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Numerical Optimisation of Multiple-Phase Systems Incorporating Transition

Costs^Ψ

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Abstract. Many important economic problems concern an intertemporal choice between alternate dynamical systems. One example is determining the optimal management of alternative production technologies. This significance has motivated a substantial theoretical literature generalising the necessary conditions of Optimal Control Theory to multiple-phase problems. However, gaining detailed insight into their practical management is difficult because suitable numerical solution methods are not available. This paper resolves this deficiency through the development of a flexible and efficient computational algorithm based on a set of necessary conditions derived for finite-time multiple-phase systems. Its effectiveness is demonstrated in an application to a complex crop rotation problem.

Keywords. Crop management, multiple-phase systems, optimal control.

JEL classification codes. C61; Q24.

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17 **1. Introduction**

18 The Maximum Principle of Optimal Control Theory (Pontryagin et al., 1962) has been utilised
19 extensively in economics (Arrow and Kurz, 1970; Seierstad and Sydsaeter, 1987; Kamien and
20 Schwartz, 1991) because of its intuitive economic interpretation (Dorfman, 1969) and the
21 significant methodological extensions to this theory developed in other fields of study, such as
22 engineering. However, despite this broad application, there has been limited treatment of
23 multiple-phase systems. These consist of multiple alternate regimes, each characterised by its
24 own dynamical system, of which only one may be active at each point in time. Selecting
25 between individual crops to plant on a given area of land is one example (Mueller et al., 1999).
26 Other examples are determining the optimal time to switch between alternative energy sources
27 (Tomiyaama, 1985; Tomiyaama and Rossana, 1989) and identifying the optimal time for a
28 government to abolish a policy, such as a capital control (Makris, 2001). In actual fact, many
29 economic decisions may be studied more precisely if cast as multiple-phase problems. For
30 example, in production theory, these are a natural means of representing choices between the
31 alternative technologies available to a firm, such as the natural and artificial recovery of
32 petroleum (Amit, 1986).

33 Switching schedules may be determined through the standard Maximum Principle if individual
34 stages are represented by piecewise-constant control variables. However, this approach is
35 inherently combinatorial and complicated significantly through the existence of transition costs
36 (see Teo and Jennings, 1991, and references therein). These limitations have motivated the
37 analysis of multiple-phase systems in which the sequence of stages is pre-assigned. This
38 approach is, in fact, relevant to many important economic problems, such as the alternative crop,
39 technology, or government policy examples outlined above. Such systems may be studied in a
40 financial options framework (Dixit and Pindyck, 1994) if no control variables are exercised

41 during the duration of a stage. In contrast, generalisation of the Maximum Principle (Pontryagin
42 et al., 1962; Kamien and Schwartz, 1991) is required if instrument variables are defined within
43 independent phases. Such conditions have been derived for two-stage systems with costless
44 transition (Tomiyama, 1985; Tomiyama and Rossana, 1989) and switching costs (Amit, 1986).
45 The latter framework has also been extended to include three stages (Mueller et al., 1999) and an
46 infinite horizon (Makris, 2001).

47 Though this theory is well established, the practical management of multiple-phase problems is
48 difficult to study given a distinct lack of suitable optimisation algorithms. Gradient-based
49 methods (Judd, 1998) are difficult to apply to a multiple-phase system incorporating control
50 variables in each stage because the state and costate equations are piecewise defined and the
51 performance index has, by definition, discontinuous derivative(s) with respect to the control
52 variable(s) within each stage (see section 2). Transition costs also introduce step discontinuities
53 into the adjoint and Hamiltonian trajectories along an optimal path. Moreover, the efficient
54 computation of optimal strategies for multiple-phase problems of realistic complexity through
55 dynamic programming (Rust, 1996) is non-trivial in most instances. This is intuitive given the
56 large state and policy spaces typically encountered within such applications.

57 This paper presents a novel computational algorithm for the solution of multiple-phase optimal
58 control problems incorporating transition costs. It involves the iterative improvement of switch
59 points utilising a root-finding procedure. This approach is inspired by the use of shooting
60 methods to solve boundary value problems (Ascher et al., 1995; Stoer and Bulirsch, 2002). The
61 algorithm presented here is based on a set of necessary conditions derived for a finite-time
62 multiple-phase system with different endpoint constraints and n phases. This derivation is
63 necessary because previous theoretical studies have ignored alternative endpoint constraints,
64 consequently narrowing their applicability, and the prior analysis of finite-time systems has been

65 limited to either two (Tomiyama, 1985; Amit, 1986; Tomiyama and Rossana, 1989) or three
66 regimes (Mueller et al., 1999). The effectiveness of the algorithm is demonstrated in an
67 application to a complex multiple crop control problem incorporating strong nonlinearities and
68 stiff process equations. This algorithm appears to be the first in Economics to solve general
69 multiple-phase problems and provides practitioners with the opportunity to study these systems
70 in considerable detail, a luxury not afforded in the analytical constructs to which they have
71 previously been restricted.

72 The model and necessary conditions are presented in Section 2. Section 3 describes the
73 numerical algorithm and discusses its implementation. An application of this algorithm to a
74 multiple crop problem is presented in Section 4. Section 5 presents conclusions and
75 recommendations for further research. The parameter values for the numerical application are
76 presented in an appendix.

77 **2. Model and Necessary Conditions**

78 This section formally defines a model for a multiple-phase system and presents a set of
79 necessary conditions required for its solution.

80 *DEFINITION 2.1. A general multiple-phase system is assumed to incorporate an m -dimensional*
81 *state vector $x(t) = \{x^1(t), x^2(t), \dots, x^m(t)\}$ of continuous functions, piecewise continuous*
82 *differentiable over the time interval $t = [t_0, \dots, t_n]$ and belonging to $X \in R^m$, and a v -*
83 *dimensional vector of control functions $u(t) = \{u^1(t), u^2(t), \dots, u^v(t)\}$, piecewise continuous in*
84 *$t = [t_0, \dots, t_n]$ and belonging to $U \in R^v$. The state variables are assumed fixed at the initial time*
85 *and are denoted x_0 . The state variables free at the terminal time are denoted x_n^i , for*
86 *$i = [1, 2, \dots, d]$. Terminal state variables x_n^i , for $i = [d + 1, \dots, m]$, are fixed. \square*

87 This model concerns multiple-phase systems with a given switching sequence and fixed number
 88 of stages. Relaxation of these assumptions adds significant complexity but would nevertheless
 89 be a valuable extension of this work.

90 DEFINITION 2.2.¹ A multiple-phase switching system is defined as $\Xi = \{T, K, \vartheta\}$ where,

- 91 1. T is a set of discrete controls known as switching times that dictate the termination of one
 92 phase and the start of the next,
- 93 2. $K = \{k_1, k_2, \dots, k_n\}$ is a finite, fixed, and exogenously determined sequence of discrete
 94 (integer) states that indexes individual continuous dynamical systems, $\vartheta = \{\vartheta_k\}_{k \in K}$, where
 95 $\vartheta_k = [X, f_k, U]$. The ordinal ranking of sequences is defined over the closed interval
 96 $j = [1, 2, \dots, n]$,
- 97 3. X is a continuous state space where $X \in \mathbb{R}^m$,
- 98 4. f_k is the vector of state equations for each stage k , and
- 99 5. U is the set of admissible controls lying in \mathbb{R}^v . □

100 DEFINITION 2.3. A control input for a multiple-phase switching system Ξ consists of a set of
 101 vectors $\chi_\Xi = \{t, u\}$ where,

- 102 1. $t = \{t_1, t_2, \dots, t_{n-1}\}$ is a sequence of real numbers denoting switching times, the moment t_j
 103 at which stage k_j is terminated and the stage k_{j+1} becomes active. It follows that regime
 104 k_j is active over the interval $[t_{j-1}^+, t_j^-]$, where t_{j-1}^+ is the moment just after t_{j-1} and t_j^- is
 105 the moment just before t_j ,

¹ This definition is loosely based on the hybrid system defined in Branicky et al. (1998).

106 2. $t = t_n$ is a freely determined terminal time, and

107 3. $u = \{u_1, u_2, \dots, u_n\}$ is a collection of control functions defined for each stage in sequence K .

108 □

109 It is possible for switching times to accumulate in this model. Consequently, not all regimes in
110 the predefined sequence must be activated. For example, it may be optimal for two consecutive
111 switching times, such as t_j and t_{j+1} , to coalesce (that is, $t_j = t_{j+1}$), in which case, movement
112 from k_j to k_{j+2} will occur without the activation of k_{j+1} . This allows for the case where the
113 operation of a stage or number of stages in sequence K is not contained in the optimal solution.

114 The state variable is continuous at the switching times in this model. However, jumps within the
115 state variable (Vind, 1967) may be accommodated with manipulation of the necessary
116 conditions (see Seierstad and Sydsaeter, 1987).

117 DEFINITION 2.4. A trajectory (Γ) for a multiple-phase switching system Ξ and control sequence
118 \mathcal{X}_Ξ is admissible over the interval $t = [t_0, t_1, \dots, t_{n-1}, t_n]$ if it satisfies Definition 2.1 and the
119 continuous dynamics $\dot{x} = f_j(x(t), u_j(t))$, for $[t_{j-1}^+, t_j^-]$ and $j \in J$, for a predefined switching
120 sequence $K = \{k_1, k_2, \dots, k_n\}$. □

121 These definitions permit the classification of a general multiple-phase optimal control problem.

122 PROBLEM 2.1. For a multiple-phase system Ξ identify an admissible trajectory that maximises
123 the objective functional,

124
$$J = e^{-rt_n} G(x(t_n), t_n) + \sum_{j=1}^{n-1} e^{-rt_j} C_j(x(t_j)) + \sum_{j=1}^n \left[\int_{t_{j-1}^+}^{t_j^-} [e^{-rt} F_j(x(t), u_j(t))] dt \right], \quad (1)$$

125 *subject to,*

126 $\dot{x} = f_j(x(t), u_j(t)), \text{ for } [t_{j-1}^+, t_j^-] \text{ and } j = [1, 2, \dots, n] \text{ given } K = \{k_1, k_2, \dots, k_n\},$ (2)

127 $t_j \text{ free for } j = [1, 2, \dots, n],$ (3)

128 $x(t_j) \text{ free for } j = [1, 2, \dots, n-1],$ (4)

129 $x_0 \text{ fixed},$ (5)

130 $x_n^i(t_n) \text{ free, for } i = [1, \dots, d], \text{ and}$ (6)

131 $x_n^i(t_n) \text{ fixed for } i = [d+1, \dots, m],$ (7)

132 *where r is a discount rate, $G(x(t_n), t_n)$ is a terminal reward function, $C_j(x(t_j))$ is a switching*
133 *cost function for the j th phase, and $F_j(x(t), u_j(t))$ is a single-valued reward function on*
134 *$X^m \times U^v$ for the j th phase. Functions $G(\cdot)$, $C(\cdot)$, and $F(\cdot)$ are all real-valued functions that are*
135 *once continuously differentiable in the relevant arguments. The terminal value function G is*
136 *defined for $x_n^i(t_n)$, where $i = [1, \dots, d]$. □*

137 The terminal reward function $G(x(t_n), t_n)$ is defined as a salvage value in economic applications
138 of optimal control. The switching cost function is a cost accruing to the termination of one stage
139 and the start of another. (These can be understood as terminal value functions for individual
140 regimes.) They are a pertinent feature of many multiple-phase systems. For example, it can be
141 costly to remove one crop and establish another (Mueller et al., 1999) or invest in the productive
142 capacity required for the artificial recovery of petroleum (Amit, 1986). Both the terminal value
143 function $G(\cdot)$ and the switching cost function $C(\cdot)$ are dependent on the state variable ($x(t_j)$).

144 The latter is included because it is likely to exist in a number of important multiple-phase
 145 problems. For example, the herbicide dose required for the establishment or removal of a crop
 146 may be dependent on weed density. Or, investing in a new production technology may require
 147 an initial outlay that is dependent on the current capacity of the existing firm.

148 THEOREM 2.1. Consider a multiple-phase system Ξ described by Definitions 2.1-2.4. For
 149 $j = [1, 2, \dots, n]$ and switching sequence $K = \{k_1, k_2, \dots, k_n\}$, let $(x^*(t), u_j^*(t), t_j^*)$ denote the
 150 admissible trajectory that maximises the value of J in Problem 2.1. This is the optimal trajectory
 151 Γ^* .

152 Define a Hamiltonian function for each regime k_j as,

$$153 \quad H_j(x(t), u_j(t), \lambda_j(t), t) = e^{-rt} F_j(x(t), u_j(t)) + \lambda_j(t) f_j(x(t), u_j(t), t), \quad (8)$$

154 across the interval $[t_{j-1^+}, t_{j^-}]$.

155 An optimal trajectory Γ^* requires,

$$156 \quad \text{i) } \quad \text{initial condition } x_0 = x(t_0) \text{ for fixed initial state variable(s) } x_0, \quad (9)$$

157 ii) n m -dimensional vectors of real-valued, piecewise continuous adjoint functions

158 $\lambda_j(t) = \{\lambda_j^1(t), \lambda_j^2(t), \dots, \lambda_j^m(t)\}$, defined across $j = [1, 2, \dots, n]$ and piecewise continuously

159 differentiable over the interval $[t_{j-1^+}, t_{j^-}]$, that satisfy,

$$160 \quad \dot{\lambda}_j^T(t) = - \frac{\partial H_j(x(t), u_j(t), \lambda_j(t), t)}{\partial x(t)}, \quad (10)$$

161 where $\lambda_j^T(t)$ denotes the transpose of the n adjoint vectors,

162 iii) *optimal control function(s) that satisfy,*

$$163 \quad \text{Max}_{u_j(t)} H_j(x(t), u_j(t), \lambda_j(t), t) \quad \text{for all } t \in [t_{j-1}^+, t_{j-}^-], \quad (11)$$

164 iv) *an adjoint vector $\lambda_n(t_n)$ that satisfies,*

$$165 \quad \lambda_n^T(t_n) = \frac{\partial e^{-rt_n} G(x(t_n), t_n)}{\partial x(t_n)}, \quad (12a)$$

166 *for state variables $x_n^i(t_n)$, where $i = [1, \dots, d]$, free at the terminal time and defined in G ,*

167 NOTE: $\lambda_n^T(t_n) = 0$ replaces (12a) for those state variables $x_n^i(t_n)$, where $i = [1, \dots, d]$, that are
168 not defined in G , (12b)

169 NOTE: $x_n^i(t_n) = x(t_n)$ replaces (12a) and (12b) for fixed terminal state variables $x_n^i(t_n)$, where
170 $i = [d + 1, \dots, m]$, (12c)

171 v) *a terminal time that satisfies,*

$$172 \quad H_n(x(t), u_n(t), \lambda_n(t), t) \Big|_{t_n} + \frac{\partial e^{-rt_n} G(x(t_n), t_n)}{\partial t_n} = 0, \quad (13a)$$

173 *if no terminal value function is defined, then the equivalent of (13a) is,*

$$174 \quad H_n(x(t), u_n(t), \lambda_n(t), t) \Big|_{t_n} = 0, \quad (13b)$$

175 *if, instead, the terminal time is fixed, then no additional necessary condition is required, as*

$$176 \quad t = t_n, \quad (13c)$$

177 vi) *adjoint vectors that satisfy the boundary conditions,*

$$178 \quad \lambda_j^T(t_{j^-}) + \frac{\partial e^{-r_j} C_j(x(t_j))}{\partial x(t_j)} = \lambda_{j+1}^T(t_{j^+}), \quad (14)$$

179 *at switching times $t = \{t_1, t_2, \dots, t_{n-1}\}$ and $j = [1, 2, \dots, n-1]$,*

$$180 \quad \text{vii) } H_j(x(t), u_j(t), \lambda_j(t), t) \Big|_{t_{j^-}} - \frac{\partial e^{-r_j} C_j(x(t_j))}{\partial t_j} = H_{j+1}(x(t), u_{j+1}(t), \lambda_{j+1}(t), t) \Big|_{t_{j^+}}, \quad (15)$$

181 *for those switching times in $t = \{t_1, t_2, \dots, t_{n-1}\}$ for which $t_{j-1} < t_j < t_{j+1}$ holds,*

$$182 \quad \text{viii) } H_j(x(t), u_j(t), \lambda_j(t), t) \Big|_{t_{j^-}} - \frac{\partial e^{-r_j} C_j(x(t_j))}{\partial t_j} \leq H_{j+1}(x(t), u_{j+1}(t), \lambda_{j+1}(t), t) \Big|_{t_{j^+}}, \quad (16)$$

183 *for those switching times in $t = \{t_1, t_2, \dots, t_{n-1}\}$ for which $t_{j-1} = t_j < t_{j+1}$ holds, and*

$$184 \quad \text{ix) } H_j(x(t), u_j(t), \lambda_j(t), t) \Big|_{t_{j^-}} - \frac{\partial e^{-r_j} C_j(x(t_j))}{\partial t_j} \geq H_{j+1}(x(t), u_{j+1}(t), \lambda_{j+1}(t), t) \Big|_{t_{j^+}}, \quad (17)$$

185 *for those switching times in $t = \{t_1, t_2, \dots, t_{n-1}\}$ for which $t_{j-1} < t_j = t_{j+1}$ holds. \square*

186 PROOF. An extensive proof is provided in a mathematical appendix available at
187 www.are.uwa.edu.au/home/derivation.

188 Necessary conditions (8)-(13) are analogous to the standard Maximum Principle (Seierstad and
189 Sydsaeter, 1987). This follows the definition of a multiple-phase problem as a set of n dynamical
190 systems. In contrast, switching conditions (14)-(17) are not found in standard control problems.
191 These describe how individual systems are linked over time under optimal management. These
192 conditions appear in similar form in the models of Amit (1986), Mueller et al. (1999), and
193 Makris (2001). It is demonstrated here that they generalise to a finite-time multiple-phase model

194 with n regimes, positive switching costs, and alternative endpoint constraints. Equations (14)
195 and (15) are also equivalent to the smooth pasting and value-matching conditions found in
196 applications of stochastic control in finance (Brekke and Oksendal, 1994; Dixit and Pindyck,
197 1994).

198 Equation (14) determines the optimal level of the state variable(s) at each switching time ($x(t_j)$)
199 (these are referred to as transition states in the following). The shadow price variables, $\lambda_j^T(t_j)$
200 and $\lambda_{j+1}^T(t_j)$, represent the marginal adjustment in optimal value accruing to a change in the
201 state variable within the corresponding stage when switching time t_j is approached from below
202 or above respectively. The second term in (14) represents the marginal transition cost for the
203 active regime. Equation (14) states that it is optimal to switch when the marginal value of a
204 change in the state variable is equivalent between stages.

205 Switching conditions (15)-(17) describe the management of optimal switching times given the
206 relative value of alternate stages. The value of a Hamiltonian function $H_j(x(t), u_j(t), \lambda_j(t), t)$
207 evaluated at a given time represents the shadow price of altering the length of this phase. The
208 second term in each of conditions (15)-(17) is the rate at which transition costs change over time
209 within regime j . Equation (15) states that it is optimal to switch to the subsequent regime at time
210 t_j if the rate at which the capital value of each stage changes over time is equal at that point.
211 Regime j should not be activated if its total value, reflected through its Hamiltonian and
212 switching cost functions, is dominated at each potential switching time by that of the successive
213 regime. This is described in (16). Moreover, the successive regime should not be adopted if there
214 is no time t_j at which its capital value matches that earned within the active phase. This is stated
215 in equation (17).

216 Necessary conditions (14)-(17) are not required if T is empty. In this instance, Theorem 2.1
 217 collapses to the standard Maximum Principle. The state variable(s) could be fixed for a given
 218 switching time t_j . In this instance, equation (14) is no longer required for the determination of
 219 $x(t_j)$. Alternatively, the control input $\chi_{\bar{z}}$ may contain fixed switching times. Necessary
 220 conditions (15)-(17) are not required in this case.

221 The boundary conditions are obviously affected if switching cost functions $e^{-rt_j} C_j(x(t_j))$
 222 and/or their relevant derivatives are not defined. If switching costs do not exist or are
 223 independent of the state vector, condition (14) requires equality between the adjoint variables of
 224 stages j and $j+1$. That is, $\lambda_j^T(t_j) = \lambda_{j+1}^T(t_j)$. Likewise, equation (15) simplifies to a requirement
 225 of equality between the total capital value of each regime at the switching time; that is,
 226 $H_j(\cdot)\big|_{t_j} = H_{j+1}(\cdot)\big|_{t_j}$; if switching costs are not defined or are independent of time. (Switching
 227 costs will be a function of time in most economic problems because of discounting.) These
 228 results are analogous to the Weierstrass-Erdmann corner conditions (Seierstad and Sydsaeter,
 229 1987) from variational calculus, which are also required when state and/or control variables are
 230 subject to inequality constraints (Pontryagin et al., 1962). This equivalency highlights the close
 231 symmetry between multiple-phase problems with fixed and free stage sequencing, if the latter is
 232 incorporated utilising piecewise constant controls and transition costs do not exist.

233 **3. Algorithm**

234 Theorem 2.1 may be used to identify analytical solutions to multiple-phase problems of low
 235 dimension. However, such solutions are extremely difficult to obtain, even in systems
 236 incorporating only weakly non-linear differential equations. This section consequently describes
 237 an optimisation algorithm suited to the study of more complex problems.

238 The following algorithm is motivated by the structure of Theorem 2.1, which infers
 239 decomposition into two distinct stages. The first concerns the solution of each phase as an
 240 independent control problem at each iteration. The second concerns the updating of the switch
 241 points using the switching conditions (14) and (15) and a bisection technique (Stoer and
 242 Bulirsch, 2002). Bisection successively reduces the size of an interval where a root is bound
 243 between function values that are opposite in sign. Bisection is utilised here as other root-finding
 244 methods, such as the Newton, Broyden and secant methods (Ortega and Rheinboldt, 1970; Judd,
 245 1998), require continuity of the switching conditions. Newton's method also requires derivative
 246 information that is not available in this instance. The existence of a solution to an interval
 247 bisection technique is guaranteed for a continuous function through the intermediate value
 248 theorem, provided the initial function evaluations are opposite in sign. The step discontinuity
 249 that occurs at each switch point (given the presence of transition costs) does not void this
 250 condition in computational application given its equivalence to a continuous function whose root
 251 is located between two floating-point numbers (Press et al., 1992).

252 ALGORITHM 3.1

253 PURPOSE: Identify an optimal control sequence χ_{Ξ} for the multiple-phase system Ξ .

254 INITIALISATION:

- 255 a) Determine a fixed stage sequence K . Define the maximum number of permissible
 256 iterations (\hat{i}). Define the stopping tolerance ε . Define a set of initial conditions
 257 $\Lambda = \{t_0, x_0\}$. Provide estimates for the optimal switching times (t_j for $j = [1, 2, \dots, n-1]$)
 258 and the transition states ($x(t_j)$ for $j = [1, 2, \dots, n-1]$) for $i = \{1, 2\}$.
- 259 b) Optimise each phase k_j , for $j = [1, 2, \dots, n-1]$, as a fixed point control problem utilising

260 conditions (8)-(11) and (12c) and (13c). (12c) and (13c) are determined by the estimates
 261 of t_j and $x(t_j)$. Optimise the terminal stage utilising conditions (8)-(11) and the
 262 relevant terminal conditions from (12)-(13).

263 c) Obtain $\lambda_j^T(t_j)$ and compute $H_j(t_j)$ for all j . Ensure that

264
$$\left(\lambda_j^1(t_j) + \left(e^{-r_j} C_j(x(t_j)) \right)_{x(t_j)}^1 - \lambda_{j+1}^1(t_j) \right) \left(\lambda_j^2(t_j) + \left(e^{-r_j} C_j(x(t_j)) \right)_{x(t_j)}^2 - \lambda_{j+1}^2(t_j) \right) < 0$$
 and

265
$$\left(H_{t_j}^1(t_j) - \left(e^{-r_j} C_j(x(t_j)) \right)_{t_j}^1 - H_{j+1}^1(t_j) \right) \left(H_{t_j}^2(t_j) - \left(e^{-r_j} C_j(x(t_j)) \right)_{t_j}^2 - H_{j+1}^2(t_j) \right) < 0$$
 where

266 numeric superscripts denote the iteration number, $(\cdot)_x$ denotes the derivative of the term

267 enclosed in brackets with respect to the subscripted variable (x in this example), and

268 $t_j^1 < t_j^2$ and $x(t_j^1) < x(t_j^2)$.

269 MAIN COMPUTATION:

270 For $i=3:\hat{i}$

271 1. Form switch points for the current iteration using the midpoint formulas

272
$$t_j^i = (t_j^{i-1} - t_j^{i-2}) / 2$$
 and
$$x(t_j^i) = (x(t_j^{i-1}) - x(t_j^{i-2})) / 2.$$

273 2. Optimise each phase k_j for $j = [1, 2, \dots, n-1]$ as a fixed point control problem utilising

274 conditions (8)-(11) and (12c) and (13c). Optimise the terminal stage utilising conditions

275 (8)-(11) and the relevant terminal conditions in (12)-(13). Obtain $\lambda_j^T(t_j)$ and compute

276 $H_j(t_j)$ for all j .

277 3. If
$$\left(\lambda_j^i(t_j) + \left(e^{-r_j} C_j(x(t_j)) \right)_{x(t_j)}^i - \lambda_{j+1}^i(t_j) \right) \left(\lambda_j^{i-2}(t_j) + \left(e^{-r_j} C_j(x(t_j)) \right)_{x(t_j)}^{i-2} - \lambda_{j+1}^{i-2}(t_j) \right) > 0$$

278 then $x(t_j^i) = x(t_j^{i-2})$ and $x(t_j^{i-1}) = x(t_j^{i-1})$. Else, $x(t_j^i) = x(t_j^{i-1})$ and $x(t_j^{i-2}) = x(t_j^{i-2})$.

279 4. If $\left(H_{t_j}^i(t_j) - \left(e^{-rt_j} C_j(x(t_j)) \right)_{t_j}^i - H_{t_{j+1}}^i(t_j) \right) \left(H_{t_j}^{i-2}(t_j) - \left(e^{-rt_j} C_j(x(t_j)) \right)_{t_j}^{i-2} - H_{t_{j+1}}^{i-2}(t_j) \right) > 0$ then

280 $t_j^i = t_j^{i-2}$ and $t_j^{i-1} = t_j^{i-1}$. Else, $t_j^i = t_j^{i-1}$ and $t_j^{i-2} = t_j^{i-2}$.

281 5. Stop and print output if $t_j^i - t_j^{i-1} < \varepsilon$ and $x(t_j^i) - x(t_j^{i-1}) < \varepsilon$ or

282 $\left(\lambda_j^i(t_j) + \left(e^{-rt_j} C_j(x(t_j)) \right)_{x(t_j)}^i - \lambda_{j+1}^i(t_j) \right) < \varepsilon$ and $\left(H_j^i(t_j) - \left(e^{-rt_j} C_j(x(t_j)) \right)_{t_j}^i - H_{j+1}^i(t_j) \right) < \varepsilon$

283 for all j .

284 6. If $i = \hat{i}$, then stop and report progress; else go to Step 1.

285 The boundary conditions for each individual control problem in step (b) in the initialisation and
 286 step (2) in the main computation are well-defined following the prior definition of the switching
 287 times and the transition states. It is natural to question whether the designation of these fixed
 288 points will affect satisfaction of the optimality condition (11) for interior solutions, $(H_j(\cdot))_u = 0$
 289 for $j = [1, 2, \dots, n]$, as the weak variation δu in equation (A.14) in the accompanying
 290 mathematical appendix (available at www.are.uwa.edu.au/home/derivation) is no longer entirely
 291 arbitrary but must now satisfy these endpoint constraints. However, it may be shown that (11)
 292 holds despite this induced restriction (see Kamien and Schwartz, 1991, Section II.6).

293 The approach taken in Algorithm 3.1 resembles the single shooting algorithm used for the
 294 solution of two-point boundary value problems commonly defined by the necessary conditions
 295 of the standard Maximum Principle. The single shooting algorithm involves integration of the
 296 state and costate equations using an Initial Value Problem method and updating of the
 297 unspecified initial condition(s) through use of a root-finding method until the given endpoint
 298 condition(s) are satisfied to sufficient accuracy (Keller, 1968; Osborne, 1969; Ascher et al.,
 299 1995). Their stability is significantly increased through division of the problem into multiple
 300 intervals that reduce the length of each integration (Lipton et al., 1982; Stoer and Bulirsch,

301 2002). This method, known as multiple shooting, may be adapted to analyse multiple-phase
302 problems (see Bulirsch and Chudej 1995 for a two-phase example). However, in contrast to
303 Algorithm 3.1, an expensive approximation of the Jacobian matrix is typically required for the
304 non-linear equation solver at each iteration and this solver is also required to enforce the
305 continuity of each state variable at the switching time (Pesch, 1994; Stoer and Bulirsch, 2002).

306 Phases are bypassed if equation (15) is satisfied for consecutive switching times at a single
307 moment. However, this algorithm does not cater for the situation where (16) and (17) hold as
308 inequalities. These may be incorporated in simple problems utilising mathematical programming
309 (see Mueller et al., 1999). However, this requires that the differential equations governing the
310 dynamic behaviour of the state and costate variables are explicitly solvable. Algorithm 3.1 does
311 not face such restrictions and is therefore capable of solving problems of much greater
312 complexity.

313 The following application is programmed in MATLAB version 7.1 (Miranda and Fackler,
314 2002). Each sub-problem (phase) is solved utilising a variant of the MISER parameterisation
315 algorithm of Teo et al. (1991), which is engineered to operate more efficiently in an iterative
316 scheme. This algorithm involves an approximation of control functions within each phase
317 through interpolation with sets of linear basis functions and solution of the discretised problem
318 using non-linear programming (NLP). Adjoint and state equations are integrated explicitly over
319 the length of a stage using a differential algebraic equation method (Ascher et al., 1995)
320 following the definition of an initial guess of the optimal control. These control histories are
321 subsequently iteratively improved using NLP, with the integration of the process equations
322 repeated at each step to calculate the required gradients, until an optimal solution is obtained. A
323 sequential quadratic programming (SQP) NLP algorithm (Gill et al., 1981) is used because it is
324 the most robust and efficient method presently available for this form of optimisation (Betts et

325 al., 1993; Betts and Gablonsky, 2002). Control parameterisation is adopted for the solution of
326 each phase due to its efficiency and improved convergence relative to other methods.
327 Approximation of control variables utilising basis functions introduces some degree of
328 suboptimality but this is significantly reduced as the number of such functions in each phase is
329 increased, with an optimum of around twenty knot points (Teo et al., 1991), which is
330 subsequently adopted in the following application.

331 It is well known that the bisection technique employed in Algorithm 3.1 will converge linearly
332 to a root in $\log(\mu_0 / \varepsilon) / \log(2)$ iterations, where μ_0 is the size of the initial interval and ε is the
333 stopping tolerance (Press et al., 1992). A loose stopping criterion ($\varepsilon = 0.0001$) is utilised in the
334 outer iteration in the following application so that numerical errors generated in the optimisation
335 phase do not detrimentally affect convergence (Judd, 1998).

336 There are a number of ways to improve the efficiency of Algorithm 3.1. First, solution time is
337 often significantly decreased through using an optimal trajectory from the previous iteration as
338 an initial guess for the next. Solution time may be reduced by up to 80 percent. However, this
339 strategy must be carefully implemented to prevent poor results from affecting convergence.
340 Second, parallel processing may be used to solve each independent phase.

341 **4. Application**

342 This section describes the application of Algorithm 3.1 to a complex multiple-phase control
343 problem.

344 Annual ryegrass (*Lolium rigidum*) is the most economically important weed constraining crop
345 production in Western Australia (Pannell et al., 2004). Moreover, nearly half of the annual
346 ryegrass populations in the primary grain-growing region of this state (the West Australian
347 wheat belt) are estimated to be resistant to regular selective herbicides (Llewellyn and Powles,

2001). This reduces producer profit through forcing substitution towards less cost-effective substitutes, such as the mechanical collection of weed seeds at harvest. The adoption of grain legumes and the greater profitability of cereals, relative to livestock activities, in many farming systems in this region motivate continuous cropping (Pannell, 1995; Poole et al., 2002). However, the inclusion of regular pasture phases has the potential to delay or help to minimise the effects of herbicide resistance through permitting the use of a wide range of weed control strategies (Powles et al., 1997), such as grazing, the use of non-selective herbicides, or green-manuring. The economics of herbicide resistance and the utilisation of non-chemical treatments have been investigated previously (Gorrdard et al., 1995, 1996; Pannell et al., 2004). Yet, the optimal management of multiple phases and pasture treatments has not been studied because significant methodological difficulties have been predicted (see, for example, Gorrdard et al., 1995, p. 73). These may be overcome, however, through the use of Algorithm 3.1.

It is assumed that a producer wishes to determine the optimal management of a single field in the eastern wheat belt of Western Australia. The goal of the producer is to determine the optimal management of two phases in a steady-state field rotation. The initial phase involves lucerne (*Medicago sativa*) pasture and the second phase involves wheat (*Triticum aestivum*) cropping. Stationarity of the steady-state cycle is imposed through requiring equality between the initial ($x(t_0)$) and terminal ($x(t_2)$) state vectors. Algorithm 3.1 is not limited to the solution of this type of problem, however, and may easily be extended to deal with any feasible problem defined by Problem 2.1.

It is assumed that crop yield is detrimentally affected by the population of a single weed, annual ryegrass. There is one switching time (t_1) and the terminal time (t_2) is free. The latter determines the length of the second phase in the rotation. Two state variables are required to represent the weed seed population because of herbicide resistance (Gorrdard et al., 1995,

372 1996). First, $x^s(t)$ is the population of annual ryegrass seeds that following germination is
 373 susceptible to the selective Group A herbicide (diclofop-methyl) (Preston, 2000).² Second, $x^h(t)$
 374 is the population of seeds that following germination are resistant to this herbicide. Time
 375 notation is omitted where not required in the following discussion for notational parsimony.

376 *4.1 Pasture phase dynamics*

377 The producer's problem in the lucerne phase is,

378
$$\max_{u_i^1} F_1 = \int_{t_0}^{t_1} e^{-rt} \left(au_1^1 \left(1 - \frac{u_1^1}{b} \right) - c_{np} \left(\frac{u_1^2}{1 - u_1^2} \right) \right) dt, \quad (18)$$

379 subject to,

380
$$\dot{x}^s = x^s \left(v_1 + v_2 \left(1 - \frac{u_1^1}{u_1^1 d + l} \right) (1 - u_1^2) R \right), \quad (19)$$

381
$$\dot{x}^h = x^h \left(v_1 + v_2 \left(1 - \frac{u_1^1}{u_1^1 d + l} \right) (1 - u_1^2) R \right), \quad (20)$$

382
$$x_0 = \{x^s(t_0), x^h(t_0)\}, \quad (21)$$

383
$$x_1 = \{x^s(t_1), x^h(t_1)\}, \quad (22)$$

384
$$t_1 \text{ fixed}, \quad (23)$$

² Resistance to a single herbicide is studied to focus attention on the intertemporal management of herbicide resistance.

385 where v_j denotes the size of the control vector for phase j , r is the discount rate, u_1^1 is the
386 sheep stocking rate, a and b are parameters describing the relationship between stocking rate and
387 profit, c_{np} is the cost of achieving 50 percent weed control utilising alternative weed control
388 treatments available during the pasture phase (u_1^2) (Gorrdard et al., 1995),
389 $v_1 = -g - (1 - g)M_{seed}$ where g is the germination rate and M_{seed} is the natural mortality rate of
390 ungerminated seeds, $v_2 = g(1 - M_{plant})$ where M_{plant} is the natural mortality rate of germinated
391 seeds, d and l are parameters describing the strength of the relationship between grazing rate and
392 weed control, and R is the number of seeds produced by a single weed. Equation (21) is the set
393 of initial conditions and terminal conditions (22)-(23) will be determined by the estimated
394 switch points in Algorithm 3.1.

395 4.2 Cereal phase dynamics

396 The producer's problem for the cereal phase is,

$$397 \max_{u_2^2} F_2 = \int_{t_1^+}^{t_2} e^{-rt} \left(py_0(1 - \eta u_2^1) \left((1 - z) + z \left(\frac{b}{s + gW(t)} \right) \right) - c_h u_2^1(t) - c_{nc} \left(\frac{u_2^2}{(1 - u_2^2)} \right) - c_{cest} \right) dt - e^{-rt_2} c_{lest},$$

398 (24)

399 subject to,

$$400 \dot{x}^s = x^s (v_1 + v_2 e^{-qu_2^1} (1 - u_2^2) R),$$

401 (25)

$$401 \dot{x}^h = x^h (v_1 + v_2 (1 - u_2^2) R),$$

402 (26)

$$402 x_1 = \{x^s(t_1), x^h(t_1)\},$$

403 (27)

$$403 t_1 \text{ fixed,}$$

(28)

404 $x_2 = \{x_0^s(t_0), x_0^h(t_0)\},$ (29)

405 t_2 free, (30)

406 where p is a constant price, y_0 is weed-free yield, η is the proportion of yield lost to
 407 phytotoxic damage for a given dosage (measured in kilograms of active ingredient per hectare)
 408 of selective herbicide (u_2^1), z is the maximum proportion of grain yield lost at high weed density,
 409 s is a crop-dependent density parameter, g is a constant representing the competitiveness
 410 between the weed population and the wheat crop, $W(t)$ represents the total weed population, c_h
 411 is the cost of the selective herbicide dose, c_{nc} is the cost of achieving 50 percent weed control
 412 utilising alternative weed control treatments available during a cropping phase (u_2^2) (Gorddard et
 413 al., 1995), c_{cest} is a fixed cost representing the establishment costs of wheat, c_{lest} is a fixed cost
 414 representing the establishment costs of lucerne, and q is a parameter designating the strength of
 415 the relationship between ryegrass mortality and selective herbicide dosage. The weed population
 416 is defined as $W(t) = W^s(t) + W^h(t)$, where W^s is the susceptible weed population and W^h is
 417 the herbicide resistant weed population. These are related to the susceptible and resistant seed
 418 populations through $W^s = x^s g(1 - M_{plant})e^{-qu_2^1}(1 - u_2^2)$ and $W^h = x^h g(1 - M_{plant})(1 - u_2^2)$.

419 The initial conditions (27)-(28) for the second phase will be determined by the estimated switch
 420 points in Algorithm 3.1. The terminal condition (29) is required given the cyclical nature of this
 421 problem discussed above. A terminal value function ($e^{-rt_2}c_{lest}$) is required in (24) to reflect
 422 establishment costs for the subsequent lucerne phase in the cycle.

423 The effective removal of lucerne requires careful grazing management and the application of
 424 non-selective herbicides (Bee and Laslett, 2002). A switching cost function for t_1 is therefore

425 defined as $e^{-rt_1}c_{lrem}$, where c_{lrem} is the fixed cost of lucerne removal. This is obviously not a
426 function of the state variables so condition (14) will hold as $\lambda_1^T(t_1) = \lambda_2^T(t_1)$ at $x(t_1)$ in this
427 example. An interesting extension of this work would be the inclusion of a relationship between
428 herbicide application when lucerne is removed and the density of annual ryegrass plants. This
429 would require better information and the inclusion of plants, rather than seeds, as state variables.
430 Moreover, this would require manipulation of Theorem 2.1 as a jump in the state variables
431 would occur at the switching time. This extension may provide little additional insight, however,
432 as two ryegrass plants or less are present at the switching time under optimal management of
433 both scenarios in the following application.

434 The parameter values for this application and a brief description of their estimation is provided
435 in Table 1 in Appendix 1. All values are expressed in 2004 Australian dollars. More detailed
436 information on the estimation of parameters may be obtained from the author on request.

437 *4.3 Model output*

438 The first scenario represents an established resistance problem, with an initial susceptible seed
439 ($x_0^s(t_0)$) population of 70 seeds m^{-2} and an initial herbicide resistant seed ($x_0^h(t_0)$) population of
440 35 seeds m^{-2} . The model solves after fifteen iterations. The optimal trajectories for both seed
441 populations are shown in Figure 1. Here, the optimal switching time is denoted with a vertical
442 line labeled t_1 .

443 *Insert Figure 1 near here*

444 Figure 1 displays that both seed populations decline significantly over the duration of the lucerne
445 pasture phase (phase one). This follows a combined use of grazing, at a constant rate of around
446 7.64 Dry Sheep Equivalents (DSE) per hectare, and alternative treatments that are utilised at

447 around 70 percent intensity over this stage. This demonstrates the value of an integrated weed
448 management strategy for reducing weed burdens before a subsequent cropping phase begins.
449 The pasture phase is utilised for just over three years ($t_1 = 3.3$). This is less than the length of
450 the cropping phase (phase two) that continues for four years in the cycle. This finding is intuitive
451 because of the higher profitability of cereal cropping relative to grazing systems at low weed
452 densities in this dryland environment.

453 The continuity of the state variable at the switching time (t_1) is observable in Figure 1.
454 Discontinuity in the time derivatives of the state variables is also obvious given that the state
455 trajectories experience a point of non-differentiability (corner) at t_1 . This, of course, follows
456 naturally from the piecewise definition of the constituent phases.

457 The second scenario involves an initial susceptible seed population of 70 seeds m^{-2} and no
458 herbicide resistance. The optimal trajectories for the susceptible seed population for the “with
459 resistance” and “without resistance” scenarios are shown in Figure 2. The switching times for
460 these cases are labeled t_1 and t_1' respectively. These trajectories demonstrate a number of
461 important concepts. First, the length of the cropping phase increases significantly, from around
462 four years to six years, when herbicide resistance is not present. This underlies a moderate
463 increase in the optimal terminal time, from $t_2 = 7.326$ years to $t_2 = 8.33$ years. This extension
464 in the length of the cereal phase follows an increase in its value, as wheat yield is not
465 constrained by resistant weeds and the ineffectiveness of the efficient selective herbicide.
466 Second, the lucerne phase finishes a year earlier ($t_1 > t_1'$) when there is no herbicide resistance.
467 This follows a reduction in the relative profitability of the pasture phase. Last, the susceptible
468 weed population at the switching time ($x^s(t_1)$) is significantly lower given an increase in the
469 marginal value of in-pasture weed control. This greater level of control is achieved through a 2
470 percent increase in the mean stocking rate (from 7.6407 DSE/ha to 7.797 DSE/ha) and a 19.6

471 percent increase in the mean intensity of alternative treatments (from 69.86 percent to 83.54
472 percent).

473 *Insert Figure 2 near here*

474 Alternative weed control treatments are used at a significant intensity over the cereal phase when
475 herbicide resistance constrains production (Figure 3a) because of the ineffectiveness of the
476 selective herbicide against resistant weeds. This decreases producer profit given the increasing
477 marginal cost associated with the utilisation of alternative treatments. The main cost of herbicide
478 resistance consequently appears to arise from higher weed control costs and not significantly
479 higher weed burdens (see Figure 2). This reinforces survey evidence (Llewellyn and Powles,
480 2001) and output from simulation modelling (Pannell et al., 2004) that identifies little difference
481 in weed density between fields under standard management practice both with and without
482 herbicide resistance. In contrast, the higher profitability of the cereal phase when herbicide
483 resistance is not present arises from the steady application of both selective herbicide (Figure 3b)
484 and alternative treatments (Figure 3c) at moderate intensities.

485 *Insert Figure 3 near here*

486 **V. Conclusions**

487 There appears to be no general framework for the numerical optimisation of multiple-phase
488 systems in which control variables are defined in each stage. This is a significant limitation
489 because such systems arise in many important situations, such as determining the optimal time
490 to switch between production technologies, energy sources, and land uses. The computational
491 algorithm presented in this paper offers a flexible and efficient platform for the solution of
492 multiple-phase problems in which the number and sequence of phases is pre-assigned. However,

493 this framework does not explicitly permit switching times to accumulate. Removing this
494 limitation would increase its flexibility and is consequently a valuable area for further work.

496 **Table 1:** Parameter values for the two-phase herbicide resistance model.

Parameter	Value	Source
r	$r=0.05$	Pannell et al. (2004)
a, b	$a=25.316, b=14.879$	Non-linear least squares estimates from a simulated relationship between stocking rate and lucerne profitability, based on Mott (1960).
c_{np}, c_{nc}	$c_{np} = c_{nc} = \$5$	These are estimates of the cost of 50 percent control from unpublished estimates in the Resistance and Integrated Management simulation model (Pannell et al., 2004).
c_h	$c_h = \$40$	DAWA (2004)
g	$g = 0.8$	Gill (1996)
M_{seed}, M_{plant}	$M_{seed} = 0.55, M_{plant} = .05$	Unpublished data in RIM model (Pannell et al., 2004)
d, l	$d = 1.1111, l = 0.5$	The parameter d is determined from the maximum level of annual ryegrass control reported for grazing sheep (90 percent) (Pearce and Holmes, 1976; unpublished RIM estimates) using $d=(1/\text{ceiling})$. The parameter l is selected to fit the functional form to available data (Reeves and Smith, 1975; Pearce and Holmes, 1976; unpublished RIM estimates), with d fixed.
q	$q = 7.451$	Gorrdard et al. (1995, 1996)
p	$p = \$185$	Estimate for wheat price after legume pasture, taken from RIM model (Pannell et al., 2004).
y_0	$y_0 = 1.82$ tonnes	Weed-free yield for continuous wheat crop (1.3 tonnes) (Pannell et al., 2004) is increased by 40 percent because of higher nitrogen, decreased disease, and improved soil structure after lucerne phase (Latta and Devenish, 2002).
η	$\eta = 0.1448$	Gorrdard et al. (1995, 1996)
z, s, k	$z = 0.6, s = 105, k = 0.33$	Pannell et al. (2004)
c_{cest}	$c_{cest} = \$82$	Pannell et al. (2004)
c_{lest}, c_{lrem}	$c_{lest} = \$58.50,$ $c_{lrem} = \$21.25$	Calculated from information in DAWA (2004)

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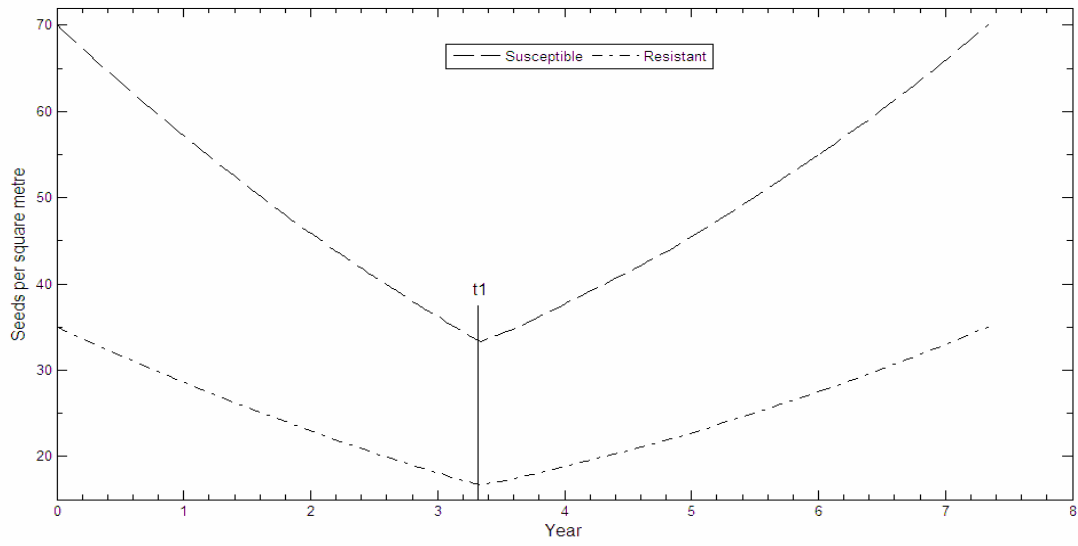
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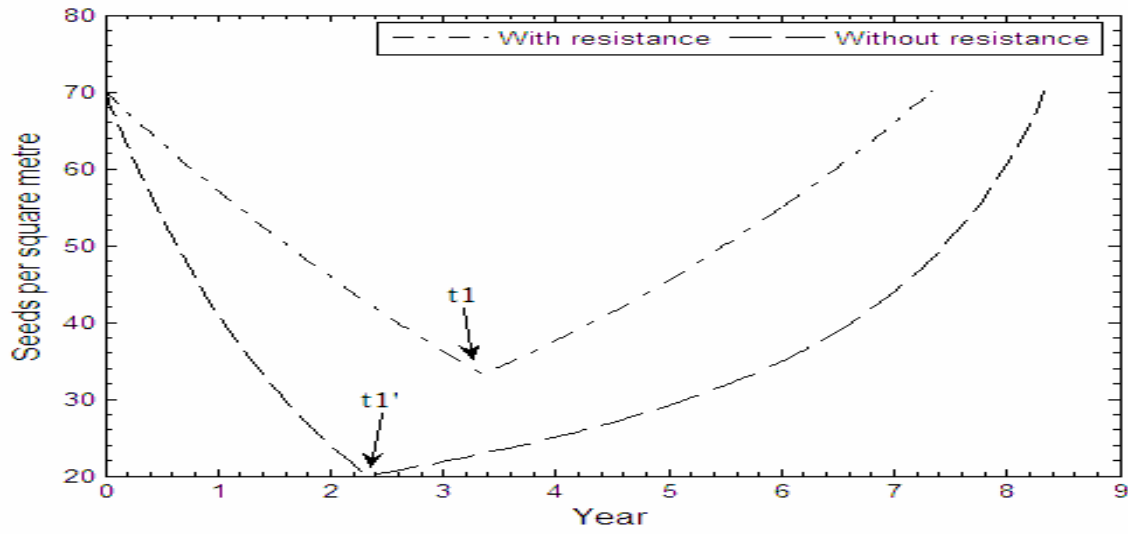
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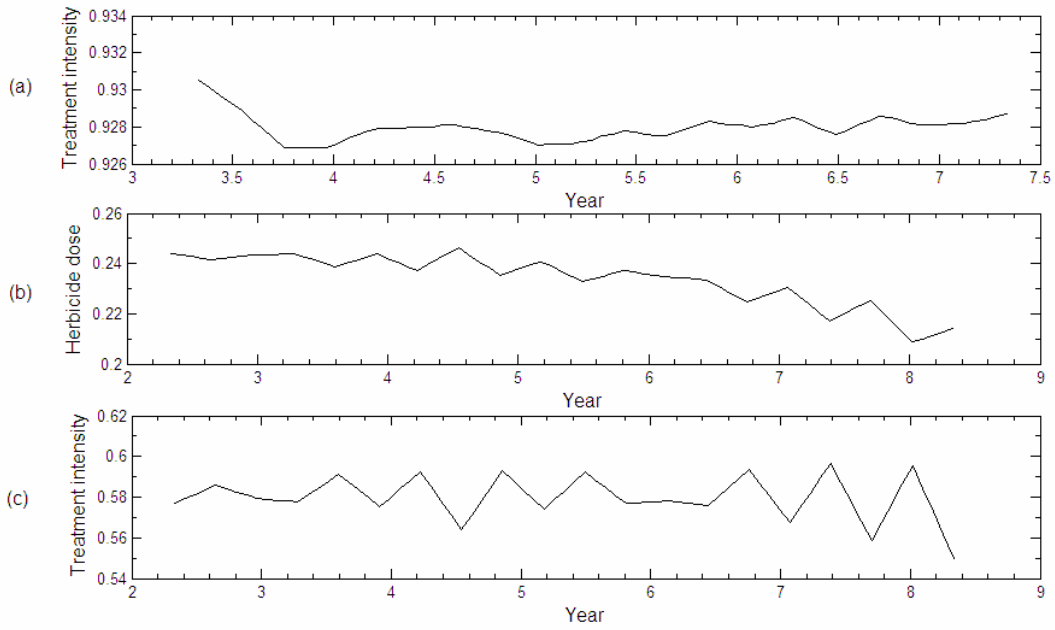
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602 **Figure 1.** Optimal trajectories for susceptible and resistant annual ryegrass seeds over a lucerne
 603 pasture – wheat crop rotation.



604

605 **Figure 2.** Optimal trajectories for susceptible annual ryegrass seeds with and without herbicide
 606 resistance over a lucerne pasture – wheat crop rotation.



607

608 **Figure 3.** (a) Intensity of alternative treatments with herbicide resistance, (b) selective herbicide
 609 dose (kilograms of active ingredient applied per hectare) without herbicide resistance, and the
 610 (c) intensity of alternative treatments without herbicide resistance. All of these treatments are
 611 applied in the second (crop) phase.

612