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Optimal weed population control using nonlinear programming

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Abstract A dynamic optimization model for weed infestation control using selective herbicide application in a corn crop system is presented. The seed bank density of the weed population and frequency of dominant or recessive alleles are taken as state variables of the growing cycle. The control variable is taken as the dose–response function. The goal is to reduce herbicide usage, maximize profit in a pre-determined period of time and minimize the environmental impacts caused by excessive use of herbicides. The dynamic optimization model takes into account the decreased herbicide efficacy over time due to weed resistance evolution caused by selective pressure. The dynamic optimization problem involves discrete variables modeled as a nonlinear programming (NLP) problem which was solved by an active set algorithm (ASA) for box-constrained optimization. Numerical simulations for a case study illustrate the management of the *Bidens subalternans* in a corn crop by selecting a sequence of only one type of herbicide. The results on optimal control discussed here will

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give support to make decision on the herbicide usage in regions where weed resistance was reported by field observations.

Keywords Mathematical modeling · Population dynamics · Nonlinear programming · Weed management

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1 Introduction

Weeds grow naturally in agricultural soils and are highly competitive for resources that are necessary to the crop growth. The competition between weeds and crop plants occurs when two or more plants share the available resources for their growth and development which are limited in a common ecosystem. A plant may inhibit another by limiting its resources consumption. For this reason, the weed control strategies are essential to maximize the productivity of a crop.

The weed management aims to avoid losses due to competition, to benefit crop conditions, to avoid further infestation and to protect the environment. The main method of weed control is the use of herbicide. However, it is of most importance to understand the evolution of resistance in weed population.

The development of resistance to herbicide in agricultural weed population is common and well known. There has been an increasing interest in modeling the resistance evolution in weed populations (Maxwell et al. 1990; Diggle et al. 2003; Gressel 2009; Neve et al. 2011).

Resistance is essentially a natural phenomenon which occurs in weed populations, but it is only noticed when a selection pressure is applied. The repeated application of one or more herbicide modes of action in a weed population selects individuals of species that can survive the herbicide treatment (Powles and Shaner 2001). This phenomenon characterizes a selection pressure, thereby increasing the proportion of resistant individuals in the next generation.

The weed resistance to herbicide occurs on account of an evolutionary process. The development of herbicide-resistant (R) weed biotypes is due to the selection pressure caused by intensive herbicide use. The functions of the gene frequencies of dominant and recessive alleles due to the selective pressure imposed by the herbicide follow the principles of population genetics (Britton 2003).

Optimization strategies are used in several weed management programs (Jones and Cacho 2000; Jones et al. 2006; Kotani et al. 2009, 2011). In these papers, dynamic programming techniques are used to find the optimal strategies. In Jones and Cacho (2000) and Jones et al. (2006), the optimal level of weed control that maximized economic benefits was obtained in terms of a single herbicide dose sequence. The Pontryagin Maximum Principle and dynamic programming were used in solving the considered optimal control problem. Kotani et al. (2009, 2011), using a dynamic model of weed management, proposed an optimal decision rule for the removal of weeds, including whether or not to eradicate them.

Optimal control problem is also used in agriculture to control pest population. In Rafikov and Balthazar (2005), an optimal control problem is developed as a management strategy to maintain the density of the pest population in the equilibrium below some economic injury level. In this management strategy, the Pontryagin Maximum Principle was used to drive the pest ecosystem equilibrium to the desired level and dynamic programming to stabilize the ecosystem level. In Christiaans et al. (2007), an optimal pest control is formulated to determine the optimal crop return by applying pesticides and fertilizers in a ecosystem with two species in a predator–prey relationship.

In modeling the weed population growth under control, an important effect to consider is the resistance to herbicides. In this paper, the Jones and Cacho (2000) weed population model is extended to incorporate the resistance dynamics. In addition, we proposed a weed control strategy aimed at reducing the use of herbicide, maximizing economic returns and minimizing the environmental impacts caused by excessive use of herbicide, using a nonlinear programming (NLP) solved by an active set algorithm (ASA) for box-constrained optimization. The numeric solutions for a sequence of one single herbicide doses considering two herbicides are presented.

2 Population model considering the weed resistance dynamics

2.1 Weed population dynamic model

The weed dynamics we consider consists of the weed seed bank and seedling densities denoted as x_t and y_t, respectively, which follows closely (Jones and Cacho 2000). Let t denoted the production cycle, the weed population model with the resistance phenomenon in which all the parameters are assumed to be nonnegative, has the following form

$$y_t = x^g \delta x_t, \ x_{t_0} = x_0 \tag{1}$$

$$y_t^a = (1 - \rho(u_t))y_t \tag{2}$$

$$x_t^r = \exp[\gamma \ln y_t^a / (\mu + \varepsilon \ln y_t^a)] \tag{3}$$

$$x_t^n = \kappa x_t^r - \eta + \xi \tag{4}$$

$$x_{t+1} = x_t^n + (1 - \Psi)(1 - \delta)x_t, \tag{5}$$

with parameters defined in Table 1.

The structure of the model (1)–(5) is based on the life cycle of weeds in which the initial population x_0 is the seed bank of viable and non-germinated seeds present in a single agricultural field. In the model, (1) describes the emergence plants from the seed bank, (2) the relative survival of emerged seedlings determined by the weed management strategies employed during each iteration, (3) describes the survived mature plants produced by seeds, (4) describes the proportion of new seeds. Finally, in (5), the newly produced seeds are added to the soil seed bank at the end of the growing season.

The propagation of x_t^r described by (3) was constrained to zero when $y_t^a < 0.5$ plants per m^2, due to the nature of the functional form used, as it degenerates to $e^{\frac{\gamma}{\varepsilon}}$ as y_t^a approaches zero.

Equations (1)–(5) can be condensed by forward substitution (y_t given by (1) into (2), then y_t^a into (3) and so on), yielding the following equation

$$x_{t+1} = g(x_t, u_t), \tag{6}$$

where

$$g(x_t, u_t) = (1 - \Psi)(1 - \delta)x_t + \kappa \exp\left(\frac{\gamma \ln\left((1 - \rho(u_t))\, x^g \delta x_t\right)}{\mu + \varepsilon \ln\left((1 - \rho(u_t))\, x^g \delta x_t\right)}\right) - \eta + \xi.$$

The dynamics of weed seed bank is given in (6), in which ρ describe the herbicide-induced mortality of seedlings in cycle t where the control variable is described by u_t and determined by the weed management strategy employed during each iteration.

Table 1 Population dynamic model variables and parameters

x_t	Weed seed bank density in cycle t (m^{-2})
y_t	Seedlings in cycle t (m^{-2})
y_t^a	Density of mature plants (m^{-2})
x_t^r	Seeds resulting from the reproduction of weeds (m^{-2})
x_t^n	New seeds added to the seed bank in cycle t (m^{-2})
x^g	Proportion of germination
δ	Annual germination rate of weed seeds
u_t	Dose of herbicide in cycle t (L ha^{-1})
ρ	The herbicide-induced mortality of seedlings
$\gamma,\ \mu,\ \varepsilon$	Regression coefficients (Medd et al. 1995)
κ	Survival rate of new seeds
η	Seed export such as removal of seeds at harvest (m^{-2})
ξ	Import of seeds (m^{-2})
Ψ	Death rate of dormant seeds

2.2 Dose–response model

The relationship between herbicide doses and plant response is of fundamental importance to understand herbicide efficacy and mode of action. The dose–response is usually analyzed using a log-logistic curve (Christensen et al. 1990; Streibig and Kudsk 1993; Seefeldt et al. 1995) and is used to quantify plant sensitivity to a herbicide (Karam et al. 2004; Dan et al. 2010). Resistant plants have a lower sensitivity to herbicide and their dose–response function differ from the dose–response function of susceptible plants. This difference is used to detect cases of resistance to a herbicide (Moss 1999).

A logistic model to be fitted to the survival data is as follows:

$$\rho(u) = c + \frac{d - c}{1 + \exp[b(\ln(u) - \ln(GR_{50}))]}, \tag{7}$$

where ρ is the induced mortality, c is the lower asymptotic values of ρ and d is the upper asymptotic values of ρ, the parameter GR_{50} is the herbicide rate which produces a survival-level halfway between the lower limit zero and upper limit d, u is the herbicide dose and the parameter b denotes the relative slope around GR_{50} (Seefeldt et al. 1995). The fitted logistics model was used to estimate the rate of herbicide that causes 50 % grow reduction (GR_{50}). The parameters b, c, d and GR_{50} can be determined experimentally.

One of the advantages of using the curve described by (7) is that the parameters are biologically meaningful. The upper limit d corresponds to the mean response of the control and the lower limit c is the mean response at very high doses. The dose–response (7) is supposed to determine the reduction in mortality of weeds if an herbicide is applied. Then, if the herbicide is not applied it is equal to zero, in others words, $\lim_{u\to 0} \rho(u) = c = 0$.

We formulated a model for the resistance dynamics based on the detection of resistant biotypes to a herbicide via the dose responses. We make the following assumptions: (1) the parameters c and d in both resistant (R) and susceptible (S) biotype dose–response curves are close, (2) the slope b is parallel for different GR_{50} under the same resistant mechanism (Tind et al. 2009; Christoffoleti 2002), (3) the parameter GR_{50} varies according to the proportion of R and S biotypes, and it is commonly used to estimate the herbicide efficacy (Tind et al. 2009; Powles and Preston 2011).

The adopted dose–response function is thus given by

$$\rho(u_t) = c_S + \frac{d_S - c_S}{1 + \exp[b_R(\ln(u_t) - \ln(GR_{50t}))]}, \tag{8}$$

where c_S indicates the minimum mortality and is taken from the S biotype dose–response curve, d_S indicates the maximum mortality (Christoffoleti 2008) and is taken from the S biotype dose–response curve to reflect the maximum mortality, b_R is taken from the resistant biotype dose–response curve around the parameter GR_{50t} which is modeled as a function of R and S biotypes, because in this population both biotypes are present.

In this paper, we assume that the weed management strategy depends on different mortality responses from resistant and susceptible seedlings. Then, we used proportions of both seedlings present in the weed population described as a convex relationship as follows:

$$\mathrm{GR}_{50t}(R_t) = R_t\mathrm{GR}_{50R} + (1 - R_t)\mathrm{GR}_{50S}, \tag{9}$$

where GR_{50R} and GR_{50S} are the doses necessary to reduce to 50 % the resistant and susceptible biotype dose–responses, respectively, and R_t is the resistance to herbicides in cycle t obtained as a function of the allele frequency given by the Fisher–Haldane–Wright (FHW) equation which describes the population genetics (Britton 2003). Therefore, model (9) captures informations about both populations R and S, present in the seed bank in cycle t.

The dose–response function is then dependent not only on the herbicide dose u_t but also on the resistance R_t. This has effect on the modeling of the seed bank, which will be described in Sect. 3.2.

2.3 Weed resistance dynamic model

For most weeds, the behavior predicted by the FHW equation (Britton 2003) efficiently represents species with rapid breeding, sexually generating seed through pollen, very different generations from each other, isolated populations and greater interaction within the same population. Therefore, the FHW equation is used to describe the genetic evolution of the weed resistance.

2.3.1 Selection pressure for the dominant and recessive allele frequencies

The function of genetic frequencies of dominant and recessive alleles under selective pressure is described next (Britton 2003). Let the allele frequencies at the end of the gametic phase of generation t be p_t and q_t. Let the ratio $w_{\mathrm{AA}} : w_{\mathrm{Aa}} : w_{\mathrm{aa}}$ define the probability of survival from zygotic phase to breeding phase for the various genotypes. According to Britton (2003), w_{aa} is usually assumed to be equal to 1, such that w_{AA} and w_{Aa} are the relative selective values of genotypes **AA** and **Aa**. With p_t^2, $2p_tq_t$ and q_t^2 genotype frequencies, at the beginning of the zygotic phase the ratios of the genotypes **AA**, **Aa** and **aa** at the breeding phase were modified to

$$w_{\mathrm{AA}}p_t^2 : 2w_{\mathrm{Aa}}p_tq_t : w_{\mathrm{aa}}q_t^2 \tag{10}$$

and the alleles **A** and **a** frequencies are now in the ratio

$$w_{\mathrm{AA}}p_t^2 + w_{\mathrm{Aa}}p_tq_t : w_{\mathrm{Aa}}p_tq_t + w_{\mathrm{aa}}q_t^2. \tag{11}$$

Finally, the change in allele **A** frequency at the end of the gametic phase may be described by

$$p_{t+1} = \frac{w_{\mathrm{AA}} p_t^2 + w_{\mathrm{Aa}} p_t q_t}{w_{\mathrm{AA}} p_t^2 + 2w_{\mathrm{Aa}} p_t q_t + w_{\mathrm{aa}} q_t^2}, \tag{12}$$

which can be written in the recursive form as

$$p_{t+1} = p_t + \sigma(p_t), \tag{13}$$

where

$$\sigma(p_t) = p_t q_t \frac{(w_{\mathrm{AA}} - w_{\mathrm{Aa}}) p_t + (w_{\mathrm{Aa}} - w_{\mathrm{aa}}) q_t}{w_{\mathrm{AA}} p_t^2 + 2w_{\mathrm{Aa}} p_t q_t + w_{\mathrm{aa}} q_t^2}.$$

This is the FHW introduced earlier which describes the change in gene frequencies at period $t + 1$.

We represent the weed seed bank as genetic material that participates in the selection process. In this process, the dormancy seeds do not undergo selective pressure, but the adult plants do. Finally, eliminating dead and germinated seeds from the existing bank and adding the new seeds into it, we obtain

$$p_{t+1} = p_t + \chi_t \sigma(p_t), \tag{14}$$

with $\chi_t < 1$, and

$$\chi_t = \frac{x_t^n}{x_t}.$$

Equation (14) can be written as

$$p_{t+1} = v(x_t, p_t, u_t), \tag{15}$$

where

$$v(x_t, p_t, u_t) = p_t + \chi_t \sigma(p_t).$$

The dynamic of seed bank, represented by χ_t, considers the proportion of new seeds to be added in the seed bank in the next generation. This factor is important because of the allele frequencies' change in each generation thus it is necessary to represent more accurately the allele frequencies of the seed bank.

The ratio of the evolution advantages relative to the selection in (14) is given by

$$\begin{bmatrix} w_{\mathrm{AA}} & w_{\mathrm{Aa}} & w_{\mathrm{aa}} \end{bmatrix}^T = Es + \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}^T, \tag{16}$$

where s is the coefficient of strength of selection for dominant and recessive alleles and E is a vector that defines the relative selective values of genotypes **AA** and **Aa** given by:

$$E = \begin{cases} [\,1\;1\;0\,]^T, & \text{if dominant} \\ [\,1\;0\;0\,]^T, & \text{if recessive.} \end{cases} \tag{17}$$

2.3.2 Resistant genotype

The initial population is the viable seed bank, non-germinated seeds found in agricultural fields. Within this seed bank, S and R individuals exist in numbers determined by the initial frequency of resistant alleles.

The percentage of resistant genotype R_t can be introduced by knowing the plant phenotype. The proportion of new seeds of each genotype (**AA**, **Aa**, **aa**) is determined by the population genetics.

The cases of dominant and recessive alleles are studied. In the case of the resistance being connected to recessive alleles, the homozygous **aa** ($(1 - p_t)^2$) is responsible for the trait. In the case of dominant alleles, the homozygous **AA** (p_t^2) and the heterozygous **Aa** ($2p_t(1-p_t)$) are responsible for the resistance.

The model for the resistant genotype follows the Hardy–Weinberg equilibrium and is formulated as

$$R_t = \begin{cases} p_t^2 + 2p_t(1 - p_t), & \text{if dominant} \\ (1 - p_t)^2, & \text{if recessive.} \end{cases} \tag{18}$$

Therefore, the resistance dynamic model for selective pressure taken into account the seed bank is given by (14)–(18).

2.4 Multiple resistance dynamic model

The most intractable problems of herbicide resistance involve weeds which exhibit multiple herbicide resistance. The phenomenon of multiple herbicide resistance can be seen as the expression of different herbicide modes of action. Multiple herbicide-resistant weeds may possess from two to various distinct resistance mechanisms and may exhibit resistance to different herbicide (Powles and Preston 2011). The weeds with multiple herbicide resistance have a speed up evolution of resistance dynamics to the herbicide, where each herbicide shows a different selection pressure.

In Maxwell et al. (1990), Diggle et al. (2003) and Gressel and Segel (1978), the segregation of the allele frequencies was considered to use different herbicide modes of action to control the weed infestation. We do not consider the segregation of the allele frequencies in the weed population model.

The weed population and resistance dynamics are thus described by (1)–(9) and (14)–(18). The dose–response parameters are defined according to the selected herbicide.

3 Weed management optimization problem

Differing from Jones and Cacho (2000), we propose a dynamic optimization model for weed control considering the resistance evolution to a certain herbicide.

3.1 Defining the economic model

The economic problem faced by decision maker is to determine the levels of input of all production factors, including weed control, which maximize net returns and minimize environmental impacts. The crop yield denoted Y, which is a function of the weed density, the weed resistance and the weed control, is represented in the form of

$$Y = h(x_t, p_t, u_t). \tag{19}$$

This function can be separated in equations for the weed-free yield denoted Y_0, the yield loss associated with the weed density, the weed allele frequencies and the weed control denoted Y_L and the yield loss associated to phytotoxic effects of herbicide denoted Y_p. The crop yield is thus obtained as

$$Y = Y_0(1 - Y_L)(1 - Y_p). \tag{20}$$

Cousens (1985) argued that the appropriate loss function that describes yield loss as a function of weed density is a rectangular hyperbola function

$$Y_L = \frac{aD}{1 + \frac{a}{m}D}, \tag{21}$$

where a is the percentage of yield loss per unit weed density (m^{-2}), m an estimate of the maximum yield loss of a weed crop relative to the yield of a weed-free crop and D a function of weed density which estimates the efficiency of the herbicide dose $\rho(u_t, R_t)$

$$D = y_t(1 - \rho(u_t, R_t)), \quad 0 \leq \rho \leq 1,$$

with $\rho(u_t, R_t)$ given by (8).

The yield loss associated to phytotoxic effects of herbicide was estimated as Pandey and Medd (1990)

$$Y_p = \varphi u_t,$$

where φ is an adjusted parameter that depends on the applied herbicide.

The economic model maximizes net returns and minimizes the weed resistance, for a initial level of weed infestation. Thus, the profit function denoted π is defined as:

$$\pi(x_t, p_t, u_t) = P_y Y(x_t, p_t, u_t) - P_u u_t - C, \tag{22}$$

where P_y is the crop price, P_u is the per unit cost of weed control, C is the constant application cost for the weed control input (machinery and labor) and cost of the production of the remaining production factors. The profit function (22) is determined not only by the control variable but also by the weed density x_t and weed resistance p_t.

3.2 Optimization model

Let u be the applied herbicide dose. Using (5) and (14), the dynamic model for the seed bank density and allele frequencies for applied herbicide is written in terms of functions g and v, respectively, as

$$g(x_t, p_t, u_t) = x_{t+1} \tag{23}$$

$$v(x_t, p_t, u_t) = p_{t+1}, \tag{24}$$

where g represents the change in the seed bank and v the change in the allele frequencies in time t.

The vector field, which represents the speed of the dynamics evolution, is chosen as $[g\ v]^T$, where the first element represents the evolution of the seed bank density and the second the allele frequencies for applied herbicide.

We point out that due to (6) and (15) the vector field is dependent on both state variables x_t and p_t as opposed to previous models where either the seed bank density or the allele frequency in populations were considered separately. Here we model the behavior of the seed bank density as well as the allele frequency in the seed population and therefore interactions between the equations in the system modeling are expected to happen. The proposed model captures these interactions through the dose–response and resistance functions analysis.

The optimization model that considers a single herbicide application strategy is modeled as a NLP problem. The variables are the seed bank x_t, the allele frequencies p_t, the herbicide dose u_t which should be applied at each time. Then, the NLP problem is formulated as

$$\max_{u_t} J(x, p) = \sum_{t=0}^{T} \alpha^t \pi(x_t, p_t, u_t) \tag{25}$$

subject to

$$x_{t+1} = g(x_t, p_t, u_t), \quad x(0) = x_0 \tag{26}$$

$$p_{t+1} = v(x_t, p_t, u_t), \quad p(0) = p_0 \tag{27}$$

$$0 \le u(t) \le u_{\max} \tag{28}$$

$$x_t, p_t, u_t \in \mathbb{R}$$

where J is the objective function, π the smooth function (22), T is the planning horizon, $\alpha^t \in (0, 1)$ the discount rate (Kennedy 1986) and $u_{\max}$ the highest dose of herbicide allowed in the field. The objective function J is a smooth nonlinear and generally concave function. The state variables are x_t and p_t and u_t represents the control variable.

The optimal control theory can be used to determine the annual rate of herbicide that maximizes the objective functional. An important role in this problem are the costate variables, denoted by λ_t e β_t, which are similar to the Lagrange multipliers. The costate variables are inserted in the optimal control problem through the Hamiltonian function. Following Kennedy (1986), the Hamiltonian function for the weed management problem is established as follows:

$$\begin{aligned} H_t(\lambda_{t+1}, \beta_{t+1}, x_t, p_t, u_t) = \pi(x_t, p_t, u_t) + \alpha\lambda_{t+1} g(x_t, p_t, u_t) \\ + \alpha\beta_{t+1} v(x_t, p_t, u_t). \end{aligned} \tag{29}$$

The Hamiltonian function H_t is the net profit obtained from an existing level of the state variables, x_t and p_t and control u_t plus the value of any change in the stock of the state variables valued at the costate variables λ_{t+1} e β_{t+1}. When g_t is multiplied by λ_{t+1}, this result is converted to a monetary value and represents the rate of change of the economic value of the seed bank corresponding to herbicide dose applied, the same occurs when v_t is multiplied by β_{t+1}. In general, this value can be viewed as the future profit effect of weed population change (Jones and Cacho 2000).

According to Kennedy (1986), the first-order conditions for a resource management problem, given by the Maximum Principle of Pontryagin, are

$$\frac{\partial H_t}{\partial u_t} = P_y \frac{\partial Y}{\partial u_t} - P_u + \alpha\lambda_{t+1} \frac{\partial g}{\partial u_t} + \alpha\beta_{t+1} \frac{\partial v}{\partial u_t} = 0 \tag{30}$$

$$\alpha\lambda_{t+1} = -\frac{\partial H_t}{\partial x_t} = -P_y \frac{\partial Y}{\partial x_t} - \alpha\lambda_{t+1} \frac{\partial g}{\partial x_t} \tag{31}$$

$$x_{t+1} = \frac{\partial H_t}{\partial \lambda_{t+1}} = g(x_t, p_t, u_t) \tag{32}$$

$$\alpha\beta_{t+1} = -\frac{\partial H_t}{\partial p_t} = -P_y \frac{\partial Y}{\partial p_t} - \alpha\beta_{t+1} \frac{\partial v}{\partial p_t} \tag{33}$$

$$p_{t+1} = \frac{\partial H_t}{\partial \beta_{t+1}} = v(x_t, p_t, u_t), \tag{34}$$

where (30) is the maximum principle, the standard conditions for maximization with respect to u_t, (31) and (33) correspond to the costate equation and (32) and (34) are a re-statement of the equation of motion relative to the seed bank and the allele frequency, respectively. The set of equation (30)–(34) allows the solution of the unknown optimal trajectories, that are state variables x^* and p^*, control u^* and costate λ^* and β^* variables. The state variables depend on the initial state of the system x_0 and p_0. Although x_0 and p_0 are given, λ_1 and β_1 are unknown and an additional condition, known as the transversality condition, is required to obtain a unique solution. In this problem, where the final time T is given, and the final state x_T is free, the transversality condition is $\lambda_{T+1} = 0$ e $\beta_{T+1} = 1$.

To solve the NLP given by (25)–(28), we use an algorithm proposed by Hager (2006) called active set algorithm (ASA). This algorithm is described in Sect. 4 next.

4 Solution of the nonlinear programming problem

The nonlinear programming problem considered is a mathematical programming problem with discrete variables, nonlinear constraints and a nonlinear objective function.

This paper is concerned with a nonlinear programming problem based in box-constrained optimization problem given by (25)–(28), where (25) is the objective functional with J a real-valued, continuously differentiable function defined on the set (28).

To solve the NLP problem, the active set algorithm (ASA) is used (Hager 2006). We consider that the box (28) is replaced by a nonempty, closed and concave set. The solution of the corresponding problem yields the optimal control strategy.

4.1 Active set algorithm

We implemented the box-constrained optimization problem using an nonlinear programming problem (NLP) strategy to solve the weed control problem. In the NLP strategy, the decision variable is u_t and the state space equation has u_t as inputs. Thus, the NLP method is used to obtain an optimal control u_t^*.

The optimization problem (25)–(28) has a box constrained for the control variables, thus it is then necessary to use a box-constrained method. Therefore, the ASA method proposed by Hager (2006) available at Hager (2009) is used. This algorithm consists of a non-monotone gradient projection step, an unconstrained optimization step and a set of rules for branching between the two steps.

The ASA method global convergence to a stationary point is established in Hager (2006). Hager (2006) also showed that the ASA method is superior to the L-BFGS-B (Byrd et al. 1995), the SPG2 v. 2.1 (Birgin et al. 2000), the GENCAN (Birgin and Martínez 2002) and the TRON v. 1.2 (Lin and Moré 1999) methods in terms of CPU time.

Algorithm 1 describes the problem to solve the weed control problem using the ASA method. We emphasize that Algorithm 1 is applied to the general box constraint problem with both upper and lower bounds. To implement the problem, it is necessary to choose the input parameters of the weed control problem.

The functional objective (25), the state functions (26)–(27), the Jacobian of $f = [g\ v]^T$ and the box-constrained (28) are given as input of the Algorithm 1. The problem outputs are the optimal control u_t^* and its corresponding optimal states x_t^* and p_t^*. In Algorithm 1, the stopping condition used in ASA algorithm was $d_k = P(u_k - G_k) - u_k$, where P denotes the gradient projection onto the domain of f and $G_k = \nabla f(u_k)$ the gradient at the iterate u_k from ASA. For more details see Hager (2006).

Algorithm 1: NLP problem routine

Input: objective function J, state space functions g and v, Jacobian of $f = [g\ v]^T$, lower and upper bounds $0.005 \leq u_k \leq u_{max}$

Output: optimal control

Initialize $k = 0$, u_0 (starting guess), n (number of years), nx (number of state variables) and nc (number of control variables);

Choose error tolerance $\epsilon \in [0, \infty)$;

Choose initial values x_0, $p_0 > 0$, $u_0 \in [0.005,\ u_{max}]$;

while $\| P(u_k - G_k) - u_k \| > \epsilon$ **do**

  Execute the ASA program loaded from Hager (2009);

  Set $u_{k+1} = u_k$;

  $k = k + 1$;

end

Optimal control = $[u_k^*]$;

return.

5 Results

A case study with the *Bidens subalternans* in a corn crop by applying two herbicides is presented. The *Bidens subalternans* is a highly competitive weed, with great adaptability on farm soils, which is due to its high seed production combined with dormancy mechanisms.

The *Bidens subalternans* has dominant allele with nuclear resistance (Tranel and Wright 2002). This species shows multiple resistance to the acetolactate synthase (ALS) and the photosystem two (PS2) inhibitors (Gazziero et al. 2008; Karam 2011; Heap 2011).

The effective use of herbicide in weed management depends on the knowledge of the characteristics of the herbicide active ingredient. The atrazine herbicide is a well-known herbicide in the class of triazine and it can be applied for pre-emergent (root-absorbed) and post-emergent (foliage-absorbed) control of weed. Its mechanism of action is by inhibition of PS2, causing a series of irreversible damage to plant cells and can be classified as a nonsystemic herbicide (Carvalho et al. 2010). Due to its large use around the world and low soil absortion, the herbicide atrazine is more harmful to the environment (Ralebitso 2002). The nicosulfuron is a systemic, post-emergent (foliage-absorbed) herbicide and working in ALS inhibitors in weeds (Anderson et al. 1998). The nicosulfuron herbicide is widely used in corn crop to weed control, with negative effects on the environment (Oliveira et al. 2009). Therefore, the effective weed control can be accomplished by combining the characteristics of individual herbicides when integrated with weed biological information.

As the model output was particularly sensitive to the initial seed bank density (*B. Subalternans* population size) and initial frequency of R alleles, we defined a scenario for simulation. The scenario considered an initial seed bank of 500 (seeds m^{-2}) and an initial allele frequency of 0.1 following the characteristics of the area where the seeds were collected. In the simulation, two herbicides (nicosulfuron and atrazine) were considered for post-emergent (foliage-absorbed) control of the weed population. The weed control problem was simulated over a 10 years period.

The parameter values of the dose–response model, ρ, were obtained by curve fitting from experimental data of herbicide-induced mortality using the R Statistical Software. The data were collected in a controlled environment setup conducted in Embrapa Milho e Sorgo (see Table 2). The dose–response curves are shown in Fig. 1. The parameter values of the adopted dose–response model (8) used are presented in Table 3.

Table 2 Dose–response model parameter values for nicosulfuron and atrazine from experimental data

Herbicide	Biotype	*b*	*c*	*d*	GR_{50}
Nicosulfuron	Susceptible	−0.80721	−3.06521	102.65965	8.57764
	Resistant	−1.28707	−0.30570	34.41258	36.12024
Atrazine	Susceptible	−1.38747	−1.30678	105.86746	783.09583
	Resistant	−0.68405	0.12445	212.9900	57375.0

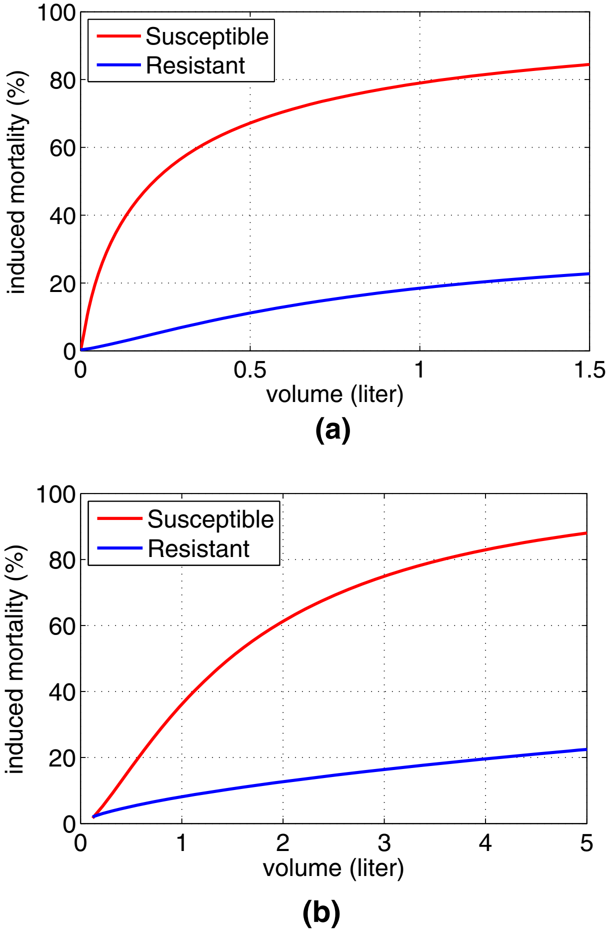

Fig. 1 Herbicide-induced mortality for resistant and susceptible seedlings for **a** nicosulfuron and **b** atrazine herbicides

The parameter values of the population and economic models used in the annual corn harvest system 2013/2014 (IMEA 2014) are reported in Table 4.

We used the bound-constraints maximization solver ASA to solve the NLP problem. The code was written in C programming language. All experiments were run on a 2.27 GHz Intel core i5 processor 3 Gb of RAM memory and Windows 7 operating system. The NLP algorithm for the weed problem runs relatively fast, and the average processing time is around 2 s.

Table 3 Dose–response model parameter values for nicosulfuron and atrazine used in weed resistance model proposed

Herbicide	b_R	c_S	d_S	GR_{50S}	GR_{50R}
Nicosulfuron	−1.28707	−3.065216	102.65965	8.577645	36.12024
Atrazine	−0.68405	−1.30678	105.86746	783.09583	57375.00

Table 4 Parameter values used in the numeric simulation (1 = nicosulfuron and 2 = atrazine)

Population parameters	Value
δ (%)	60.00
ψ (%)	30.00
η (m^{-2})	0.00
ξ (m^{-2})	0.00
κ (%)	35.00
x^g (%)	80.00
γ	6.80
μ	2.00
ε	0.67
Economic parameters	
P_y (R\$ ton^{-1})	534.40
Y_0 (ton ha^{-1})	8.64
C (R\$ ha^{-1})	954.73
P_u^1 (R\$ L^{-1})	42.90
P_u^2 (R\$ L^{-1})	12.40
u_{max}^1 (L ha^{-1})	1.50
u_{max}^2 (L ha^{-1})	5.00
α	0.90
φ^1	8.90×10^{-3}
φ^2	2.70×10^{-3}
a	1.58×10^{-2}
m	4.83×10^{-1}

5.1 Weed population equilibrium

Consider the dynamic model involving both the seed bank density and the allele frequency which describes the herbicide resistance, (5) and (14), respectively. Fixing the dose u_t and initial conditions, the equilibrium points for this system are the fixed points (x^*, p^*) such that $(x_t, p_t) = (g(x_t, p_t, u_t), v(x_t, p_t, u_t))$. In other words, the fixed points satisfy

$$x_{t+1} = x_t \tag{35}$$

$$p_{t+1} = p_t. \tag{36}$$

In (3), when $y_t^a < 0.5$ plants per m^2, we set $x_t^r = 0$. Thus, for $\eta = 0$ and $\xi = 0$ the population model becomes the linear model:

$$\begin{aligned} x_{t+1} &= (1-\Psi)(1-\delta)x_t \\ p_{t+1} &= p_t. \end{aligned} \tag{37}$$

As the eigenvalues are $\lambda_1 = (1-\Psi)(1-\delta) < 1$ and $\lambda_2 = 1$, the linear model (37) is marginally stable. Table 5 shows the equilibrium points for a fixed dose of nicosulfuron and atrazine. The phase plane of the model is shown in Fig. 2.

Table 5 Dynamic model equilibrium points for nicosulfuron and atrazine

Herbicide	Dose (L ha^{-1})	P_1	P_2	P_3
Nicosulfuron	0.107	$(0,\ p_0)$	$(10,\ 1)$	$(245,\ 1)$
Atrazine	4.500	$(0,\ p_0)$	$(17,\ 1)$	$(227,\ 1)$

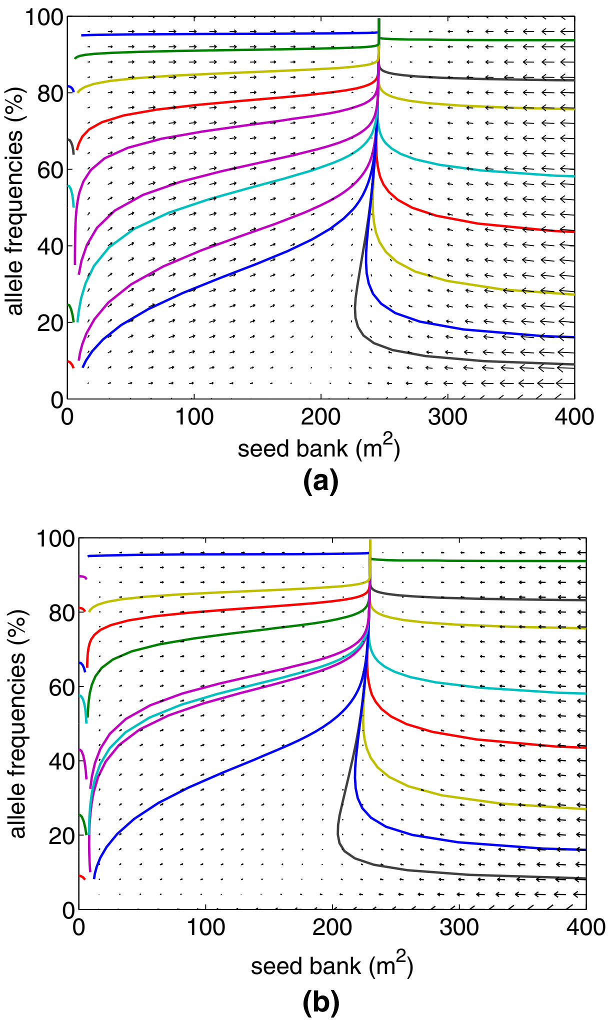

Fig. 2 Phase plane for fixed dose **a** nicosulfuron; **b** atrazine with selective pressure $s = 0.3$

In the particular context of nonlinear system analysis, a phase plane is a visual display of the behavior of the model variables as it shows the solutions of the dynamic model and their behavior in the neighborhood of each equilibrium point can be qualitatively determined. The phase plane showed in Fig. 2 depicts the solution of the seeds density versus the allele frequency in the time (years) considering different initial conditions denoted as (x_0, p_0). In each simulation was used 1000 cycles for both nicosulfuron and atrazine herbicides. In this figure, we observed that exists three equilibrium solutions, as shown in Table 5.

For the nonlinear model described here, P_2 is an unstable equilibrium solution as the solutions starting near the equilibrium point or equilibrium solution move away from the equilibrium solution. Similarly, P_3 is a stable equilibrium solution as the solutions starting near the equilibrium all converge to the equilibrium P_3 as time increases. Finally, for small seed density, the solutions are solutions of the linear model and approach P_1 given by $x = 0$ and p_0 which is thus said to be a marginally stable equilibrium point.

The phase plane is useful to define the correct weed management strategy in terms of the herbicide doses to be applied. Moreover, the phase plane indicates that the allele frequencies do not decrease even if the weed population reaches low levels, in other words, the allele frequencies have kept an existing trait.

5.2 Genetic frequencies

The genetic frequency using the FHW (13) are compared to the FHW (14) model using the seed bank (5) with (8)–(9) and (18). Figure 3 illustrates the dynamics of the allele frequency to (13) model and (14) model using the seed bank with nicosulfuron applied and weak selection for a dominant allele. The dynamics of the allele frequency is similar in both models which means that the weed population model proposed follows the population genetic principles.

5.3 Optimal control strategy

We evaluated the dynamics of the seed bank and the resistance evolution. The net average from the NLP problem for two herbicides in an annual application bases is compared to the

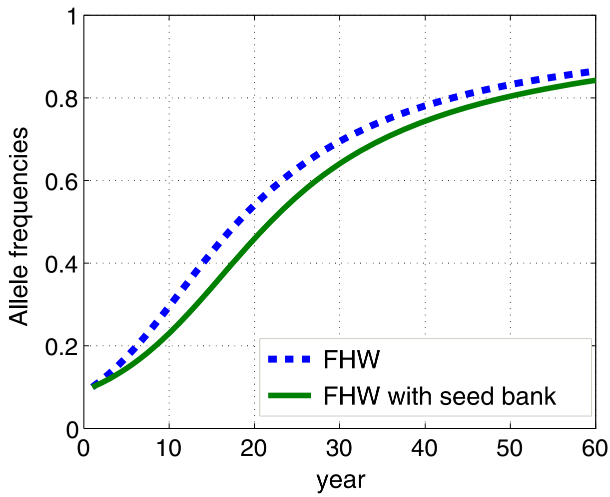

Fig. 3 Allele frequencies (—) FHW model (14) using the seed bank (5) with (8)–(9) and (18) and (– –) FHW model (13) for *Bidens subalternans* with dominant allele, nicosulfuron applied and weak selection $s = 0.2$

profit of the conventional harvest system with a constant application dose. The seed bank x^* and allele frequency p^* obtained from the NLP problem were simulated over a 10-year period for an initial seed bank of 500 (seeds m^{-2}) and an initial allele frequency of 0.1. This initial allele frequency indicates that the population resistant is close to be agronomically detectable. The simulation results were obtained using the strategies described in Sect. 4.1.

Figure 4a shows the seed bank and Fig. 4b the resistant allele frequency responses given by the optimum solution herbicide doses. We noticed in Fig. 4a that the seed bank decreased over time and the change in the seed bank was similar for the both herbicides with a NLP control strategy, but we also noticed that the nicosulfuron herbicide is better than the atrazine herbicide to control weeds, this may be explained by the dose–response curves obtained (see Fig. 7).

In Fig. 4b, we noticed that the NLP solution yielded a significantly retard in the allele frequency of the resistant biotypes. The resistant allele frequency increased from 10 % to

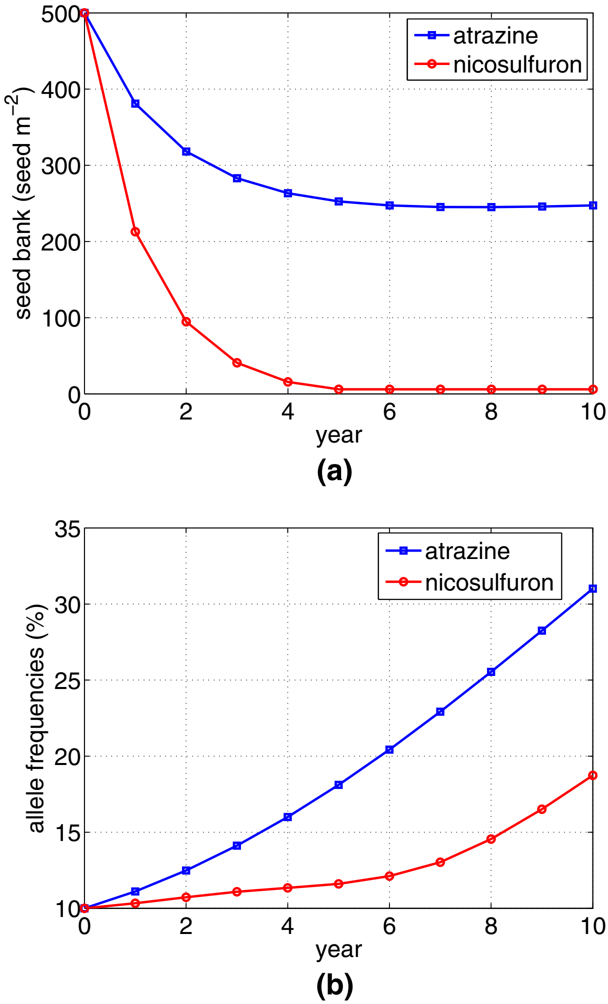

Fig. 4 Optimal results using the NLP optimal strategy for a 10-year simulation. **a** Optimal seed bank for nicosulfuron and atrazine. **b** Optimal resistant allele frequency for nicosulfuron and atrazine

around 30 % in a 10-year simulation under atrazine herbicide application while the resistant allele frequency of the nicosulfuron herbicide increased from 10 % to around 20 % in the same period of time. Note that, the seed bank control for atrazine herbicide showed a higher level of seeds which reflected also in the level of resistance. Therefore, the adopted optimum strategy was able to reduce the herbicide doses, minimizing the environment damage.

However, the weed control strategy adopted was satisfactory as compared to the conventional management which leads to higher values of resistance. Therefore, the use of new techniques of management that considers optimization strategies can help meeting environmental goals and not only the increase in profit.

Risks of resistance were reduced when a herbicide constant application was replaced by decreasing herbicide doses but maintaining efficacy in the seed bank control. However, not all herbicide application impacted the same selection pressure. Application of a soil residual her-

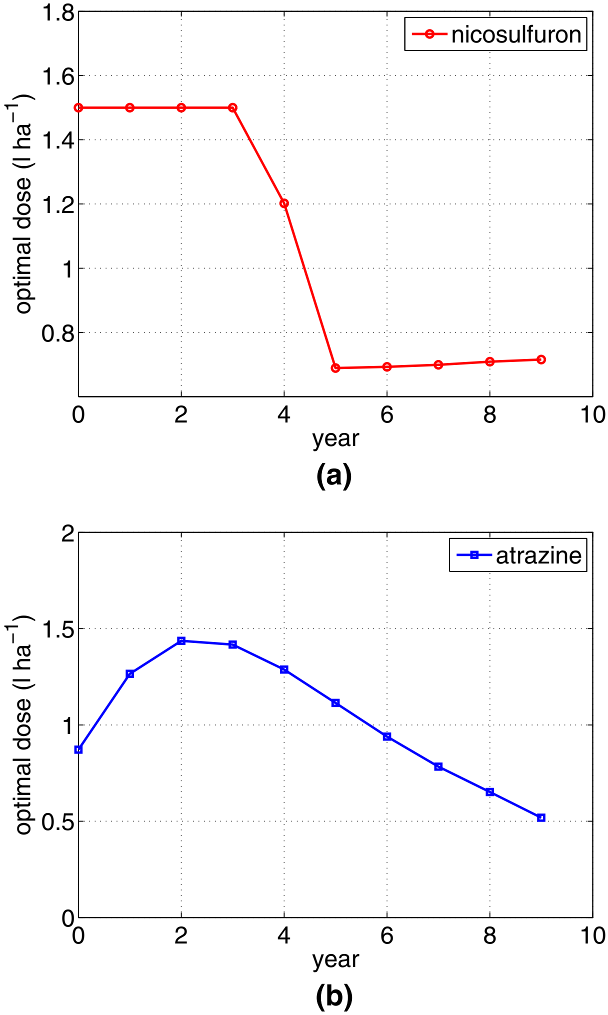

Fig. 5 Optimal dose u^* using NLP strategy for a 10-year simulation. **a** The nicosulfuron herbicide was applied. **b** The atrazine herbicide was applied

bicide at the time of crop sowing season can provide control of *Bidens subalternans* well into the growing season and significantly reduce the rate and risk of herbicide resistance evolution.

Variation occurred in the time of development of resistance. In general, resistant populations increases more slowly where the germination fraction was low (0.1) (not simulated as the type of weed considered has a high germination fraction). For both types of treatment, the resistance was delayed.

In the simulation scenario, the weed population was controlled for both herbicides applied (see Fig. 4a). Figure 5 illustrates the decreasing in herbicide doses given by the optimal control strategy for both herbicides. Thus, the decrease in herbicide doses is important to reduce the environmental impact caused by excessive use of herbicides.

5.4 Weed resistance impact on the solution

Considering the weed resistance to herbicides, we compared the solution of the NLP problem with a conventional strategy. The conventional strategy is based on the application of the

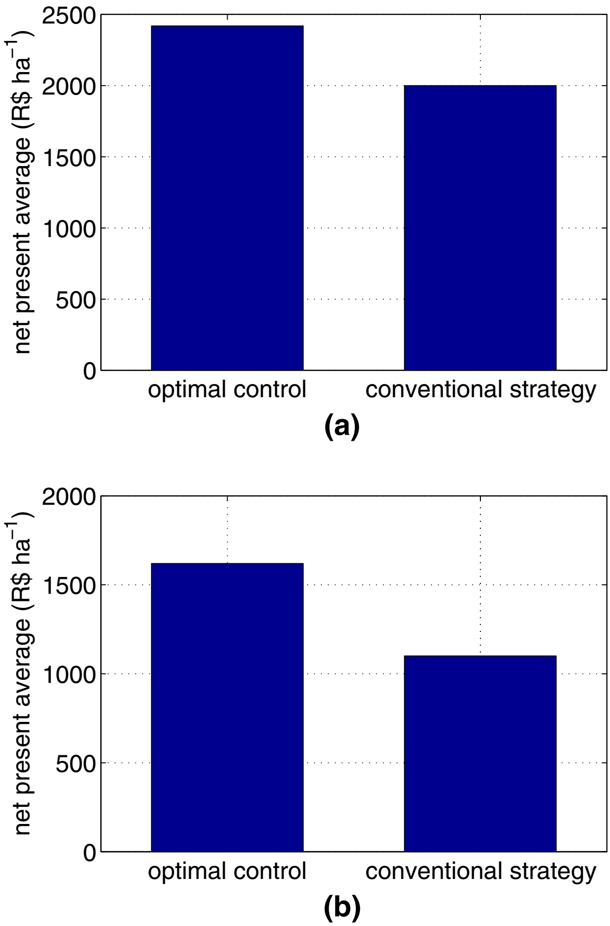

Fig. 6 Comparison of net values obtained with the optimal control approach for the application of **a** nicosulfuron and **b** atrazine herbicides and the conventional strategy for a 10-year simulation

maximum dose recommended for the field, following the recommendation indicated on the product label.

The net present values are given in Fig. 6 which indicates that the NLP result is economically superior to the conventional strategy results. In Fig. 6, we noticed that the profit using optimal control strategy for nicosulfuron herbicide was around 20 % superior when compared to the conventional strategy and in case of atrazine herbicide application the profit was around 50 % superior. This fact is due to the price of each unit of product used and the difference showed in weed control by dose–response curves as each herbicide have a different mode of action.

With the goal of maximizing crop returns with minimal environmental effects of herbicides, the formulated optimal control problem to define optimal management strategies for controlling weed population affecting the agricultural production achieved its purpose.

The sensitivity analyses indicated that the model was sensitive to variations in population size and seed bank dynamics. The solution is more sensitive to the initial condition and it is

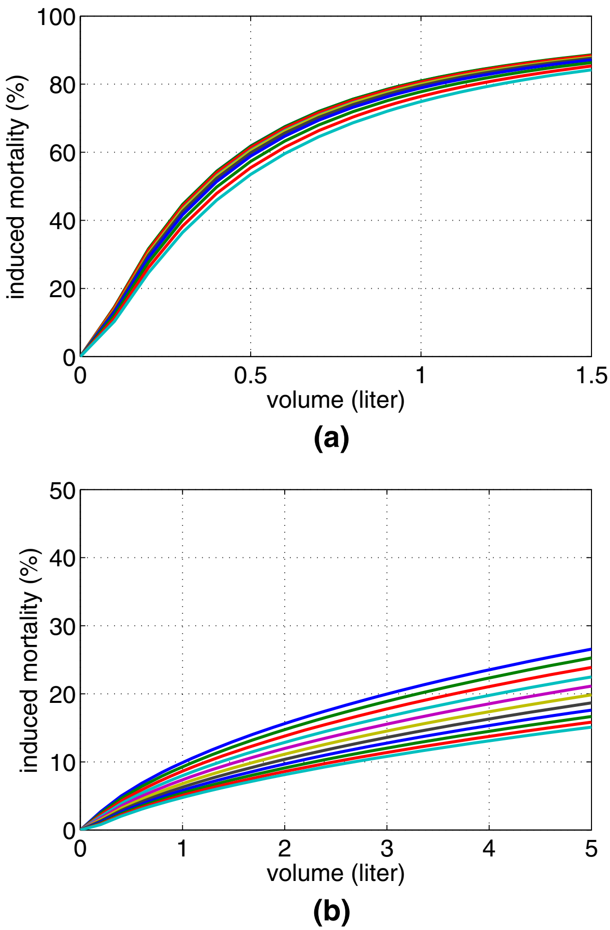

Fig. 7 Herbicide-induced mortality using the adopted dose–response curve (8) considering the optimal allele frequency p^* for **a** nicosulfuron and **b** atrazine herbicides

the most difficult parameter to select. The initial population sizes clearly vary from field to field. The annual germination rate, survival rate of new seeds and seed mortality, are clearly influenced by variable climatic and other environmental variables. All these factors contribute to the complexity of the weed population model which makes the study of weed population dynamics the key on agricultural production scenario.

The parameter values of the adopted dose–response model (7) were obtained by curve fitting from experimental data of herbicide-induced mortality (see Table 2). The resulting curves obtained according to (8) for the nicosulfuron and atrazine herbicides are illustrated in Fig. 7.

We noticed in Fig. 7 that the nicosulfuron herbicide is more efficient in weed control than the atrazine herbicide, since the nicosulfuron herbicide showed around 90 % control of weeds while the atrazine herbicide showed around 20 % control. This fact will be reflected in the production cost, the seed bank and the resistance evolution. We observed that the curves obtained using the adopted dose–response function (8) illustrated the change of dose–response curve due to the increase of resistance in the period of time of the

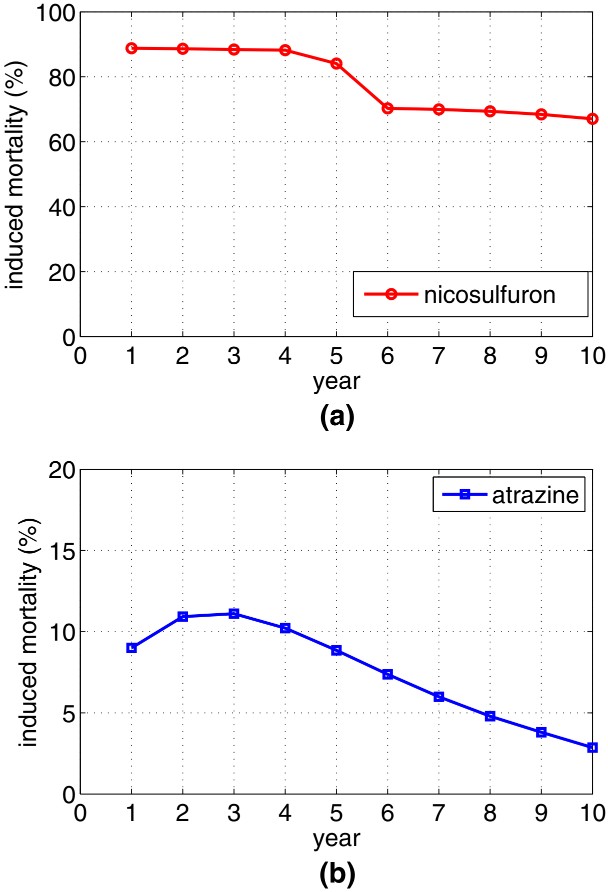

Fig. 8 Herbicide-induced mortality obtained with NLP optimal strategy, u^* and p^*, for the application of **a** nicosulfuron and **b** atrazine herbicides for a 10-year simulation

simulation. Therefore, the more resistant plants in the field the less is the efficiency of control applied.

The variation in the mortality rate of plants obtained with the optimal strategy NLP is illustrated in Fig. 8. We noticed that the mortality rate decreases due to the presence of weed resistant. Thus, with the increase of the resistance occurs a reduction in the efficiency of control applied to both herbicides. In this scenario, nicosulfuron was recommended as the herbicide resistance manifests slower and has higher profit while compared to the treatment made with atrazine herbicide.

Moreover, Maxwell et al. (1990) showed that the influence of herbicide efficiency on the evolution of resistance has important management implications. Reducing the control efficiency may delay the resistance evolution due to minimization of selection pressure for resistance. The results presented in this paper confirm these conclusions.

Several proposed strategy to reduce the risk of herbicide resistance evolution use herbicide rotation, sequences and mixture, these had been investigated in Diggle et al. (2003) and Neve et al. (2011). Our modeling analysis has shown that the continuous use of a single herbicide application for long period of time increases the selection of resistant byotype, thus the optimal control of weed can contribute to reduce the herbicide resistance.

6 Conclusions and discussion

In this work, we discussed an optimal weed control to support resource management and control in agriculture and a dynamic optimization model which considers the population resistance under selection pressure imposed by the use of herbicide is established. We proposed a single herbicide sequence to control weed infestation by maximizing economic returns and retarding the weed resistance evolution. The results are promising as they indicate that decreased herbicide doses are economically superior to both single herbicide sequences when compared to a conventional practice. In addition, the developed model is useful to explain the evolution of herbicide resistance and to demonstrate that the allele frequency in a population plays an important role in weed management.

The results on optimal control discussed here takes into account important requirements arising in resource management and control in agriculture and will give support to make decision on the herbicide usage in regions where weed resistance was reported by field observations. It is probable that herbicide resistance will only be readily apparent in the field after years of evolution and the practice of herbicide management is essential to retard the resistance evolution in the field. The absence of field management at many locations where the resistance has evolved and lack of detailed knowledge on the precise number of variables involved in the evolution of resistance make model validation problematic as detailed model validation can only be achieved with long-term field experiments and these can be troublesome. Considering these facts, we believe that combining weed dynamic modeling and field observations provides good practice to support resource management. Further work includes the use of rotation of herbicides to improve the control on the seed bank.

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