods and techniques in ecology, and may act to improve the capacity of humans to successfully manage ecological systems. As increasingly complex problems arise at the interface between ecological systems and human civilisation, developing more advanced control strategies will become increasingly important. In response to this increased complexity, an increase in the capability of OC methods is needed, as current mathematical tools are not always suited to modelling complex ecological systems.

From the promising GA results produced in this study, an EA approach appears to possess the potential to contribute towards meeting the requirements of not only current ecological OCPs, but also future, more complex OCPs. This potential of EAs lies not only in their accuracy as an OC method in ecology, but also in the adaptability of an EA approach to OCPs, and the reduced mathematical theory requirements. Further investigation in this regard is thus warranted so as to produce useful ecological management strategies, capable of addressing pertinent ecological issues, using a combination of OCT and an EA approach.

Appendix A

Statistics Regarding Genetic Algorithm Results in Chapter 4

A.1 Introduction

The first of two comparative chapters, the performance of a GA was compared to classic OC methods by means of two ODE-based OCPs in Chapter 4. The first case study considered a predator-prey OCP and was solved using both a GA and the indirect FBSM. In the second case study, a GA was applied by the current author, and the results were compared to solutions obtained in literature using two different direct method-based solvers.

The optimal solutions presented in the main text were the solutions with minimum fitness (minimisation OCPs) across 30 runs of the GA for each set of circumstances considered. This criterion was chosen due to the fact that in most GA applications, a classical solution is not necessarily available as a means by which to nominate the *best* solution. This definition of best, however, corresponds to the OCPs themselves, which sought to minimise the objective.

A number of different chromosome lengths were used to construct controls in both case studies. Furthermore, two different quadrature methods were used to approximate the objective value, and the GA was compared to multiple solution methods/solvers. To give the reader an idea of the consistency of GA performance across the 30 runs and all combinations considered, basic descriptive statistics are next given. Statistics pertaining to the predator-prey problem are given in Section A.2, and those regarding the dengue OCP in Section A.3.

A.2 Predator-Prey Statistics

In line with the reporting of solution error in Chapter 4, the percentage relative difference (% *error*) between the GA and FBSM objective values were calculated for each and every run of the GA. These are given in Table A.1 to four significant decimal places, along with the associated variance and standard deviation of each average % *error*. While RS solutions were more accurate overall, all solutions produced had extremely low variability between runs.

Table A.1: Statistics regarding the percentage difference between the FBSM's objective function value and those produced by the GA (across 30 runs) in the predator-prey OCP.

Control	**Average % error**	**Variance**	**Standard Deviation**
	Riemann Sum Results		
$\mathbf{u_1}$	0.005321	1.6051×10^{-19}	4.006393×10^{-10}
$\mathbf{u_5}$	0.0003067	2.4316×10^{-8}	0.001559
$\mathbf{u_{25}}$	0.001969	4.01186×10^{-7}	0.0006334
$\mathbf{u_{50}}$	0.005270	1.9199×10^{-6}	0.001386
	Composite Simpson's Results		
$\mathbf{u_1}$	0.02580	2.1131×10^{-16}	1.4537×10^{-8}
$\mathbf{u_5}$	0.02489	6.1083×10^{-7}	0.0007816
$\mathbf{u_{25}}$	0.01751	3.8312×10^{-6}	0.001957
$\mathbf{u_{50}}$	0.01254	5.9593×10^{-6}	0.002441

A.3 Dengue Statistics

Basic statistics are reported analogously for the dengue OCP in Tables A.2 and A.3, depending on the direct software with which the GA was compared. In Table A.2, the average % *error* corresponding to the chromosome lengths of $n = 25$ and $n = 50$ are given in bold as these percentages are lower than that of the optimal solutions reported in the main text[1].

This is due to the definition of the *best*. Solutions more similar to those produced by the DOT_{CVP} software were generated by the GA and are given in Table A.4. Since a comparison is not always available with classic OC methods, the definition of best could not simply be the GA solution with the least % *error*. However, these results show that a GA is capable of producing solutions with equivalent, or better accuracy, than popular direct methods.

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[1] The GA's objective was lower than the DOT_{CVP} software, but greater than the *IPOPT* software.

Table A.2: Statistics regarding the percentage difference between the DOT_{CVP} software's objective function value and those produced by the GA (across 30 runs) in the dengue OCP.

n	**Average % error**	**Variance**	**Standard Deviation**
	GA vs. $\mathbf{DOT_{CVP}}$: Riemann Sum Results		
1	17.9786	2.1294×10^{-8}	0.0001459
5	0.1613	0.02719	0.1649
25	**8.7262**	1.0231	1.01146
50	**7.6760**	1.8875	1.8369
	GA vs. $\mathbf{DOT_{CVP}}$: Composite Simpson's Results		
1	18.09653	2.09207×10^{-8}	0.0001446
5	0.2497	0.06145	0.2479
25	**8.6268**	1.2887	1.1352
50	**7.8530**	1.8369	1.3553

Table A.3: Statistics regarding the percentage difference between the *IPOPT* software's objective function value and those produced by the GA (across 30 runs) in the dengue OCP.

n	**Average % error**	**Variance**	**Standard Deviation**
	GA vs. *IPOPT*: Riemann Sum Results		
1	33.3522	2.7205×10^{-8}	0.0001649
5	13.2131	0.03474	0.1864
25	3.1675	1.3071	1.1433
50	4.3546	2.4114	1.5529
	GA vs. *IPOPT*: Composite Simpson's Results		
1	33.4855	2.6728×10^{-8}	0.0001635
5	13.3131	0.07850	0.2802
25	3.2799	1.6464	1.2831
50	4.1545	2.3468	1.5319

Table A.4: The GA-produced objective function values most like the DOT_{CVP} solutions.

	Riemann Sum Results		**Composite Simpson's Results**	
n	$\mathbf{J(c_A^*, c_m^*, \alpha^*)}$	**% $\mathbf{DOT_{CVP}}$**	$\mathbf{J(c_A^*, c_m^*, \alpha^*)}$	**% $\mathbf{DOT_{CVP}}$**
25	0.06393	4.4537	0.06456	3.5124
50	0.06389	4.5204	0.06495	2.9361

Appendix B

Alternative Control in the Raccoon-Rabies Optimal Control Problem

B.1 Introduction

In the PDE-based raccoon-rabies OCP, the control form implemented in the GA had to be predefined in order to constrain chromosome length. Consequently, the user-defined control form impacted on the optimal strategy. In addition to the diffusive control implementation that was presented in Chapter 5, a control form involving terms proportional to population classes is examined in this Appendix. This control form is investigated to determine whether bait distribution is generated differently by the GA when the control form is altered.

B.2 Control Formulation and Encoding

Similarly to Chapter 5, a PDE was once again constructed, and was comprised of diffusive and reductive terms. Two diffusion terms, namely D_1 and D_2, were used, but unlike the previous implementation (Section 5.5), a term $k\dfrac{R}{(S+I)}$ was formulated and included in the PDE to allow the bait quantity to decrease proportionally to the ratio of vaccinated to unvaccinated raccoons. This allows the bait distribution to decrease faster as the proportion of immunised raccoons in the population becomes larger. In this instance, $k \in [0, 1]$ was assumed constant.

The PDE is given by: $$\frac{\partial v}{\partial t} = D_1(x,y,t)\, v_{xx} + D_2(x,y,t)\, v_{yy} - kv\frac{R}{(S+I)}.$$

Initial bait distribution was determined in the same manner as before (Section 5.5), with the GA selecting 50 values with which to accomplish initialisation. Both D_1 and D_2 were generated almost identically to the previous implementation however, since only a single reduction constant was used to reduce vaccination rate, 20 initial diffusion terms were generated, to allow the vaccination strategy to change at each week.

B.3 Associated Genetic Algorithm Results

The optimal solutions at weeks $t = 1$, $t = 11$ and $t = 20$ under this alternative control formulation are given in Figures B.1, B.2 and B.3 respectively. Analogous to the GA results presented in Chapter 5, the alternative control formulation resulted in susceptible (S), infected (I) and vaccinated (R) raccoon classes much like the FBSM throughout the vaccination strategy. Very similar trends and densities were observed in these population classes at all points in the domain, throughout the 20 week strategy.

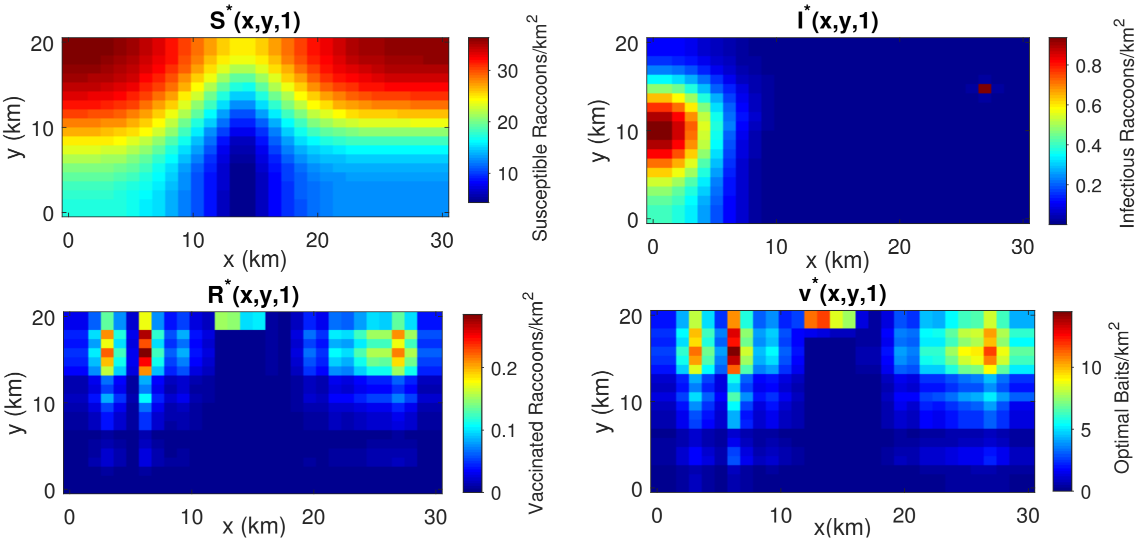

Figure B.1: Alternative control formulation: The GA-derived optimal solution at week 1

Once again, optimal bait distribution differed from the FBSM strategy. Initially (Figure B.1), the GA placed baits similarly to the strategy shown in Chapter 5. From there on, bait distribution followed the trends seen in the susceptible raccoon population, albeit with a time lag. Baits were placed throughout Ω_F in the alternative strategy. The final bait density at $t = 20$ (Figure B.3) was much higher than that observed in the previous GA solution.

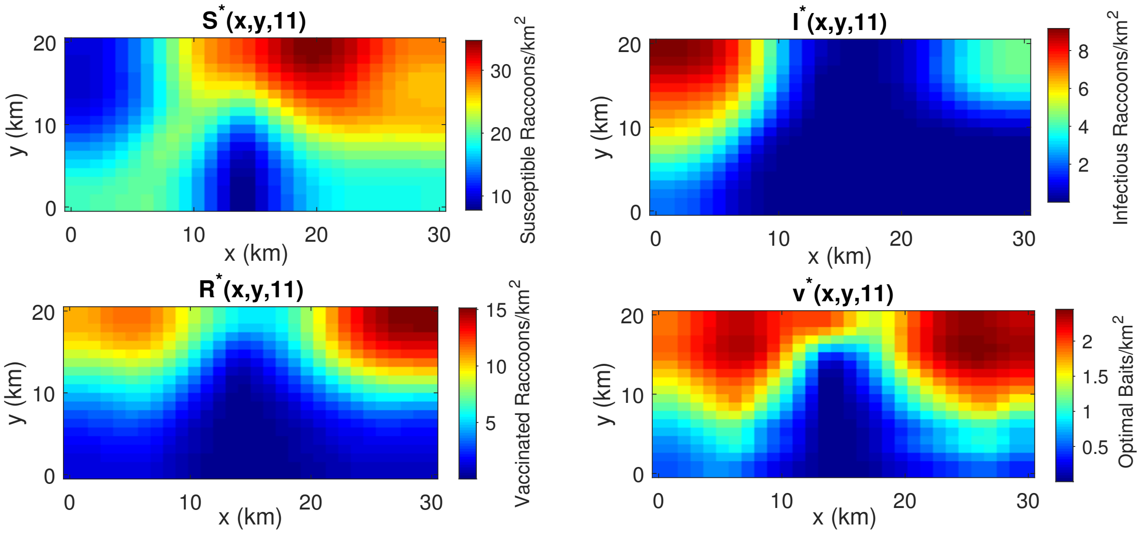

Figure B.2: Alternative control formulation: The GA-derived optimal solution at week 11

It can clearly be seen that the GA control form radically alters the optimal GA bait distribution strategy. It is therefore likely that the control form and initialisation is responsible for the differences seen between the GA and FBSM solutions, both here (Figures B.1, B.2 and B.3) and as discussed in Section 5.5.3 of Chapter 5 (Figures 5.7, 5.8 and 5.9). The effect on disease transmission within the raccoon population itself, however, is minimal. Although the control form plays a role in GA solutions, the success or failure thereof may therefore also be dependent on the OCP to which the GA is applied. Seemingly, the raccoon-rabies OCP is robust to variations in bait distribution strategies.

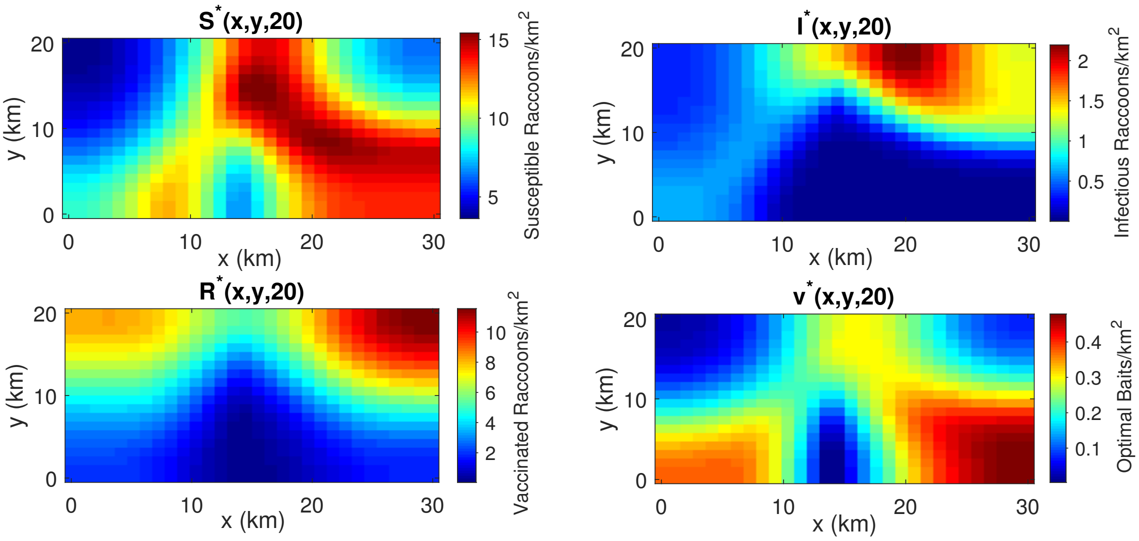

Figure B.3: Alternative control formulation: The GA-derived optimal solution at week 20

Appendix C

The Unsuitability of Classic Optimal Control Methods in the Bee Optimal Control Problem

Typically, highly constrained, non-linear OCPs of large dimension, such as in wind turbine design (Wang et al., 2017), present standard, mathematical OC methods with great difficulty. Excessive complexity when applying classic OC methods is not limited to these factors however, and can instead arise from the unconventionality of an OCP which prevents these problems from fitting into common classical frameworks.

The OCP constructed in Chapter 6 to conserve wild bee populations by controlling habitat placement considered optimal layout design within a domain. Layout design optimisation problems have been solved using classic OC methods, however, these problems usually consider a set number of components requiring optimal placement, failing which, they are solved using modern computational methods like GAs (Wu, Yang and Zhu, 2021). Wind turbine layout designs are almost exclusively solved using GAs or particle swarm optimisation, due to the difficulty and often intractability of classic OC approaches (Tao, Xu, Feijóo, Zheng and Zhou, 2020).

In some instances, mathematical methods like linear programming methods can be used, however the entire problem, including constraints, must be linear, and only a fixed number of components requiring placement can be considered (Pourvaziri, Pierreval and Marian, 2021).

Where the configuration of components as well as properties of components, for instance, dimension, interact however, the control method used plays a crucial role since the optimal configuration is dependent not merely on distance, but also on each specified location (Lyu, Abdelkhalik and Gauchia, 2019). For example, Lyu et al. (2019), who made use of the built-in GA function in MATLAB to solve a layout design OCP in wave energy converters, found that buoys placed in the centre of an array have a disproportionate impact on total performance.

The conservation OCP (Section 6.3) was atypical in the sense that the control was concerned with the number, location and combination of different habitat types, subject to the effects these interventions would elicit on the foraging behaviour of wild bees within the control-determined arrangement and composition of habitat in a domain. Where the number and location of components has been considered in analogous layout design OCPs with two competing objectives, simulation methods have been developed due to the intractability of classic OC methods (Derhami, Smith and Gue, 2020).

In the event that the OCP was solvable using classic OC methods, significant mathematical expertise would be required to adapt algorithms to solve it in a classical OC framework. Moreover, classic OC methods would automatically become more complex due to the non-linear relationships and inequality constraints in the OCP. In this particular OCP (Section 6.3), the inequality constraints could easily be taken into account in the GA approach by adjusting chromosome length (Section 6.4.3), whereas incorporating inequality constraints in classic OC methods introduces significant complexity. How the OCP could be solved using classic OC methods could not be ascertained by the current author and it was thus considered reasonable to assume that the OCP was not solvable using classic OC methods.

Additional assumptions in the GA approach, including the pre-design of agricultural land (for example the placement and shape of crop fields, as well as dimensions of borders and margins) are also in accordance with OCPs concerning layout design in literature. Derhami et al. (2020), for example, made use of analysis to pre-emptively constrain the components whose configuration was optimised according to the influence of the components on one another, and both limit and to an extent, pre-design domain layouts. Similarly, in wind farm design problems, the grids on which GAs are used to determine optimal layouts, are subjected to predetermined subdivision based on experimental observations in controlling the location of wind turbines (Wu et al., 2021).

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