Numerical Methods for Optimal Control with Binary Control Functions Applied to a Lotka-Volterra Type Fishing Problem*

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Summary. We investigate possibilities to deal with optimal control problems that have special integer restrictions on the time dependent control functions, namely to take only the values of 0 or 1 on given time intervals. A heuristic penalty term homotopy and a Branch and Bound approach are presented, both in the context of the direct multiple shooting method for optimal control. A tutorial example from population dynamics is introduced as a benchmark problem for optimal control with $0-1$ controls and used to compare the numerical results of the different approaches.

1 Introduction

Optimal control problems have long been under investigation and it is well known that for certain systems, in particular linear ones, bang-bang controls are optimal. On the other hand it is not clear what to do if the feasible set of a control is a priori restricted to two (or more) discrete values only and the optimal switching structure cannot be guessed due to the complexity of the model under consideration.

Optimal control problems with the mentioned restriction to 0-1 values in the controls arise whenever a yes-no decision has to be made, as is e.g. the case for certain types of valves or pumps in engineering, certain investments in economics, discrete stages in transport or application of laws in given time periods. Such problems are typically nonlinear and already difficult to solve without combinatorial apects.

Although some mixed integer dynamic optimisation problems, namely the optimisation of New York subway trains that are equipped with discrete acceleration stages, were solved in the early eighties [3], the so-called indirect methods used there do not seem appropriate for generic large-scale optimal control

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problems with underlying nonlinear differential algebraic equation (DAE) systems. Therefore efforts have to be undertaken to bring together methodology of and new results for indirect methods in this context (see e.g. [24]) and the so-called direct methods, particularly the direct multiple shooting method [4] and direct collocation [23, 29].

Several authors have been working on optimal control problems with discrete valued control functions: [7] investigate a water distribution network in Berlin with such on/off pumps, using a problem specific nonlinear continuous reformulation of the control functions; [28] treat powertrain control of heavy duty trucks with a tailored heuristics in the context of direct multiple shooting that fits into the model predictive control context; [15, 22] use a switching time approach related to the one described in Section 3.3 to deal with problems where only a finite set of controls, e.g. velocities of submarine vessels, is feasible; [8] focus on problems in robotics, applying a combination of Branch and Bound and direct collocation [26].

Other publications in the field of mixed integer dynamic optimisation deal with time independent integer variables (e.g. [20]) or state dependent (autonomous) switches (e.g. [6]) that are both not the topic of this paper.

The paper is organised as follows. In Section 2 a short introduction to numerical methods for optimal control is given, in particular to the direct multiple shooting method [4]. In Section 3 extensions to treat additional integer restrictions are presented. An optimal control problem with a 0-1 restriction in the controls is presented in Section 4 and is used as a benchmark problem further on. Numerical results are given and compared in Section 5. Section 6 concludes.

2 Numerical Methods for Optimal Control

The optimal control problems we refer to in this section and that are later on to be extended, are of the form

$$
\begin{array}{ll}
\min\limits_{p,u,x,z} & \int_{t_0}^{T} L(x(t),z(t),u(t),p)dt \; + E(x(T),z(T),p) \\
\text{s.t.} & \dot{x}(t) = f(t,x(t),z(t),u(t),p), \quad t \in [t_0,T] \\
& \quad 0 = g(t,x(t),z(t),u(t),p), \quad t \in [t_0,T] \\
& \quad 0 \le c(t,x(t),z(t),u(t),p), \quad t \in [t_0,T] \\
& \quad 0 \le r_i(x(t_0),z(t_0),x(t_1),z(t_1),\dots,x(T),z(T),p) \\
& \quad 0 = r_e(x(t_0),z(t_0),x(t_1),z(t_1),\dots,x(T),z(T),p)
\end{array}
\tag{1}
$$

The system state is described by the differential and algebraic state vectors $x(t) \in \mathbb{R}^{n_x}$ and $z(t) \in \mathbb{R}^{n_z}$. The system behaviour is controlled by the control vectors $u(t) \in \mathbb{R}^{n_u}$ and the global design parameter vector $p \in \mathbb{R}^{n_p}$. The objective functional is of generalised Bolza type, containing Lagrange and Mayer terms. The differential and algebraic right hand side functions f respectively

g describe the dynamical system behavior, while the vector valued functions r_i, r_e are additional interior point constraints for given time points t_i (see Section 2.1) and c contains path constraints. The Jacobian $\partial g/\partial z \in \mathbb{R}^{n_z \times n_z}$ is assumed to be invertible, resulting in an index 1 DAE.

There are several approaches to treat optimal control problems of this form. For an overview and comparison between indirect and direct methods, sequential and simultaneous approaches (in particular single shooting, multiple shooting and collocation) we refer to [1]. We investigate extensions in the context of the direct multiple shooting method, therefore we will give a brief introduction in Section 2.1.

2.1 Direct Multiple Shooting

The direct multiple shooting method [4, 17] is used to transform the infinite dimensional optimisation problem (1) into a finite dimensional one that can be treated efficiently with tailored nonlinear optimisation methods, e.g. sequential quadratic programming (SQP). This transformation is performed by a piecewise parameterisation of the control functions, a relaxation of the path constraints to grid points and a discretisation of the state variables. To this end the time horizon $[t_0, T]$ is divided into a number of m subintervals $[t_i, t_{i+1}]$ with $t_0 < t_1 < \cdots < t_m = T$, the so-called multiple shooting intervals.

Parameterisation of the controls. For each interval the function space that the optimal control function $u(t)$ can be chosen from is reduced to a finite dimensional one. Then a piecewise approximation $\hat{u}$ of the control functions u on this grid is defined by

$$\hat{u}(t) := \varphi_i(t, q_i), \quad t \in [t_i, t_{i+1}], \quad i = 0, \ldots, m-1 \tag{2}$$

using "local" control parameters q_i. The functions φ_i are typically vectors of constant, linear or cubic functions.

State discretisation. The basic concept of the multiple shooting method is to solve the DAE-constraints independently on each of the multiple shooting intervals. On interval i the initial value for the DAE solution is given by the so-called *node values* s_i^x, s_i^z for differential and algebraic states. The algebraic equations are relaxed (see [2], [16]). They enter as conditions in t_i into the NLP. Continuity of the state trajectory at the multiple shooting grid points

$$s_{i+1}^x = x_i(t_{i+1}) \tag{3}$$

is also incorporated by constraints into the nonlinear program (NLP). Here $x_i(t)$ denotes the differential part of the DAE solution on interval $[t_i, t_{i+1}]$ with initial values s_i^x, s_i^z. These equations are required to be satisfied only at the solution of the problem, not necessarily during the SQP iterations.

Resulting NLP. The local variables q_i, the global parameters p, that may include the time horizon length $h = T - t_0$, and the node values s_i^x, s_i^z are the degrees of freedom of the parameterised optimal control problem. If we write them in one vector $\xi = (q_i, p, s_i^x, s_i^z)$, rewrite the objective function as $F(\xi)$, subsume all equality constraints with the continuity conditions (3) into a function $G(\xi)$ and all inequality constraints into a function $H(\xi)$, then the resulting NLP can be written as

$$\min_{\xi} F(\xi) \quad \text{s.t.} \quad 0 = G(\xi), \;\; 0 \leq H(\xi) \tag{4}$$

This NLP can be solved with tailored iterative methods, exploiting the structure of the problem. For more details, see [4, 16, 17]. An efficient implementation of the described method is the software package `MUSCOD-II` [9].

3 Treatment of Binary Control Functions

We are interested in an extension of problem (1), where some or all of the control functions have the additional restriction to have values in $\{0, 1\}$. If we denote these control functions by $w(t)$ we can formulate an optimal control problem with binary valued control functions. We want to minimise the functional

$$\Phi[x, z, w, u, p] := \int_{t_0}^{T} L(x(t), z(t), w(t), u(t), p)dt \; + E(x(T), z(T), p) \tag{5}$$

subject to a system of DAEs, path and interior point constraints and additional restrictions

$$w(t) \in \{0, 1\}^{n_w}, \quad t \in [t_0, T] \tag{6}$$

that turn the problem into a combinatorial one.

For some applications restriction (6) is still too general. A certain limitation on the number of switchings must be taken into consideration, as an infinite switching from one value to the other is not applicable in practice. This might be achieved by an upper limit on the number of switches or a penalisation. In the direct multiple shooting approach a fixed finite control parameterisation inhibts infinite switching automatically.

Another possible limitation occurs when switching can only take place at time points from a prefixed given set. This limitation is motivated by machines that can only switch in discrete time steps and by laws or investments that can only be applied resp. made at certain times, e.g. on the first of a month or year. Thus we replace restriction (6) by the more general restriction

$$w(t) \in \Omega(\Psi), \quad t \in [t_0, T] \tag{7}$$

where $\Omega(\Psi)$ is defined as

$$\Omega(\Psi) := \left\{ w(t) \in \{0, 1\}^{n_w}, \text{ with discontinuities only at times } \hat{t}_i \in \Psi \right\}$$

with either

$$\Psi = \{\tau_1, \tau_2, \ldots, \tau_{n_\tau}\} \tag{8}$$

being a finite set of possible switching times or with

$$\Psi = [t_0, T] \tag{9}$$

corresponding to (6). If we write $\bar{\Omega}(\Psi)$, we mean the relaxed function space where $\{0,1\}^{n_w}$ is replaced by $[0,1]^{n_w}$. Summing up, the optimal control problems under consideration can be formulated in the following way:

$$\begin{array}{ll}
\min\limits_{x,z,w,u,p} & \int_{t_0}^{T} L(x(t), z(t), w(t), u(t), p)dt \; + E(x(T), z(T), p) \\
\text{s.t.} & \dot{x}(t) = f(t, x(t), z(t), w(t), u(t), p), \quad t \in [t_0, T] \\
 & \quad 0 = g(t, x(t), z(t), w(t), u(t), p), \quad t \in [t_0, T] \\
 & \quad 0 \leq c(t, x(t), z(t), w(t), u(t), p), \quad t \in [t_0, T] \\
 & \quad 0 \leq r_i(x(t_0), z(t_0), x(t_1), z(t_1), \ldots, x(T), z(T), p) \\
 & \quad 0 = r_e(x(t_0), z(t_0), x(t_1), z(t_1), \ldots, x(T), z(T), p) \\
 & w(t) \in \Omega(\Psi), \quad t \in [t_0, T]
\end{array} \tag{10}$$

In the following we will choose the control parameterisation intervals $[t_i, t_{i+1}]$ such that they coincide with the intervals $[\tau_i, \tau_{i+1}]$. More precisely, we choose $m = n_\tau$ and $t_i = \tau_i, i = 1, \ldots, m$. Furthermore we will use a control parameterisation (2) that is constant on these intervals.

We want to investigate possibilities to solve problem (10). In Section 3.1 we have a look at relaxations of the integer constraints and in Section 3.2 we describe a Branch and Bound algorithm for mixed integer dynamic optimisation problems. In Section 3.3 a reformulation based on optimisation of the continuous switching times is given and discussed.

3.1 Heuristics Based on Relaxation

A first approach to solve problem (10) consists of relaxing the integer requirement $w(t) \in \Omega(\Psi)$ to $\bar{w}(t) \in \bar{\Omega}(\Psi)$ and to solve a relaxed problem of form (1) first. The obtained solution $\bar{w}(t)$ can then be investigated – in the best case it is an integer feasible bang-bang solution and we have found an optimal solution for the integer problem. In case the relaxed solution is not integer, one of the following rounding strategies can be applied:

- Rounding strategy 1
  The values $w_{j,i}(t)$ of the control functions $j = 1, \ldots, n_w$ on the intervals $[t_i, t_{i+1}]$ are fixed to

$$w_{j,i}(t) = \begin{cases} 1 & \text{if } \bar{w}_{j,i}(t) \geq 0.5 \\ 0 & \text{else} \end{cases}, \quad i = 0, \ldots, m-1$$

- Rounding strategy 2
  The values of $\bar{w}_{j,i}(t)$ are summed up over the intervals, more precisely

$$w_{j,i}(t) = \begin{cases} 1 & \text{if } \sum_{k=0}^{i} \bar{w}_{j,k}(t) - \sum_{k=0}^{i-1} w_{j,k}(t) \geq 1 \\ 0 & \text{else} \end{cases}, \quad i = 0, \dots, m-1$$

- Rounding strategy 3
  As 2, but with a different threshold:

$$w_{j,i}(t) = \begin{cases} 1 & \text{if } \sum_{k=0}^{i} \bar{w}_{j,k}(t) - \sum_{k=0}^{i-1} w_{j,k}(t) \geq 0.5 \\ 0 & \text{else} \end{cases}, \quad i = 0, \dots, m-1$$

In case the relaxed solution is not integer and the gap between the objective values of relaxed and rounded problems is important, we propose the following approach to drive the values of the control function to its borders.

- Penalty term homotopy
  We consider an optimal control problem $P^k, k \in \mathbb{N}_0$ defined by

$$\begin{array}{ll} \min\limits_{x,z,w,u,p} & \Phi[x,z,w,u,p] \ + \ \sum_{i=1}^{n_w} \epsilon_i^k \ \int_{t_0}^{T} (1 - w_i(t)) \ w_i(t) \ dt \\ \text{s.t.} & \dot{x}(t) = f(t, x(t), z(t), w(t), u(t), p), \quad t \in [t_0, T] \\ & \quad 0 = g(t, x(t), z(t), w(t), u(t), p), \quad t \in [t_0, T] \\ & \quad 0 \leq c(t, x(t), z(t), w(t), u(t), p), \quad t \in [t_0, T] \\ & \quad 0 \leq r_i(x(t_0), z(t_0), x(t_1), z(t_1), \dots, x(T), z(T), p) \\ & \quad 0 = r_e(x(t_0), z(t_0), x(t_1), z(t_1), \dots, x(T), z(T), p) \\ & w(t) \in \bar{\Omega}(\Psi), \quad t \in [t_0, T] \end{array} \tag{11}$$

  with penalty parameters $\epsilon_i^k \geq 0$ for $i = 1, \dots, n_w$. P^k is similar to the relaxed version of problem (10), but additionally penalises all measurable violations of the integer requirements with a concave quadratic penalty term. The proposed penalty term homotopy consists of solving a series of continuous optimal control problems $\{P^k\}, k \in \mathbb{N}_0$ with relaxed $w(t)$. Problem P^{k+1} is initialised with the solution of P^k and $\epsilon_i^0 = 0$ so that P^0 is the relaxed version of problem (10). The penalty parameters ϵ_i^k are raised monotonically until all $w_i(t)$ are 0 or 1.

Remark 1. The algorithm may of course get stuck if the solution is driven towards an infeasible solution. This can e.g. be observed by a technique controlling the changes in the optimisation variables from one problem to the next. In such a situation several remedies are possible, e.g. a complete restart with different initial data, backtracking with a different choice of ϵ_i^k, another penalisation to get away from the current point or a transformation of the problem with an approach as described in Section 3.3.

Remark 2. A good choice for the ϵ_i^k is crucial for the behaviour of the method. A too fast increase in the penalty parameters results in less accuracy and is getting closer to simple rounding, while a slow increase leads to an augmentation in the number of QPs that have to be solved. In Section 5.1 problem specific parameters are given. A general formula is topic of current research.

Remark 3. Another possibility to penalise the nonintegrality is proposed by [25]. They introduce additional inequalities, prohibiting nonintegral domains of the optimisation space.

3.2 Branch and Bound

Mixed integer dynamic optimisation problems can be solved with methods used in mixed integer nonlinear optimisation (MINLP), see [10]. This can be accomplished by parameterising problem (10) in a way as described in Section 2. Instead of a NLP (4) the result would be a MINLP of the form

$$\begin{array}{lrcl} \min\limits_{\xi,\omega} & F(\xi,\omega) & & \\ \text{s.t.} & 0 & = & G(\xi,\omega) \\ & 0 & \leq & H(\xi,\omega) \\ & \omega_i & \in & \{0,1\}, \quad i = 1,\dots,n_w \end{array} \tag{12}$$

that can be solved with methods as Branch and Bound or Outer Approximation. In the following we assume that the objective function and the feasible set are convex. In our study we apply a Branch and Bound algorithm that is performing a tree search in the space of the binary variables. We first solve a relaxed problem with $\omega \in [0,1]^{n_w}$ and decide on which of the variables with non-integral value we shall branch, say ω_i. Two new subproblems are then created with ω_i fixed to 0 and 1, respectively. These new subproblems are added to a list and the father problem is removed from it. This procedure is repeated for all problems of the list until none is left. There are three exceptions to this rule, when a node is not branched on, but abandoned directly:

1. The relaxed solution is an integer solution. Then we have found a feasible solution of the MINLP and can compare the objective value with the current upper bound (and update it, if possible).
2. The problem is infeasible. Then all problems on the subtree will be infeasible, too.
3. The objective value is higher than the current upper bound. As it is a lower bound on the objective values of all problems on the subtree, they can be abandoned from the tree search.

A more detailed description of nonlinear Branch and Bound methods and a survey about branching rules can e.g. be found in [11]. We used depth-first search and most violation branching in our implementation.

Remark 4. On each node of the search tree a NLP resulting from an optimal control problem has to be solved, which is very costly. A more efficient way of integrating the Branch and Bound scheme and SQP is proposed by [5] and [18].

Remark 5. If the functions are non-convex, the nodes cannot be fathomed any more as feasible or better solutions may be cut off. A heuristics to overcome this is proposed in [18]. An approach using underestimations of the dynamical system is described in [21].

3.3 Switching Time Approach

Another possibility to solve problem (10) is motivated by the idea to optimise the switching structure and to take the values of the controls fixed on given intervals, as is done for bang-bang arcs in indirect methods. Of course this is only valid for feasible sets $\Omega(\Psi)$ where Ψ is given by (9). Instead of (7) we have, assuming for the sake of notational simplicity a one-dimensional control, a fixed $\hat{w}(t;\hat{t},n_{\mathrm{sw}})$ given by

$$\hat{w}(t;\hat{t},n_{\mathrm{sw}}) = \begin{cases} 0 & \text{if } t \in [\hat{t}_i, \hat{t}_{i+1}], \quad \text{i even} \\ 1 & \text{if } t \in [\hat{t}_i, \hat{t}_{i+1}], \quad \text{i odd} \end{cases}, \quad i = 0, \ldots, n_{\mathrm{sw}} \tag{13}$$

with $t_0 = \hat{t}_0 \le \hat{t}_1 \le \cdots \le \hat{t}_{n_{\mathrm{sw}}+1} = T$. The number n_{sw} and the locations $\hat{t}_j$ of the switching times are then to be optimised and we obtain

$$\begin{aligned} \min_{x,z,u,p,\hat{t},n_{\mathrm{sw}}} \quad & \int_{t_0}^{T} L(x(t), z(t), \hat{w}(t;\hat{t},n_{\mathrm{sw}}), u(t), p)dt \ + E(x(T), z(T), p) \\ \text{s.t.} \quad & \dot{x}(t) = f(t, x(t), z(t), \hat{w}(t;\hat{t},n_{\mathrm{sw}}), u(t), p), \quad t \in [t_0, T] \\ & 0 = g(t, x(t), z(t), \hat{w}(t;\hat{t},n_{\mathrm{sw}}), u(t), p), \quad t \in [t_0, T] \\ & 0 \le c(t, x(t), z(t), \hat{w}(t;\hat{t},n_{\mathrm{sw}}), u(t), p), \quad t \in [t_0, T] \\ & 0 \le r_i(x(t_0), z(t_0), x(t_1), z(t_1), \ldots, x(T), z(T), p) \\ & 0 = r_e(x(t_0), z(t_0), x(t_1), z(t_1), \ldots, x(T), z(T), p) \end{aligned} \tag{14}$$

with fixed $\hat{w}(t;\hat{t},n_{\mathrm{sw}})$ and $\hat{t}_i$ and n_{sw} as above.

If we allow that switching times fall together, $\hat{t}_j = \hat{t}_{j+1}$, this formulation can be extended in a straightforward way to n_w binary control functions and every solution $(p, w(t), u(t), x(t), z(t))$ of system (10) with a finite number of switches in $w(t)$ has an equivalent solution $(p, n_{\mathrm{sw}}, \hat{t}, u(t), x(t), z(t))$ of system (14) and vice versa.

For fixed n_{sw} we then have an optimal control problem that fits into the definition of problem (1) and can be solved with standard methods, where the interval lengths $\hat{t}_{j+1} - \hat{t}_j$ take the role of parameters that have to be determined. Special care has to be taken to treat the case where interval lengths diminish during the optimisation procedure, causing the problem to become singular. [12, 13, 19] propose an algorithm to eliminate such non-optimal bang-bang intervals.

Some authors propose to iterate on n_{sw} until there is no further decrease in the objective function of the corresponding optimal solution [22, 12, 13]. But it should be stressed that this can only be applied to more complex systems, if good initial values for the location of the switching points are available, as they are essential for the convergence behaviour of the underlying method. In

Section 5.3 we will see how this approach may drift off to an arbitrary local optimum even in the case of a one-dimensional control, only few switching events and reasonable initialisations.

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4 A Fish Population Optimal Control Problem

In this section we introduce a fish population control model as a benchmark problem for optimal control with binary control functions. This model has some oscillations that we want to bring close to a steady state. Such an optimisation objective might also be the topic of other applications, e.g. in control of pattern self-aggregation [14].

In Section 4.1 the standard textbook ordinary differential equation (ODE) model of Lotka–Volterra type is brought back to memory. This ODE model is then extended in 4.2 to a control problem by introducing a fishing allowance. In Section 4.3 we have a look at some details of this model, e.g. at the optimal relaxed solutions obtained either by a direct approach or by Pontryagins maximum principle.

4.1 ODE Model

Lotka-Volterra systems have already been under investigation for a long time and are very well studied, see e.g. [27] for an overview. In a two-species predator-prey model there are two differential states, namely the biomass of the prey $x_0(t)$ that is assumed to grow exponentially and the biomass of the predator species $x_1(t)$ that is assumed to decrease exponentially. A second coupling term standing for the probability of a contact between the two species gives a decrease in the biomass of prey and an increase in that of the predator due to eating. The system is assumed to be in a given state $x(t_0) = x_0 \geq 0$ at time t_0. All parameters typically in use in such models are assumed to be 1 for the sake of notational simplicity.

$$
\begin{aligned}
\dot{x}_0(t) &= x_0(t) - x_0(t)x_1(t) \\
\dot{x}_1(t) &= -x_1(t) + x_0(t)x_1(t) \\
x_i(t_0) &= x_{i0}
\end{aligned}
\tag{15}
$$

The plots in Figure 1 show the periodic oscillating nature of this model for a given initial state $x = (0.5, 0.7)^T$.

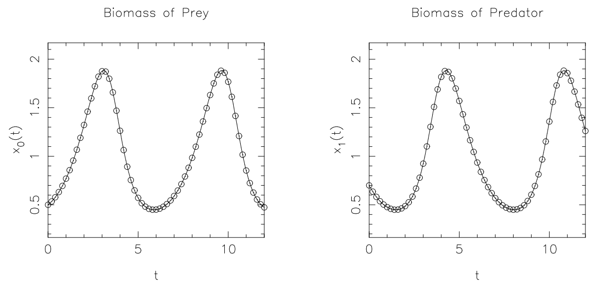

Fig. 1. Simulation of the ODE (15) for a time horizon $[t_0, T] = [0, 12]$.

4.2 Optimal Control Problem

As D'Ancona and Volterra [30] observed due to an unexpected decrease in the fishing quota after World War I – everybody expected an increase as fishing was almost completely abandoned in the war years – that there is an interconnection between the evolution of the biomasses of a system of type (15) and fishing. A very simple way to model an additional fishing aspect is the following model:

$$\begin{aligned}
\dot{x}_0(t) &= x_0(t) - x_0(t)x_1(t) \quad - c_0 x_0(t)\, w(t) \\
\dot{x}_1(t) &= -x_1(t) + x_0(t)x_1(t) - c_1 x_1(t)\, w(t) \\
x_i(t_0) &= x_{i0}\,, \quad w(t) \in [0,1]
\end{aligned} \tag{16}$$

Here $w(t)$ is a function describing the percentage of the fleet that is actually fishing at time t. The parameters c_0 and c_1 indicate how many fish would be caught by the entire fleet, we choose arbitrarily $c_0 = 0.4$ and $c_1 = 0.2$. The plots in Figure 2 show that amplitude and phase offset have changed, but that the periodic oscillating nature is kept for $w(t) = 1$.

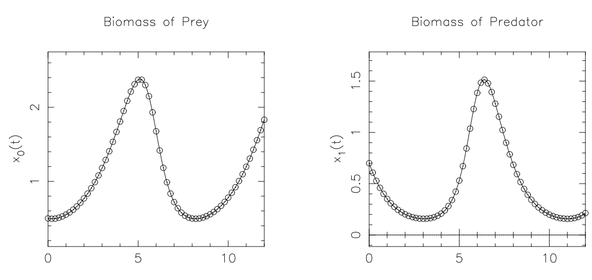

Fig. 2. Simulation of the ODE (16) with fishing for a time horizon $[t_0, T] = [0, 12]$.

One might be interested in bringing such a system close to a steady state to avoid the high fluctuations shown in Figure 2 that cause economical problems. One way to achieve this is to vary the fishing quota for a certain time span $T - t_0$. Adding an objective functional that punishes deviation from the steady state $\tilde{x} = (1,1)^T$ for $w(t) = 0$ resp. $\tilde{x} = (1 + c_1, 1 - c_0)^T$ for $w(t) = 1$ [3]

$$\min_{x,w} \int_{t_0}^{T} (x_0(t) - 1)^2 + (x_1(t) - 1)^2 \, dt$$

leads us to the following optimal control problem

$$\begin{array}{ll} \min\limits_{x,w} & \int_{t_0}^{T} (x_0(t) - 1)^2 + (x_1(t) - 1)^2 \, dt \\ \text{s.t.} & \dot{x}_0(t) \ = x_0(t) - x_0(t)x_1(t) \quad - c_0 x_0(t) \, w(t) \\ & \dot{x}_1(t) \ = -x_1(t) + x_0(t)x_1(t) - c_1 x_1(t) \, w(t) \\ & x_i(t_0) = x_{i0} \ , \quad w(t) \in [0,1] \end{array} \tag{17}$$

This optimal control problem can e.g. be solved by indirect methods or with the direct multiple shooting method. Having a look at the optimal control function $w(t)$ (see Figure 3) one notices that the percentage of the fleet that is fishing at a given time t is varying strongly on the singular arc, which would be practically very hard to achieve in the fishing example. From an economic point of view it would be easier to operate either the entire fleet or to do no fishing at all and use the manforce for different things in the meantime (on fixed time intervals corresponding to weeks). This could be achieved by laws that prohibit fishing for a certain time span. This would lead us to a model of the form

$$\begin{array}{ll} \min\limits_{x,w} & \int_{t_0}^{T} (x_0(t) - 1)^2 + (x_1(t) - 1)^2 \, dt \\ \text{s.t.} & \dot{x}_0(t) \ = x_0(t) - x_0(t)x_1(t) \quad - c_0 x_0(t) \, w(t) \\ & \dot{x}_1(t) \ = -x_1(t) + x_0(t)x_1(t) - c_1 x_1(t) \, w(t) \\ & x_i(t_0) = x_{i0} \ , \quad w(t) \in \Omega(\Psi) \end{array} \tag{18}$$

where the control function is restricted to take values of either 0 or 1 and change its value only at given time points, see definition (7) of $\Omega(\Psi)$. In our case we assume a hime horizon $[t_0, T] = [0, 12]$ and $n_\tau = 60$ equidistant time points, e.g. the start of a working week or a month, to be feasible switching points. Therefore all calculations in this paper are done using a control parameterisation of $m = 60$ intervals.

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[3] for the sake of notational simplicity we will stick to the first case, wanting a steady state for a system left alone after time T

4.3 Relaxed Solutions

The relaxed fishing problem (17) can be solved efficiently with the standard direct multiple shooting method. It is also possible to apply indirect methods, which is typically much harder for higher dimensional optimal control problems with a complex switching structure. Here we give some details to deliver a more comprising understanding of the system under investigation. We write x_i for $x_i(t)$, w for $w(t)$ and λ_i for $\lambda_i(t)$. The Hamiltonian in normalized form H and the adjoint equations of (17) are given by

$$\begin{aligned} H &:= -L(x) + \lambda^T f(x,w) \\ &= -(x_0-1)^2 - (x_1-1)^2 \\ &\quad +\lambda_0(x_0 - x_0x_1 - c_0x_0w) + \lambda_1(-x_1 + x_0x_1 - c_1x_1w) \\ \dot\lambda_0 &:= -H_{x_0} = 2(x_0-1) - \lambda_0(1 - x_1 - c_0w) - \lambda_1x_1 \\ \dot\lambda_1 &:= -H_{x_1} = 2(x_1-1) + \lambda_0x_0 - \lambda_1(-1 + x_0 - c_1w) \end{aligned}$$

The switching function $S(x,\lambda)$ is given by $S(x,\lambda) := H_w = -c_1\lambda_1x_1 - c_2\lambda_2x_2$. It can be shown, e.g. with the methods presented in [19], that the optimal relaxed control (neglecting $\Psi = \{\tau_1, \tau_2, \ldots, \tau_{60}\}$) has the form

$$w(t, x(t), \hat t) := \begin{cases} 0 & \text{for } t \in [t_0, \hat t_1] \\ 1 & \text{for } t \in [\hat t_1, \hat t_2] \\ w_{\text{sing}}(x) & \text{for } t \in [\hat t_2, T] \end{cases} \tag{19}$$

The singular control is of *order one* since the second total time derivative $S^2(x,\lambda,u)$ of the switching function $S(x,\lambda)$ contains the control explicitly. Then along a singular arc the equations $S(x,\lambda) = 0, S^1(x,\lambda) = \frac{d}{dt}S(x,\lambda) = 0$ and $S^2(x,\lambda,u) = 0$ hold from which one can compute the singular control in feedback form (the adjoint variables λ can be eliminated),

$$\begin{aligned} w_{\text{sing}} = (\ & c_0^3x_0^3 - c_1^3x_1^3 + c_0^3x_0^2x_1 - c_1^3x_0x_1^2 + 2c_0x_0x_1^2c_1^2 - 2c_1x_0^2x_1c_0^2 \\ & - 4c_0^2x_0c_1x_1^2 + 2c_0^2x_0c_1x_1 + 4c_1^2x_1c_0x_0^2 - 2c_1^2x_1c_0x_0 \\ & - x_0^3x_1c_0^3 + x_0^2x_1^2c_1^3 + x_0x_1^3c_1^3 - 2x_0^2x_1^2c_1^2c_0 + x_0^3x_1c_1c_0^2 \\ & - x_0x_1^3c_0c_1^2 - x_0^3x_1c_1^2c_0 - x_0^2x_1^2c_0^3 + 2x_0^2x_1^2c_0^2c_1 + x_0x_1^3c_0^2c_1\ ) \\ /\ (\ & c_0^4x_0^3 + 2c_0^2x_0^2c_1^2x_1 - 2c_0^2x_0c_1^2x_1 + 2c_1^2x_1^2c_0^2x_0 \\ & + c_1^4x_1^3 - c_0^3x_0c_1x_1^2 + c_0^3x_0c_1x_1 - c_1^3x_1c_0x_0^2 + c_1^3x_1c_0x_0\ ) \end{aligned} \tag{20}$$

for the singular arc $[\hat t_2, T]$. The parameters $\hat t_1$ and $\hat t_2$ can be determined to $\hat t_1 = 2.43670$ and $\hat t_2 = \hat t_1 + 1.50526$ by solving a boundary value problem. The computed initial values of the adjoint states are $\lambda_0(0) = 5.83903$ and $\lambda_1(0) = 1.53101$. The resulting optimal control $w(t)$ is shown in Figure 3, together with the optimal parameterised control obtained by appyling the direct multiple shooting method. Figure 4 shows the corresponding state trajectories. The minimum deviations obtained by these controls are $\Phi = 1.34408$ for the indirect method and $\Phi = 1.34466$ for the parameterised approximation (that takes into account $\Psi = \{\tau_1, \tau_2, \ldots, \tau_{60}\}$).

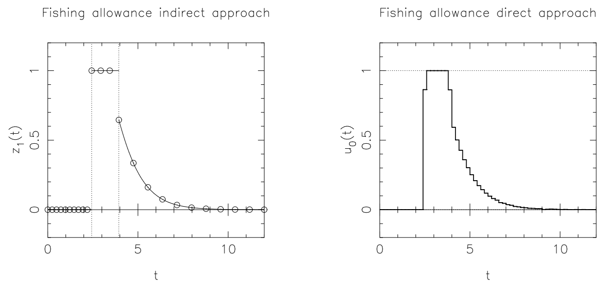

Fig. 3. Optimal controls for the relaxed problem. Left: indirect approach. Right: direct multiple shooting with 60 intervals.

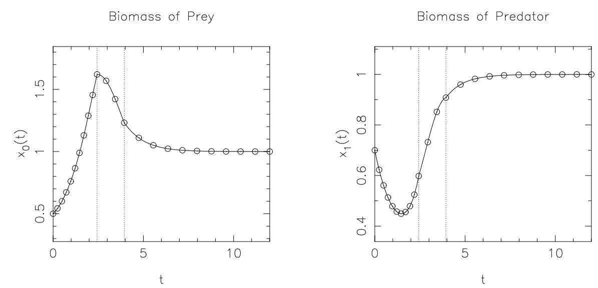

Fig. 4. Optimal states for the relaxed problem, obtained with the indirect method.

5 Numerical Results

In this section we want to show and discuss results obtained from the application of the methods described in Section 3 to the optimal control problem presented in Section 4. In 5.1 we will show how certain heuristics perform, while 5.2 gives results for the global Branch and Bound approach. In 5.3 we discuss a possible extension to a continuous optimisation of the switching points.

In all problems that had to be solved, the control was initialised with $w(t) = 0 \ \forall t \in [t_0, T]$ and the initial multiple shooting node values were obtained by integration with this fixed control. As a measurement for computational effort we consider the number of QPs to be solved (more precise would be SQP iterations as there is additional effort such as solving the ODE and linearising).

5.1 Heuristics

Heuristic solutions for problem (18) can be obtained in a number of ways. In this discussion we will focus on the rounding heuristics and the penalty term homotopy described in Section 3.1. Table 1 shows how many quadratic programs (QPs) had to be solved and what objective values were obtained. $w(t) = 0$ and $w(t) = 1$ correspond to the cases where the control is fixed to one value for the whole time horizon, thus no fishing at all or fishing all the time. The plots in Figures 1 and 2 show the respective states for these controls. They both do not require any QP to be solved, as an integration of the system with fixed controls suffices to obtain the solution. The rounding heuristics require a relaxed solution $\bar{w}(t)$ of problem (17), which takes 23 iterations. The penalty parameters for the penalty homotopy (see 3.1) are

Heuristics	# QPs	Objective value
$w(t) = 0$	0	6.06187
$w(t) = 1$	0	9.40231
Rounding 1	23	1.51101
Rounding 2	23	1.45149
Rounding 3	23	1.34996
Penalty homotopy	89	1.34898

Table 1. Number of QPs to be solved and obtained objective value for several heuristics to get a feasible solution.

chosen exponentially increasing as

$$\epsilon_i^k = \epsilon_{\text{init}} * \epsilon_{\text{inc}}^{k-1}$$

for $k \geq 1$ and $\epsilon_i^0 = 0$ to get the relaxed parameterised solution as starting point for the homotopy. A choice of $\epsilon_{\text{init}} = 10^{-4}$ and $\epsilon_{\text{inc}} = 2.1$ showed good results. A faster increase in the penalty parameters is getting closer to simple rounding, while a slower increase leads to an augmentation in the number of QPs to be solved. All problems of the homotopy were solved to an accuracy of 10^{-4}, while all other problems in this paper were solved up to 10^{-6}.

Table 1 shows that the proposed homotopy delivers a solution with an objective value of 1.34898 closer to the objective value 1.34466 of the parameterised relaxed model (17) than the rounding heuristics. As the optimal solution of (17) is a lower bound on the optimal integer solution of (18), the difference gives an indication about how good our heuristic solution is. As the relative gap of about 0.3% is known at runtime, one can decide whether the obtained solution suffices, otherwise one has to turn to global methods, where it can be used as an upper bound. This will be the topic of the next section.

5.2 Branch and Bound

Before applying a Branch and Bound approach to problem (18) we have to investigate whether the optimal control problem is convex. The feasible set is the hypercube in $\mathbb{R}^{n_w}$ and thus convex. We do not show analytically that the objective function is convex as well, but refer to Figure 5 that shows the behaviour of the objective function in the vicinity of the optimal relaxed solution – on 59 stages $w(t)$ is fixed and on one stage the value is changing. In

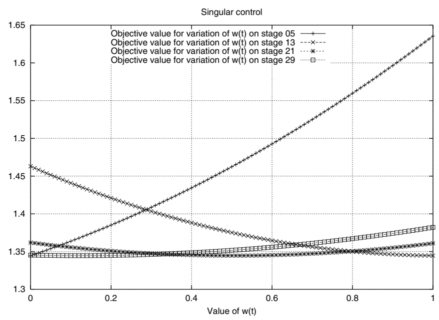

Fig. 5. The objective function in the vicinity of the optimal solution: for four selected stages the control on this stage is changing its value while the other 59 values are fixed. The trajectories give an indication for the convexity of the objective function over the feasible set.

the following, we do assume that the objective function is indeed convex for the given data. Thus we can apply a Branch and Bound approach as presented in Section 3.2. Figure 6 shows the optimal controls obtained by the Branch and Bound approach and, for comparison, a rounded control. The optimal solution on $\Psi = \{\tau_1, \tau_2, \dots, \tau_{60}\}$ is

$$w(t) = \begin{cases} 0 & t \in [\tau_i, \tau_{i+1}] \text{ and } i \in I_{\text{off}} \\ 1 & t \in [\tau_i, \tau_{i+1}] \text{ and } i \in I_{\text{on}} \end{cases}$$

with

$$I_{\text{on}} = \{13, 14, \dots, 20, 22, 25, 28\}$$
$$I_{\text{off}} = \{1, 2, \dots, 60\} \setminus I_{\text{on}}$$

Figure 7 shows the state trajectories of the biomasses that correspond to the optimal integer solution obtained by Branch and Bound. Note the non-differentiabilities in the states caused by the switching of the control function.

The behaviour of the Branch and Bound method depends very strongly on the availability of an upper bound. Table 2 gives performance data for different heuristics to get such an a priori upper bound. The first integer solution and therefore upper bound is found after branching on 33 variables, if no nodes are fathomed. The objective value of this feasible solution is 1.36614 – thus it is clear, that no heuristics will help to reduce the size of the Branch and Bound tree that delivers an upper bound above this value and it explains why two rounding heuristics perform as bad as the Branch and Bound without any upper bounding heuristics at all. Rounding strategy 3 gives a result

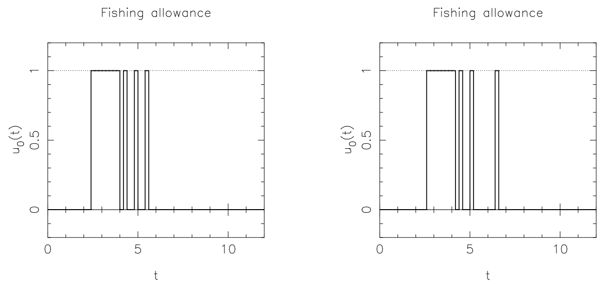

Fig. 6. Left: global optimal control obtained by Branch and Bound. Right: optimal control obtained by rounding strategy 2.

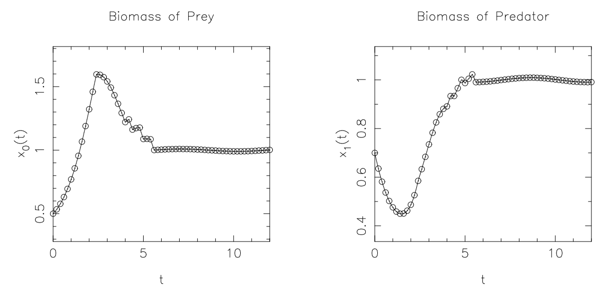

Fig. 7. State trajectories corresponding to the optimal integer solution.

Start heuristics	# Nodes	# QPs	Opt. in iter	First upper bound
None	1634	15720	1064	∞
Rounding 1	1634	15720	1064	1.51101
Rounding 2	1634	15720	1064	1.45149
Rounding 3	906	9210	336	1.34996
Penalty homotopy	757	7769	1	1.34898

Table 2. Number of nodes in the Branch and Bound tree, overall number of QPs to be solved, the node iteration when the optimal solution is found and the start upper bound for several heuristics to produce an upper bound.

close to the optimal solution, differing only on intervals $22, 23$ and $27, 28$. The solution obtained by the penalty homotopy turns out to be the global solution, although further 756 nodes have to be visited and 7680 SQP iterations are needed to verify this in our Branch and Bound implementation.

5.3 Switching Time Approach

Although we have the additional Ψ-restriction on $w(t) \in \Omega(\Psi)$ resp. $w(t) \in \bar{\Omega}(\Psi)$, it is interesting to investigate how much we could improve an obtained solution by giving additional degrees of freedom. Table 3 lists results obtained

Method	n_{sw}	# QPs	Objective value
ST after Rounding 2	8	35	1.34541
ST after B&B	8	7852	1.34604
ST after Penalty homotopy	8	171	1.34604
ST after Rounding 3	8	35	1.34616
ST after Rounding 1	2	38	1.38273
ST after Initialisation by hand	8	142	1.38273

Table 3. Switching time optimisation results.

by a switching time (ST) approach. n_{sw} and initial values for $\hat{t}_1, \dots, \hat{t}_{n_{\text{sw}}}$ are obtained by a transformation of a solution $w(t)$ of problem (18). To get this, methods investigated in 5.1 or 5.2 are used. After the transformation the controls $w(t)$ and $w(t; \hat{t}, n_{\text{sw}})$ are identical. With this start initialisation the switching times $\hat{t}$ are optimised, n_{sw} is kept constant. *Initialisation by hand* is a solution set up arbitrarily in the following way:

$$\begin{aligned} n_{\text{sw}} = 8, \hat{t}_0 = 0.0, \hat{t}_1 = 2.8, \hat{t}_2 = 4.0, \hat{t}_3 = 7.0, \hat{t}_4 = 7.4, \\ \hat{t}_5 = 8.0, \hat{t}_6 = 8.2, \hat{t}_7 = 10.0, \hat{t}_8 = 10.2, \hat{t}_9 = 12.0 \end{aligned}$$

Figure 8 shows this initialisation and the control obtained by an optimisation of $\hat{t}$, Figure 9 shows the corresponding states. Although n_{sw} is chosen such that eight switches are allowed, the optimisation procedure reduced three intervals to size zero and ends in the local solution also found by optimisation after initialisation with rounding strategy 1 (with $n_{\text{sw}} = 2$). This makes clear that it is not enough to simply increase n_{sw} without suppyling good initial values for a switching time approach. Another interesting point is that initialisation with rounding strategy 2 gives the best solution

$$\begin{aligned} n_{\text{sw}} = 8, \hat{t}_0 = 0.00000, \hat{t}_1 = 2.44093, \hat{t}_2 = 4.07798, \\ \hat{t}_3 = 4.29155, \hat{t}_4 = 4.50443, \hat{t}_5 = 4.90853 \\ \hat{t}_6 = 5.12223, \hat{t}_7 = 6.15604, \hat{t}_8 = 6.28131, \hat{t}_9 = 12.0 \end{aligned} \tag{21}$$

although it has a higher objective value than other initialisations. This is also due to the many local minima in the switching time formulation. Table 4 gives a final comparing overview over all obtained solutions in this study.

Remark 6. We do know from the maximum principle that a bang-bang control exists with the same objective function value as the solution including the singular arc, thus solution (21) is still suboptimal, n_{sw} needs to be increased (probably to infinity). Here we are content with the feasible integer solution (21), being closer than 10^{-3} to the relaxed parameterised solution.

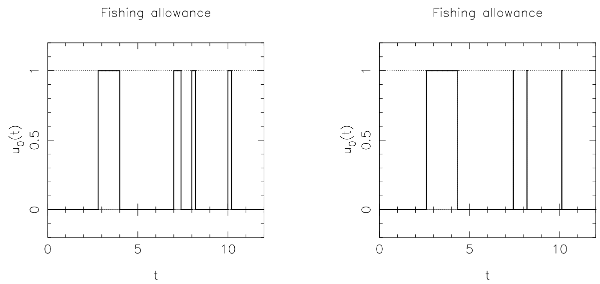

Fig. 8. Control initialisation set up by hand and resulting control after optimisation of switching points. Three intervals shrink to length zero.

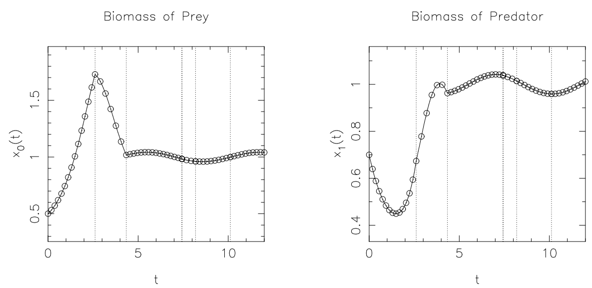

Fig. 9. State trajectories corresponding to control of Figure 8.

Method	# QPs	Objective value
Relaxed indirect	28	1.34408
Relaxed parameterised	23	1.34466
ST after Rounding 2	35	1.34541
ST after B&B	7852	1.34604
ST after Penalty homotopy	171	1.34604
ST after Rounding 3	35	1.34616
B&B	7769	1.34898
Penalty homotopy	89	1.34898
Rounding 3	23	1.34996
ST after Rounding 1	38	1.38273
ST after Initialisation by hand	142	1.38273
Rounding 2	23	1.45149
Rounding 1	23	1.51101
$w(t) = 0$	0	6.06187
$w(t) = 1$	0	9.40231

Table 4. Overview: number of QPs to be solved and obtained objective value for different approaches. Parameterisation was done with 60 multiple shooting intervals.

6 Conclusion

We have presented a benchmark problem for optimal control with $0-1$ controls that can be extended in a straightforward way to several species, other parameters or discretisations. Several heuristics and a global approach, namely a Branch and Bound strategy, have been described and applied successfully. Numerical results have been given that show the potential of a penalty term homotopy. In the special problem considered in this study it delivered the global (under a convexity assumption) optimal solution for a fixed time grid. Furthermore we showed how these methods may be used to initialise parameters in a switching time approach to deal with problems without fixed time grid.

The methods described in this paper, several heuristics and Branch and Bound, are implemented in a software package based on the direct multiple shooting method and advanced algorithms also implemented in `MUSCOD-II` and may be applied to larger-scale optimal control problems with $0-1$ controls in the future.

Future research will focus on a globalisation of the penalty term homotopy and further applications in cell biology and chemical engineering.

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