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ANALYZING COMPLEX DYNAMIC BIOECONOMIC SYSTEMS USING A SIMULATION OPTIMIZATION TECHNIQUE

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Abstract

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A hybrid approach to optimizing complex dynamic systems is introduced that employs computer simulation and theoretical conditions derived from the maximum principle to optimize non-analytic deterministic or stochastic systems. A policy problem in the area of pesticide regulation and the management of pest resistance is used in the discussion.

Key Words: Pesticide resistance, dynamic optimization, simulation, bioeconomic system

ANALYZING COMPLEX DYNAMIC BIOECONOMIC SYSTEMS USING A SIMULATION OPTIMIZATION TECHNIQUE

The use of intertemporal optimization techniques in the study of agricultural systems has expanded significantly in recent years. This shift to dynamic analysis has occurred because static neoclassical models cannot adequately address the many important problems that are connected with the multi-year nature of agricultural decision-making. The failings of static analysis are especially acute when the biological status of the agricultural system is not long-run independent of production decision-making. The perceived dominance of dynamic problems in agriculture has even led to calls for the abandonment of static analysis altogether in order to make agricultural economics more realistic and policy relevant (Trapp).

Although the movement towards dynamic economic analysis will almost certainly continue, this approach contains many problems of its own that continue to limit its empirical application. Chief among these is that most algorithms for empirical applications require that system objective functions and constraints be analytically expressed (Evtushenko). This is especially true for the maximum principle approaches that rely on boundary value, gradient, or math programming solution techniques. In addition, some specialized math programming techniques tend to require that problems be formulated in very specific, and often restricting, ways due to severe limits on computational ability. This problem has repeatedly arisen in dynamic programming applications, where the "curse of dimensionality" continues to plague complex analyses even though access to high-speed computing has greatly improved (e.g., Hornbaker and Mapp). Faced with these problems, some researchers have attempted to use digital computer simulation as a way of analyzing reduced sets of discrete policy options. However, this approach suffers from indeterminacy in the relationship between the policy sets being evaluated and the potential optimums for the system (Musser and Tew).

This paper will introduce a hybrid approach to optimizing complex dynamic systems that employs computer simulation and theoretical conditions derived from the maximum principle to optimize non-analytic deterministic or stochastic systems. This technique can potentially avoid the worst shortcomings of the standard methods and still allow researchers great flexibility in designing dynamic studies. We believe this to be the first explicit demonstration of

how this approach might be applied to a dynamic agricultural system. For illustration, a policy problem in the area of pesticide regulation and the management of pest resistance will be used throughout the discussion.

The Policy and Research Problem

Resistance can be defined as the acquired ability of a pest population to withstand a specific pesticide control treatment due to the cumulative effects of repeated exposure to the treatment. The ability of agricultural pest populations to develop genetic resistance to control measures has been known for the better part of this century, but it has only been in the last two decades that the potential severity of the problem was recognized. Producers are especially concerned about potential yield, quality, and cost effects of pest resistance. Environmentalists see a danger in the potential for increased pesticide use with increasing resistance, and thus higher residual levels of pesticides in food, water, air, and soil (Dover and Croft). Paradoxically, efforts to regulate the use of pesticides without explicitly considering resistance may itself contribute to the resistance problem, as a shrinking set of pest control alternatives forces producers to concentrate on using only one or two chemicals.

Given the emerging severity of the pest resistance/pesticide regulation problem, federal agencies continue to search for an effective way of incorporating the existence of pest resistance into their procedures for analyzing pesticide benefits and developing pest management policy (Rajotte et al.). To this end, both economists and entomologists have concentrated on investigating various theoretical and empirical aspects of pest resistance and pesticide regulations. Economists have tended to focus on the effects of resistance on pesticide use with pest resistance, and the intertemporal private and public benefits given pesticides in the presence of resistance (Knight and Norton). In general, these studies have been limited in their usefulness for policy formation by simplified characterizations of the systems involved. Biological and physical interactions within the agroecosystem are often exceedingly complex and not easily condensed in a representative economic model. This is especially true when one realizes the need to incorporate the potential use of multiple classes of pesticides to combat the pest resistance problem. On the other hand, entomologists have developed realistic, empir-

ically based computer models of resistance and the mechanisms of its development (e.g., Tabashnik). These studies have led directly to potential strategies for combating resistance. However, these strategies suffer from a lack of attention to the linkages between biology and economics in an agricultural production system. In particular, entomological models of resistance tend not to recognize the potential divergence between the interests of the producer and of society, resulting in management schemes that over-simplify the real decision-making process that needs to take place on both the local and national levels.

To emphasize the empirical complexity of investigating this type of problem, an actual management situation found in a relatively simple apple agroecosystem will be used as an example. The tufted apple bud moth (TABM -- Platynota idaeusalis Walker) is the major direct pest on apple fruit in the Cumberland/Shenandoah production region (Hull et al.) and has been successfully controlled in the past using organophosphate insecticides. An apple grower's most effective total pest control strategy has been to use limited amounts of acaracides to keep European red mite (ERM -- Panonychus ulmi Koch), an indirect pest feeding on apple tree foliage, below their economic threshold until the black ladybird beetle (BLB -- Stethorus punctum LeConte), a predator of mites, appears in the orchards to control ERM naturally (Hull et al.). This integrated pest management system is possible because of BLB's tolerance to the organophosphate pesticides used in TABM control. However, with TABM resistance to organophosphates, growers cannot count on BLB to control ERM because BLB is generally not tolerant of the other pesticide classes that are effective against TABM. Growers must then resort to increased use of acaracides to control mites. But from extensive use of acaracides problems arise. Not only do mites have the potential for rapid resistance development, but research has demonstrated that many acaracides are extremely toxic to humans and nontarget animals. In the long-run, as regulatory pressure and TABM/ERM resistance expands, the danger is that the apple pest complex will become uncontrollable and/or that there will be a net increase in the use of pesticides over what would have occurred with no regulatory action.

Formulating a model for an empirical investigation of the above apple agroecosystem proves to be an imposing undertaking. Assuming that a regulatory agency has as one of its objectives manipulating pesticide use so as to maximize, over a given planning horizon, the

total economic surplus associated with apple production and consumption, then at a minimum an empirical model would have to consider the time-varying relationships among two pest densities, predator density, two pest susceptibilities to different pesticides, predator susceptibility to the pesticides, immigration of susceptible pests and predators, environmental carrying capacities, and crop yields for both fresh and processing markets. Given the inherent nonlinearities, discontinuities, and uncertain functional forms governing these relationships, the ability to specify and estimate a suitably realistic analytic model is doubtful. It was this difficulty that led many applied entomologists to abandon differential equation simulation models of pest management with resistance in favor of complex discrete computer simulations that describe the system evolution in decidedly non-analytic ways. While directly useful for their purposes, these types of simulation models pose obstacles to the economist interested in deriving optimality-based approaches to dynamic pest and resistance management. The lack of explicit discrete or continuous analytic equations prevents straightforward application of the maximum principle through nonlinear programming or two-point boundary value solution algorithms. Dynamic programming can potentially be used, with the discrete simulations generating the states of the system for every combination of decision variable levels during each decision period. But if the computer simulation contains stochastic elements, the dimensions of the problem needs to be drastically reduced. Even if the problem at hand is simulated deterministically, the necessary state variables lead to computer storage requirements that far exceed current capabilities, and reducing its dimensions would require simplification to the point of changing the basic nature of the problem. Thus, another approach is needed to combine the realism available in the complex simulation models of entomology with the optimization theory and goals used in economics.

The Simulation Optimization Approach

Consider the general dynamic optimization problem¹

¹ The following discussion was adapted, in part, from Azadivar and Lee.

MAX
$$\int_{0}^{T} f_{0}[u(t), x(t), t] e^{-rt} dt$$
 [1]

subject to
$$\dot{x}(t) = f[u(t), x(t), t]$$
, $x(0) = x^0$ (x^0 fixed in R^n) [2]

$$x_i(T) = x_i^T$$
, $i = 1, ..., I$ (x_i^T all fixed) [3]

$$x_i(T) \ge x_i^T$$
, $i = l + 1, ..., m$ (x_i^T all fixed) [4]

$$g_j[x(t), u(t), t] \ge 0$$
 $j = 1, ..., k$ [5]

$$g_j[x(t), t] \ge 0$$
 $j = k + 1, ..., h$ [6]

$$u(t) \in U$$
, a fixed set in R^r [7]

where $f_0[u(t), x(t), t]$ may be the response of a simulation model at time t for values of v decision variables $u_1, u_2, ..., u_v$ represented by the vector u(t). Let these decision variables be constrained by membership in set U and non-negativity ([7] and [5] above), while pure state constraints include non-negativity ([6]) and terminal conditions ([3] and [4]). In addition, let $\dot{x}(t)$ denote the rate change in state variable levels, or the equations of motion. Some or all of these constraints may be non-analytic deterministic or stochastic functions represented by other responses of the same simulation model that may be generating $f_0[u(t), x(t), t]$. This formulation is completely general in that it contains both mixed and pure state constraints.

There are two main problems immediately encountered when trying to proceed towards an empirical solution to a problem of this form:

1. If $f_0[u(t), x(t), t]$, f[u(t), x(t), t], $g_i[u(t), x(t), t]$, and/or $g_i[x(t), t]$ represent simulation response functions, then they cannot be expressed analytically in terms of $\{u(t), x(t), t\}$. This makes the problem unsuitable for classical non-linear programming or boundary-value techniques, instead suggesting the need for some type of search routine through the feasible solution space. 2. Although f₀[u(t), x(t), t] can potentially be evaluated for any given {u(t), x(t), t}, even under condition (1), it may not be possible to optimize by ordinary search techniques. Most search methods proceed sequentially towards a solution by comparing system response criteria for two or more points in the feasible region. But if f₀[u(t), x(t), t] is a stochastically simulated function, comparing its mean response based on one observation at each point in the feasible region may result in the selection of a wrong direction for the next search step. Even the average of several replications at each point may be insufficient to offset stochastic characteristics in the simulated response.

Thus, from an economists viewpoint, the ideal solution procedure for this type of problem would be one that is capable of guiding the search process by incorporating some theoretical optimization conditions along with explicit use of simulation for representing non-analytic constraints, objective functions, and stochastic behavior. This can be accomplished by using a modified complex (i.e., constrained simplex) heuristic search procedure that has, as its goal, the direct optimization of the objective function subject to any number of pre-specified constraints. How this integration might be accomplished will be discussed after a description of the modified complex procedure.

The modified complex procedure (Azadivar and Lee) proposes to solve the problem

MAX
$$E[Z(u, x)] = Y(u, x)$$
 [8]

subject to
$$\phi_{j}(u, x) \stackrel{>}{=} C_{j}, \quad j = 1, 2, ..., b$$
 [9]

where *u* is a vector of discrete-valued decision variables, Z(u, x) is the random variable corresponding to observations on the simulated system, Y(u, x) is the unknown theoretical regression of Z(u, x), and $\phi_i(u, x)$ is a set of *b* constraints. The algorithm makes the following assumptions:

- 1. The theoretical regression function Y(u, x) is a real-valued, but perhaps unknown, function; and
- 2. There exists a finite constant M such that

$VAR[Z(u, x)] < M \quad \forall u .$

The basic idea behind the search procedure is to move through the feasible region as simplex vertices, each composed of a specific vector u containing decision variable levels from the set U, get closer to each other and converge towards the optimum. This movement can be random or, somewhat in analogy with the implementation of dynamic programming, exhaustive. Perhaps a better alternative, and the one advocated here, is to compare a simplex's vertices to find an inferior one. Movement is then accomplished by projecting the inferior vertex with respect to the centroid of the remaining vertices. If this new point is itself rejected, then the projection is retracted and the point moved closer to the centroid until it is no longer inferior. Then comparisons are continued to find a new inferior vertex, new projection, etc., until convergence occurs. This simplex search method is transformed into a complex search by preventing any projected vertex of the simplex from leaving the feasible region. This can be accomplished by testing each projected vertex for adherence to the constraint set. If it falls outside the constraints, then it is systematically retracted until it enters back into the feasible region. Note that, due to the complexity and stochastic nature of the objective and/or constraint functions, the solution will be approximate rather than exact, with the degree of approximation controlled by the researcher.

The procedure outlined above is directly applicable to problems involving deterministic simulation. But stochasticity in the simulation responses can lead to problems with this process. Given stochastic variation, there is no guarantee that a vertex rejected on the basis of comparing single simulations is indeed the worst point. In fact, the probability of this error increases as the variance in responses increases, and can only be ameliorated by incorporating multiple observations on the simulated response for any given vertex. One way of doing this is to calculate confidence intervals on the mean responses for a vertex. Because the confidence interval lengths will shorten as the number of simulation observations on any given vertex increases, a vertex can be rejected (with a chosen level of probability) as soon as its confidence interval is distinct and its mean is worse than adjacent vertices. If comparisons are sequentially made after small numbers of simulation runs on a set of vertices, then the total number of simulation runs for each search step can be kept to a minimum.

Simulation stochasticity in the constraint set can also lead to difficulties in directly applying the complex search method. This arises because stochastic variation implies that the constraints may never be satisfied on anything other than a probabilistic level. Thus, attaining a solution would require that the constraints be stated in terms of the maximum acceptable risk of violation. For example, a stochastic constraint from the set [9] might be expressed as

$$P[\phi_1(u, x) \le C_1] \ge 1 - \alpha_1$$
 where $0 < \alpha_1 < 1$

and α_1 is the maximum acceptable risk of violating the constraint. This representation can lead to constraints formulated in terms of upper or lower confidence limits of the type

$$HU_1(u, x) \le C_1$$
 for $P[\phi_1(u, x) \le C_1] \ge 1 - \alpha_1$

where $HU_1(u, x)$ represents the upper confidence limit on the response $\phi_1(u, x)$.

Application of the Simulation Optimization Algorithm

The complex method described above is very general and can be applied to a wide range of deterministically and stochastically simulated optimization problems. Exactly how this is accomplished will depend on the specific form of the problem being investigated and the type of information available. If the empirical problem involves analytic constraints and a simulated objective function, then it may be possible to use the necessary conditions from the maximum principle to aid in the search for optimal time-paths. In this case, initial decision variable, adjoint and state constraint multiplier levels would all have to be specified in the vertices. The problem would then entail the minimization of a function that represented the difference between calculated and required optimality conditions, subject to the adjoint, transversality, and other constraint conditions. This approach would be convenient, for it could take advantage of the requirement that the current-valued Hamiltonian be optimized in each time step, thereby allowing the optimal decision variable levels to be determined sequentially through time.

Although objective function simulation provides a case where the complex search technique can be most closely related to the standard analytic approach, the most frequent occurrence when dealing with dynamic bioeconomic models is to have simulated constraints.

In this case, complex search is used to directly optimize the objective function. As an example, reconsider the dynamic optimization problem posed in equations [1]-[7] in the light of the apple production problem discussed in the introduction:

$$\underset{U,V}{\text{MAX}} \quad \text{TES} = \sum_{0}^{T} \left\{ \sum_{h=1}^{\varepsilon} \sum_{l=1}^{\tau} \int_{0}^{(a_{h,l} y_{h,l}(t))} [D_{h,l}(\eta, t) - SY_{h,l}(\eta, U, V, t)] d\eta \right\} (1+r)^{-t} \quad [10]$$

subject to the equations of motion

$$\dot{y}_{h,i}(t) = \Omega_{h,i}[y_{h,i}(t-1), b_i(t-1), v_n(t-1), w(t-1), t]$$

$$\forall h, l, i, n$$
[11]

$$\dot{b}_{i}(t) = \Gamma_{i}[b_{j}(t-1), m_{j}(t-1), c_{j}(t-1), f_{j}(t-1), u_{k}(t-1), s_{j,k}(t-1), t]$$

$$\forall i, j, k, \text{ where } j = 1...y$$
[12]

$$\dot{s}_{i,k}(t) = \Theta_{i,k}[s_{i,z}(t-1), u_z(t-1), t]$$
[13]

 \forall i, j, k, z, where $z = 1...\psi$

$$\dot{f}_{i}(t) = \Upsilon_{i}[s_{i,k}(t-1), t]$$
[14]

$$\dot{c}_{i}(t) = \Psi_{i}[y_{h,i}(t-1), t]$$

$$\forall i, h, l$$
[15]

$$\dot{m}_i(t) = \Xi_i[t]$$
[16]

where we define

U is a fixed set of pest controls in R^{ψ}

V is a fixed set of non-pest control inputs in R^{ω}

 $u(t) \in U, v(t) \in V$

∀i, k

TES is the total economic surplus over all time periods

T is the terminal time of the planning horizon

 $D_{h,l}(\eta, t)$ is the demand function for a given crop and grade at time t

 $SY_{h,l}(\eta, U, V, t)$ is the supply function for a given crop and grade at time t

 $y_{h,l}(t)$ is the yield per acre of grade (I) for crop (h) at time t

 $a_{h,l}$ is the total number of acres producing crop h of grade 1

 $b_i(t)$ is the density of pest/predator (i) at time t

 $s_{i,k}(t)$ is the susceptibility of pest/predator (i) to control (k) at time t

 $f_i(t)$ is the fecundity of pest/predator (i) at time t

 $c_i(t)$ is the environmental carrying capacity for pest/predator (i) at time t

 $m_i(t)$ is the immigration of susceptible pest/predator (i) at time t

and the state variables are constrained as

 $y_{h,i}(t) \ge 0$, $b_i(t) \ge 0$, $s_{i,k}(t) \ge 0$, $f_i(t) \ge 0$, $c_i(t) \ge 0$, $m_i(t) \ge 0$ [17]

with $D_{h,l}$, $SY_{h,l}$, $a_{h,l}$, $y_{h,l}(0)$, $b_i(0)$, $s_{i,k}(0)$, $f_i(0)$, $c_i(0)$, and $m_i(0)$ all predefined.

Under normal circumstances, and with analytical representations for the objective and constraint equations, the next step towards a solution would be to form the current-valued Hamiltonian function and, with the presence of pure state constraints, the corresponding Lagrangian function. Sufficiency (if the solution cannot be assumed interior to the state constraints) or necessary conditions, derived from the maximum principle, could then be applied (Seierstad and Sydsaeter). This process would result in a set (in this case, a large set) of differential equations that would need to be solved for the optimal time-paths of the decision, state, and multiplier variables. But with realistically specified functions, this process usually leads to an intractable analytic problem. Approximating the solution using two-point boundary numerical techniques, or reformulating the problem in terms of non-linear programming, are alternative approaches, but they also require analytic forms for the equations of motion.

Because system complexity has, to date, prevented a realistic analytic specification of [10]-[17], entomologists have developed a discrete simulation model with which to investigate this system. This model, patterned after the SERA (Simulating the Evolution of Resistance in Arthropods) model of Tabashnik and Croft, has been greatly enhanced by Knight and is capable of handling extremely complex deterministic or stochastic systems. Thus, an appropriate approach for determining optimal decision variable levels through time would appear to be the complex search technique. Assuming a deterministic simulation of the constraint set, the procedure could be used to directly optimize the objective function [10] subject to the non-analytic constraints [11]-[16] and the non-negativity constraints [17]. Actual application of the process would entail the following:

1. Choose a number of initial vertices, each completely specifying a specific time-path of control actions to be taken over the entire planning horizon.

- 2. Simulate the entire planning period using each initial vertex and the constraints [11]-[16].
- 3. Test for conformance to the constraints [17]. This is probably most efficiently done at each time step in a simulation run, as violation of a constraint would immediately disqualify the vertex being simulated. Because, in practice, most simulation models will prevent these violations from actually occurring, the tests need to detect if the vertex would have led to a constraint violation.
- 4. Once all the initial vertices are simulated for the entire planning horizon, compare the realized value of the objective functionals to find the inferior vertex.
- Project the inferior vertex through the centroid of the remaining vertices to find a possible new vertex.
- 6. Simulate the entire planning horizon with the new feasible vertex. Compare the resulting objective functional value to the values simulated from the remaining vertices of step 4 to find a new inferior vertex.
- 7. Repeat steps 5-6 until the vertices collapse (within a specified tolerance level) to the centroid of the simplex.
- 8. The last vertex simulated can then be taken as the optimal time-path for the decision variables, with the resulting simulation describing the optimal time-path for the state variables.

Comparative Advantages of the Technique

It appears that the complex search technique has some important theoretical advantages over combined simulation/dynamic programming for optimization studies of complex systems. The most important advantage is in the use of computer resources. If approached using dynamic programming, the apple production problem above would require the simulation of every stage-state of the system. This information would then have to be stored for use in a recursive dynamic programming algorithm. In essence, every defined vertex in the feasible region would need to be evaluated. But with the complex procedure, only a small initial set of defined vertices needs to be evaluated, followed by a sequential addition of vertex evaluations until an optimum is found. In general, only a limited subset of all possible vertices will ever have to be evaluated, with only a small number of objective function values being stored at any given time. In fact, studies of theoretical deterministic systems have suggested that less than 1 percent of all possible vertices need to be evaluated before the complex search technique converges to an optimum (Azadivar and Lee). Stochastic systems would, of course, require additional simulation (the number partially depending on the probability required for the appropriate confidence limit estimates), but even analysis of these systems use significantly fewer simulations than the number of possible vertices. These factors suggest that complex search can increase the ability to investigate dynamic problems that are much more complex than previously possible. Some potential disadvantages to complex search do exist, with the primary one being the general inability to distinguish between local and global optimums. But, given the relatively small number of vertices needing evaluation before convergence, this problem can potentially be eliminated by using systematically different initial starting vertices (so as to search over different initial sectors of the feasible region) or by making sure that the initial vertices occupy significantly divergent areas of the feasible space.

Conclusions

Dynamic economic analyses of agricultural decision-making has been hampered over the years by simplistic models of the biological components in a farm production system. But discrete computer simulation, a method by which realism can be introduced to agricultural modelling, has not been widely adopted as a research tool because of the inability to relate simulation results with theoretical system optimums. The complex search simulation optimization technique presented in this paper has the potential to alleviate this shortcoming of simulation studies, thereby providing the economic researcher with a powerful tool to investigate complicated dynamic bioeconomic systems that cannot be accurately modelled using conventional analytic methods.

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