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Optimizing Complex Bioeconomic Simulations Using an Efficient Search Heuristic

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Abstract

For simulation to be truly useful for investigating many problems in agricultural economics, non-simplifying optimization techniques need to be employed. General methods for simulation optimization that do not inhibit system characterization or analysis are available, and they would appear to provide much of the mathematical and optimizing rigor demanded by economists. This paper describes the theory and algorithm of a robust and efficient simulation optimization approach, the Complex Method. An example of implementing the algorithm is illustrated using a pest management problem.

Keywords: simulation, optimization, Complex Method, hill-climbing

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Optimizing Complex Bioeconomic Simulations

Using an Efficient Search Heuristic

Richard F. Kazmierczak, Jr.[1]

INTRODUCTION

Realistic bioeconomic models are generally composed of multiple, highly non-linear biological and economic relationships. Although these bioeconomic models owe their realism to non-linearity, numerical optimization can only be directly accomplished if objective and constraint functions are analytically expressed (Evtushenko 1985). In addition, even if the models are analytically expressed, complexity can lead to difficulties in obtaining or approximating the required gradient vectors (e.g., Talpaz et al. 1978; Standiford and Howitt 1992). Linearization has been used to combat this problem, but the solution point depends on the choice of the initial path from which approximation is constructed, and thus may have no connection with the location of the true optimum (Baumol 1982). Other types of model simplification and solution methods have been developed, including combining simulation with linear, non-linear, and recursive programming (Dudley and Burt 1973; Chien and Bradford 1976; Kingma 1978; Richardson and Condra 1981). However, these alternate approaches require either drastic model simplification or specific model formulation, implying restrictions on the size of the control and/or state-space of the modeled system (Sierra and Condon 1987; Jacobson and Schruben 1989). This problem of simplification has arisen

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repeatedly in dynamic bioeconomic investigations, where the curse of dimensionality[2] continues to plague empirical implementation of theoretical models.

In an attempt to avoid unrealistic representation of agricultural systems, researchers have periodically relied on simulation. Simulation as a research tool in agricultural economics arose as the definition of an agricultural research problem was being expanded to include issues surrounding natural resources, economic development, and national economic policy (Johnson and Rausser 1977). Although simulation demonstrated its value as a practical substitute for direct physical, biological, and social experiments, the method did not necessarily lead to closed-form[3] mathematical solutions and thus continued to pose optimization problems (Anderson 1974). Path, pattern, and random searches may successfully avoid reliance on estimated analytics, but generally at the cost of extreme computational expense. In theory, simulations also can be optimized by parameter sweeps, a process where one or more model parameters are systematically and exhaustively varied and their effects on simulation responses noted (Minkoff 1987). However, the expense associated with this process often promotes simplification in the form of limited comparisons of potential policy options (e.g., Reichelderfer and Bender 1979). The *ad hoc*, non-optimizing nature of these kinds of investigations has led to reduced credibility for simulation studies (Boggess 1984; Musser and Tew 1984).

While various studies have demonstrated that simulation optimization can be used to investigate problems with a specific structure or with limited dimensions, the inability to link a general optimization process with complex bioeconomic models has contributed to the underutilization of simulation as a modeling tool in economics compared to its widespread adoption

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[2] The tendency for the computational time associated with numerical algorithms to increase exponentially with the number of variables used to define the empirical problem. This leads to unworkably long computation times for problems involving more than a few variables (Cipra 1991).

[3] In practice, the ability to derive a solution in the form of an explicit formula (Wolfram 1991).

in other disciplines. For simulation to be truly useful for investigating many problems in agricultural economics, non-simplifying optimization techniques need to be employed. General methods for simulation optimization that do not inhibit system characterization or analysis are available, and they would appear to provide much of the mathematical and optimizing rigor demanded by economists. This paper describes the theory and algorithm of a robust and efficient simulation optimization approach, the Complex Method. An example of implementing the algorithm is illustrated using a pest management problem.

THE OPTIMIZATION PROBLEM

Consider the general dynamic optimization problem

$$\max \int_0^T \phi\left[U(t), X(t), t\right] e^{-rt}\, dt \tag{1}$$

subject to the equations of motion

$$\dot{X}(t) = f\left[U(t), X(t), t\right], \quad X(0) = X^0 \quad (X^0 \text{ fixed in } \mathbb{R}^n),$$

where $\phi\left[U(t), X(t), t\right]$ is the system response at time t for w decision variables $u_1, u_2, \ldots, u_w$ represented by the vector $U(t)$. Let the decision variables be constrained in membership and non-negativity as

$$U(t) \in \bar{U}, \quad \text{a fixed set in } \mathbb{R}^w, \text{ and}$$

$$g_j[X(t), U(t), t] \geq 0 \quad \forall\, j = 1, \ldots, k,$$

while pure state constraints include non-negativity and various terminal conditions:

$$g_j[X(t), t] \geq 0 \quad \forall\, j = k+1, \ldots, h;$$

$$x_i(T) = x_i^T, \quad \forall\, i = 1, \ldots, l \quad (x_i^T \text{ all fixed}); \text{ and}$$

$$x_i(T) \geq x_i^T \ , \quad \forall \ i = l+1,\ldots,m \quad (x_i^T \ all \ fixed).$$

Some or all of these state constraints may be represented by system responses from the same model generating $\phi[U(t),X(t),t]$.

Difficulties are encountered when trying to proceed towards an empirical solution to a problem of this form. If, as is often the case when modeling bioeconomic systems over time, $\phi[U(t),X(t),t]$, $f[U(t),X(t),t]$, $g_j[X(t),U(t),t]$, and/or $g_j[X(t),t]$ represent complex response functions that cannot necessarily be expressed explicitly in terms of $\{U(t),X(t),t\}$, then the problem may be numerically intractable given that standard solution techniques rely on the calculation of gradient vectors. Specialized methods, such as response surface techniques (Myers 1971), pattern searches (Hooke and Jeeves 1961), and random searches (Smith 1973), may also be unsuitable because they either assume that the: 1) search involves a function with a known algebraic form; 2) number of available computer runs is essentially unlimited; and/or 3) number of controllable inputs under investigation is relatively small. In addition, these specialized methods generally assume that all system responses are observed without error or statistical variation. However, if $\phi[U(t),X(t),t]$ is stochastically simulated, the objective becomes one of

$$\max \quad E\left\{\int_0^T \phi[U(t),X(t),t]\, e^{-rt}\, dt\right\} = \Phi \ , \tag{2}$$

where Φ is the unknown theoretical function. If a typical search algorithm is used, then comparing the mean responses of the system based on a limited number of observations at each point in the feasible region may result in the selection of a wrong direction for the search. The ideal search heuristic would be one that incorporated theoretical optimization conditions and a flexible mechanism to account for stochastic behavior. One such technique, the Complex Method, is

applicable to situations where an analytic mathematical representation of the system is difficult to obtain, but it is possible to order the responses arising from different levels of the controllable inputs.

THE COMPLEX METHOD

The Complex Method is a general and powerful optimization algorithm that arose from the idea of applying simplexes[4] to the optimization of either physical processes or mathematical functions (Spendley, Hext, and Himsworth 1962; Nelder and Mead 1965). As a direct optimization procedure, the Complex method does not require gradients of the objective function. Instead, it operates with information on the relative response rank associated with control levels.

SIMPLEX MANIPULATION

At the core of the Complex Method is a simplex manipulation algorithm. A simplex can be geometrically defined as a convex hull of $n+1$ points, or vertices, in general position[5] in $\mathbb{R}^n$, where n denotes the number of controllable variables over which optimization is to take place. Thus, the procedure derives its name from the geometric figure that is moved through $\mathbb{R}^n$ in search of an optimum. The movement of the simplex can be broken down into six basic operations: initialization, ordering, reflection, expansion, retraction, and shrinkage (Lee 1986). In the description that follows, v_i indicates a current simplex vertex with the rank of i, where $i=0$ is the best system response and $i=w$ is the worst system response out of all the simplex's vertices. A vertex denoted by ν indicates that the vertex is either unranked or not a member of the current simplex. Angled brackets, as in $<v_0, v_1, \ldots, v_w>$, indicate that the included vertices are members of the same simplex.

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[4] Note that the relationship between simplexes of the Complex Method and the simplex method of linear programming algorithms is in name only. Where as the simplex of linear programming is a permanently rigid geometric figure defined by constraint boundaries, the Complex Method simplex is a movable, flexible geometric figure in hyperspace.

[5] Indicates that no three points defining the simplex are collinear.

To begin, a set of $w+1$ feasible vertices, each consisting of specific time-paths for each control variable, must be identified and used to define the initial simplex. A number of identification schemes can be used, ranging from those that generate the initial vertices randomly to those that attempt to distribute the initial vertices uniformly throughout the solution space (Mitchell and Kaplan 1968; Sargent 1973). Because convergence difficulties tend to arise in bounded problems if the initial simplex lies close to the edge of the feasible region, non-random selection methods have proven to be the most useful and tend to provide the largest initial coverage of the feasible region. This latter objective is desirable because convergence speed tends to be highest when the initial simplex contains the final optimum. To accomplish the non-random initiation of the simplex, the first vertex is defined as the central point of the feasible region, and includes the vector elements

$$u_w = \frac{c_w - a_w}{2} , \tag{3}$$

where c_w is the upper and a_w is the lower constraint boundary on the control variable u_w. Other initial vertices are then identified by dividing the range of all control variables into two equal sub-ranges and taking the center of each newly created sub-region as a vertex. This second operation yields $2w$ potential points in hyperspace, of which the w outermost feasible vertices are included in the initial simplex. Figure 1, where the dotted lines indicate the unknown response surface, illustrates the initialization for a simple problem of two control variables. Point A denotes the center of the bounded feasible region, while points B and C are two of the $2w$ potential vertices included in the initial simplex.

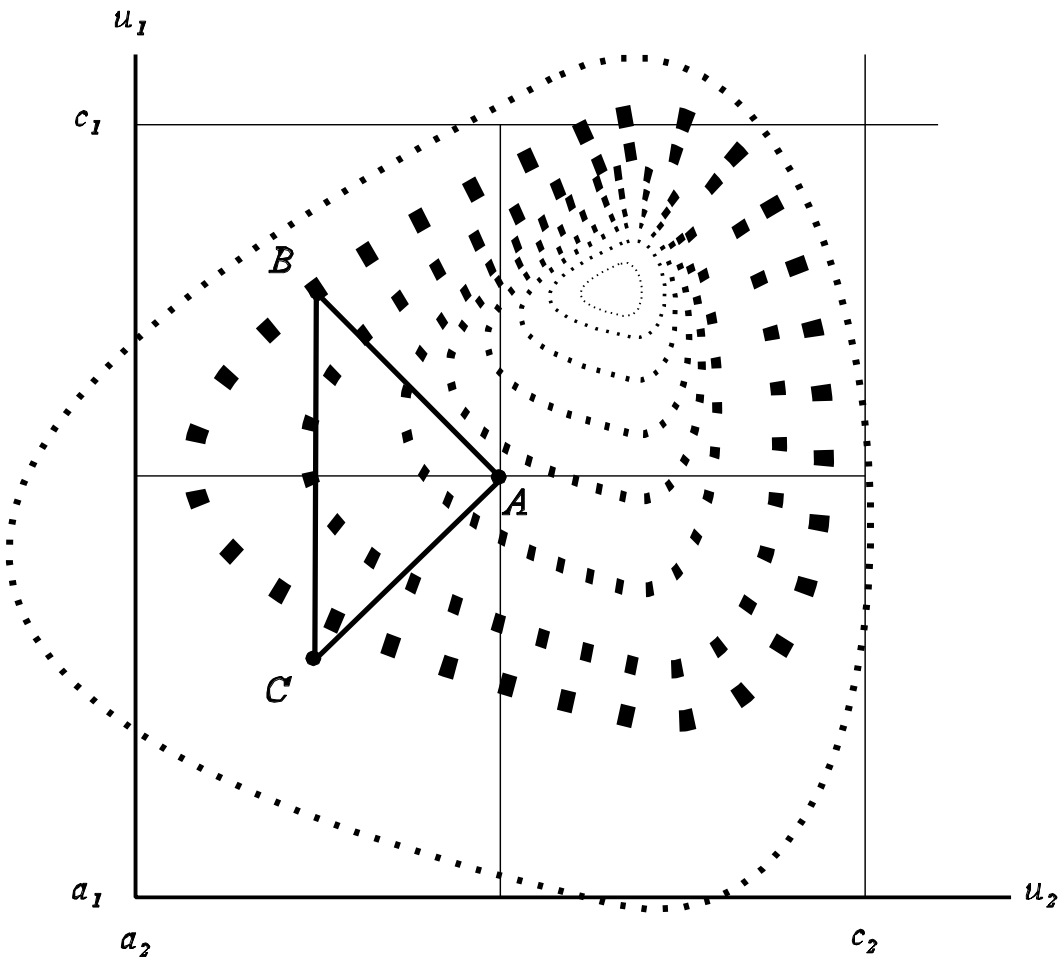

Figure 1. Initialization of the simplex given two control variables (u_1, u_2), with the unknown response surface indicated by the dotted lines.

Once an initial set of vertices are chosen, ordering occurs by whatever method is appropriate given the structure of the empirical model. In general, ordering is conducted by evaluating the system response for each individual vertex and then ranking the responses, and thus the vertices, by comparison. The initial evaluation and ordering is usually the most computationally intensive part of the simplex search algorithm because it requires $w+1$ vertex evaluations. With respect to Figure 1, the vertices would be ordered, from best to worst, as {A,B,C}.

After the initial ordering, the algorithm proceeds by moving the simplex away from the worst vertex v_w (point C in Figure 1). To do this, the centroid $\bar{v}$ (point m in Figure 2) of the current simplex vertices is calculated after excluding v_w. Thus, the centroid is the hyperspace center of the non-worst vertices, and provides a focal point through which a potentially superior vertex can be found. Calculating the centroid as

$$\bar{v} = \frac{1}{w}\sum_{i=0}^{w-1} v_i \ , \tag{4}$$

a reflected vertex v_r is obtained from

$$v_r = (1+\alpha)\bar{v} - \alpha v_w \ , \tag{5}$$

where $\alpha > 0$ is a reflection coefficient that determines how far away from the inferior vertex the reflected vertex will be located. If the simulation response of v_r (point D in Figure 2) is superior to the next-to-worst vertex v_{w-1} (point B in Figure 2), then v_r replaces the worst vertex v_w as a member of the current simplex, thus moving and changing the shape of the simplex (to ABD in Figure 2). Stopping criteria are then tested, and if not satisfied, the vertices are re-ranked and the process begins again.

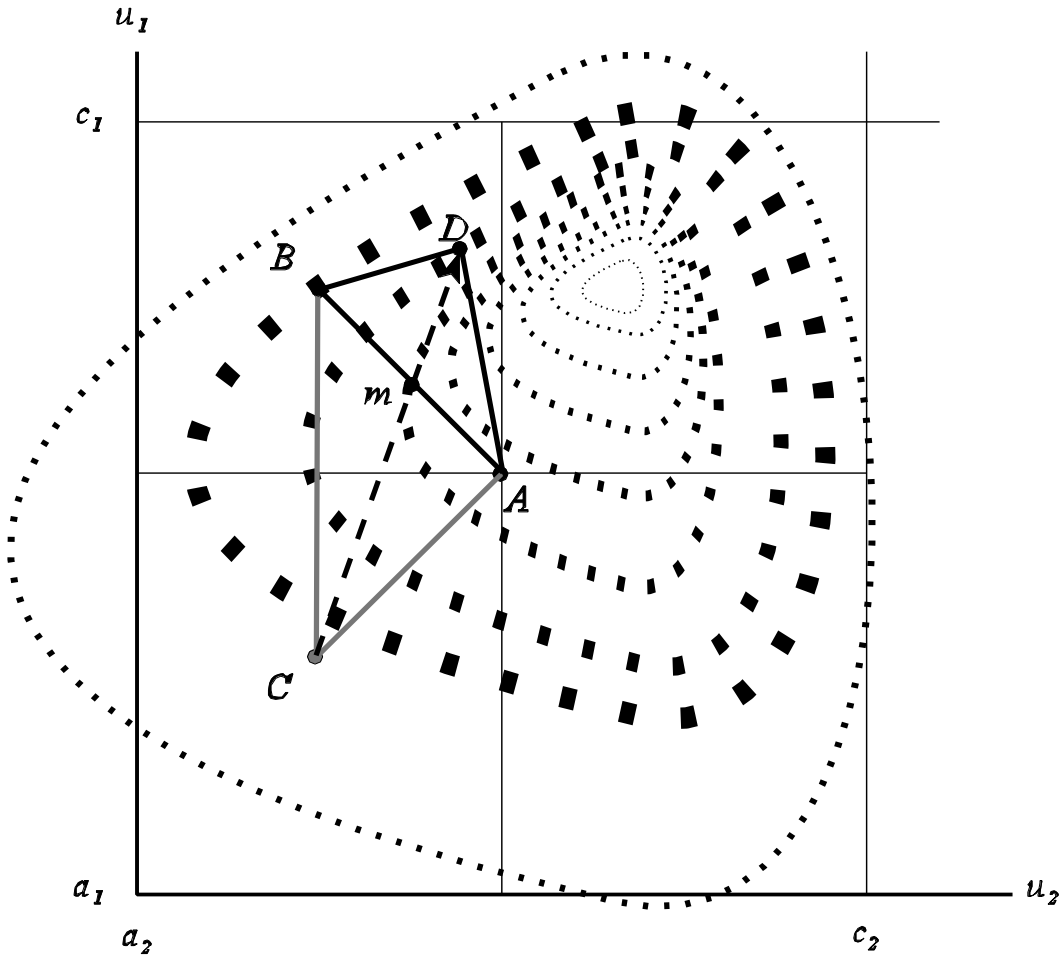

Figure 2. Reflection of an initial simplex given two control variables (u_1, u_2), with point m being the calculated centroid, the dashed arrowed line indicating the path of reflection, point D being the new, superior vertex of the simplex, and the unknown response surface indicated by the dotted lines.

It is possible for the process of reflection to yield a vertex v_r that is superior to the best vertex v_0. If this occurs, then it may be advantageous to continue the search in the direction of the original reflection. This is accomplished by calculating an expanded vertex

$$v_e = \gamma v_r + (1-\gamma)\bar{v} \ , \tag{6}$$

where $\gamma > 1$ is the expansion coefficient. For v_e superior to v_r, the new simplex is defined by replacing v_w with v_e. However, if v_e is not superior to v_r, then v_r once again replaces v_w and a new v_r is calculated after reordering.

But what happens if the v_r (point D in Figure 3) is actually inferior to v_{w-1} (point B in Figure 3), thereby making its replacement of v_w an act of futility? When this occurs, a retraction process is used to move the reflected vertex back along the projection path towards v_w. The retracted vertex is given by

$$v_c = \beta v_w + (1-\beta)\bar{v} \ , \tag{7}$$

where $0 < \beta < 1$ is the retraction coefficient. After systematically increasing β until v_c is superior to v_{w-1}, a new simplex is formed by replacing v_w with v_c (point E in Figure 3). Stopping criteria are checked, and if not satisfied, a new ranking and reflection initiated. If v_c continues to be inferior to v_{w-1}, then a shrinkage process is used to reduce the size of the simplex by moving all but the best vertex towards the best vertex:

$$v_i = \frac{1}{2}(v_0 + v_i) \quad i = 1,\ldots,w \ . \tag{8}$$

A completely new system evaluation must now be obtained for all but v_0 of the simplex, and re-ranking determined before proceeding on to a new reflection. This makes the shrinkage operation

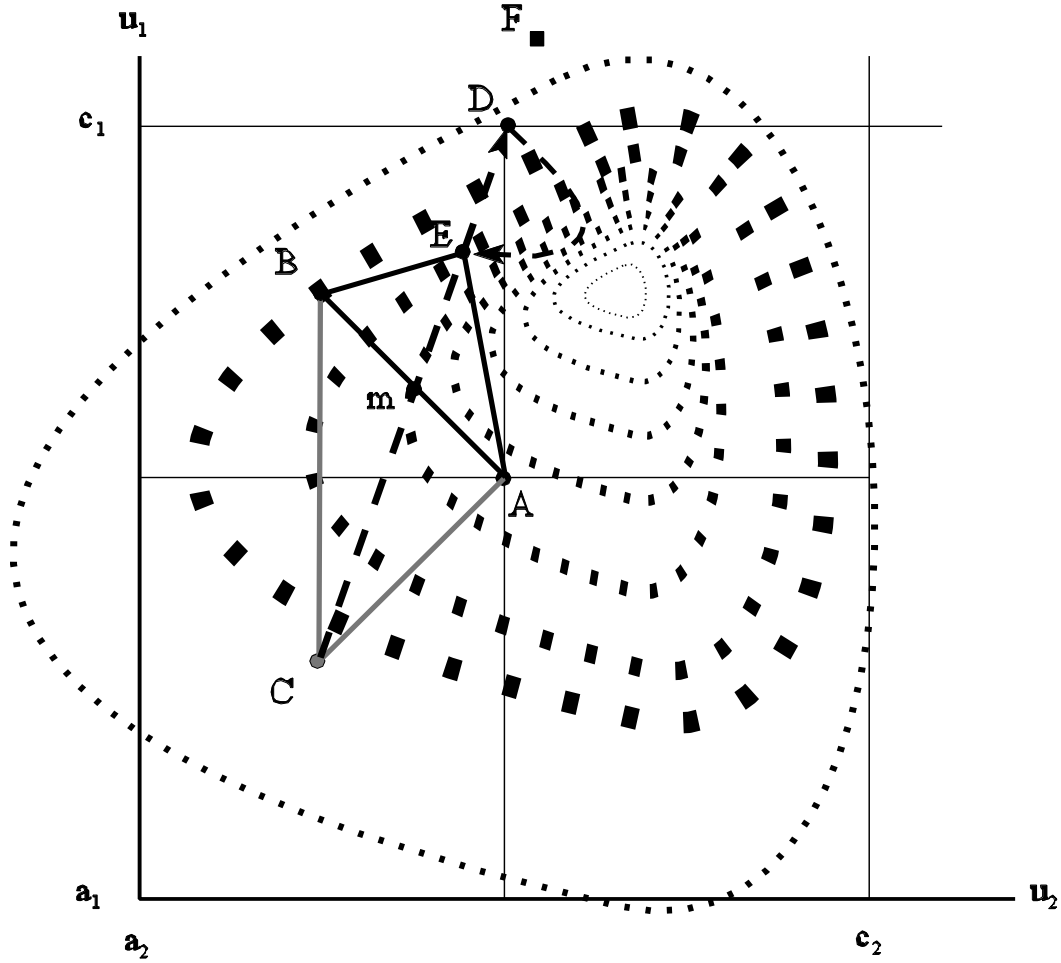

Figure 3. Reflection and retraction of an initial simplex given two control variables (u_1, u_2), with point m being the calculated centroid, the dashed arrowed line indicating the path of reflection, point D being the potential new, but inferior vertex of the simplex, point E being the retracted new vertex of the simplex, and the unknown response surface indicated by the dotted lines.

computationally expensive, but it generally represents progress due to the narrowing of the search field.

Although only alluded to in the above discussion, stopping criteria are a critical part of simplex manipulation. One potential and theoretically optimal criterion would stop the search when the simplex collapses to a single point in hyperspace. However, the success of this criterion is highly dependent on the shape of the response surface in the neighborhood of the optimum and the appropriate scaling of α, γ, and β. Other, near-optimal, criterion have also been explored. Assuming the existence of a simplex $<v_0, v_1, \ldots, v_w>$, where response values at each vertex are denoted by $\{\phi(v_0), \phi(v_1), \ldots, \phi(v_w)\}$, then Nelder and Mead (1965) proposed to define an optimizer $\phi(v_0^*)$ as when

$$\frac{1}{w}\sum_{i=0}^{w}\left[\phi(v_i) - \bar{\phi}\right]^2 < \epsilon \ , \tag{9}$$

where

$$\bar{\phi} = \frac{1}{w}\sum_{i=0}^{w}\phi(v_i) \quad \textit{and} \quad \epsilon > 0 \ . \tag{10}$$

In other words, the stopping criteria halts the search when the standard error of the response values of all simplex vertices are less than the tolerance level ϵ, or when the simplex has collapsed to a pre-defined size. Note that this stopping criteria can fail if the initial simplex is too small relative to the tolerance level ϵ, but the choice of an arbitrarily small ϵ involves a trade-off with the number of iterations the optimization process must execute. Of course, the interior of the remaining simplex could be exhaustively searched for the true optimum.

CONSTRAINTS AND STOCHASTICITY

As presented above, the simplex manipulation makes no provisions for preventing a projected vertex from leaving the feasible region. This can be accomplished by testing each projected vertex for adherence to the constraint set. If the projected vertex falls outside the constraints (as does point F in Figure 3), thus violating a control variable bound, then it can be set equal to the constraint limit. If the projected vertex results in a violation of explicit and/or implicit simulated response constraints, then it can be systematically retracted until it enters back into the feasible region (Box 1965).

While directly applicable to problems involving deterministic simulation, simplex manipulation also can be generalized to stochastic systems. Given that system stochasticity results in a situation where there is no guarantee that a vertex rejected on the basis of comparing single simulations is indeed the worst point, the probability of an erroneous rejection increases as the variance in system responses increases. This variance problem can only be addressed by incorporating multiple observations on the simulated response for any given vertex. One way of doing this is to calculate batch-mean confidence intervals for each 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 the other vertices of the simplex. If confidence interval calculations and comparisons are sequentially made after a small numbers of simulations on a set of vertices, then the total number of simulations for each search step can be minimized.

Stochasticity in the simulation constraint set can also lead to problems 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 (Azadivar and Lee 1988). For example, a stochastic constraint might be expressed as

$$P\left[f_1(U,X,t) \le C_1\right] \ge 1-\alpha_1 \ . \tag{11}$$

where $0<\alpha_1<1$ and α_1 is the maximum acceptable risk of violating the constraint. This representation can lead to constraints formulated and evaluated in terms of upper or lower confidence limits:

$$HU_1(U,X,t) \le C_1 \quad for \quad P\left[f_1(U,X,t) \le C_1\right] \ge 1-\alpha_1 \tag{12}$$

$$HL_1(U,X,t) \ge C_1 \quad for \quad P\left[f_1(U,X,t) \ge C_1\right] \ge 1-\alpha_1 \ ,$$

where $HU_1\langle U,X,t\rangle$ represents the upper confidence limit and $HL_1\langle U,X,t\rangle$ the lower confidence limit on the equation of motion $f_1\langle U,X,t\rangle$.

CONVERGENCE

In an early work on the nature of iterative solution procedures, Ortega and Rheinboldt (1970) examined methods of the form

$$v_{k+1} = v_k - \omega_k \alpha_k p_k \qquad k = 0,1,\ldots \tag{13}$$

for finding the critical points of a function $\phi: \mathbb{R}^n \to \mathbb{R}^1$, where $\alpha \in \mathbb{R}^1$ is a step-length parameter and $\omega \in \mathbb{R}^1$ is a relaxation parameter. The authors demonstrated that an iterative maximizer must have the property

$$\phi\langle v_{k+1}\rangle \ge \phi\langle v_k\rangle \qquad k = 0,1,\ldots \tag{14}$$

where ϕ is bounded from above. Wolfe extended their analysis to show that the optimizer should also be able to satisfy

$$\lim_{k\to\infty} \frac{\nabla\phi(v_k)^T P_k}{\| P_k \|} = 0 \tag{15}$$

and

$$\lim_{k\to\infty} \nabla\phi(v_k) = 0 \tag{16}$$

where $\nabla\phi$ denotes the gradient vector of ϕ and $\| P_k \|$ denotes the Euclidean norm of P_k. This section will sketch the sufficient conditions associated with equations [14] through [16] and present a convergence theorem for the Simplex Method. A preliminary proof of the theorem is relegated to the appendix.

To begin, consider the fact that the Nelder-Mead algorithm yields at least three distinct sequences of vertices that can be examined. These include the best approximate solutions $\{v_0^k\}$, the worst approximate solutions $\{v_w^k\}$, and the centroids of all the simplexes, $\{\bar{v}^k\}$. The sequence $\{v_0^k\}$ trivially satisfies condition [14] because $\{v_0^k\}$ is replaced by $\hat{v}$ only if $\phi(\hat{v}) > \phi(v_0^k)$. Demonstrating condition [15] or [16] for sequence $\{v_w^k\}$, however, requires a concavity assumption on ϕ such that

$$\phi[\alpha v_1 + (1-\alpha)v_2] > \alpha\phi(v_1) + (1-\alpha)\phi(v_2) \qquad \alpha \in [0,1] \tag{17}$$

where concavity also suggests the inequality

$$\phi\left(\sum_{i=1}^{w} \alpha_i v_i\right) > \sum_{i=1}^{w} \alpha_i \phi(v_i) \tag{18}$$

when $\alpha_i > 0 \ \forall \ i$ and $\sum_{i=1}^{w} \alpha_i = 1$. With these additional assumptions, the vertices of any simplex S_k will have response values greater than $\phi\left(v_w^k\right)$ such that, if a reflected vertex is accepted,

$$\phi\left(v_r^k\right) \geq \phi\left(v_{w-1}^k\right) > \phi\left(v_w^k\right) \tag{19}$$

If, however, a contraction vertex is accepted or the simplex is shrunk, then

$$\phi\left(v_w^{k+1}\right) > \phi\left(v_w^k\right) \tag{20}$$

and condition [15] or [16] holds for all $\{v_w^k\}$. In fact, this line of reasoning suggests that every sequence $\{v_i^k\}$ has the non-decreasing property.

Having demonstrated the potential viability of sequences $\{v_0^k\}$ and $\{v_w^k\}$, the sequence $\{\bar{v}^k\}$ remains to be examined. Consider the simple example in Figure 4, where the vertices of a simplex S_k are v_0 and v_1, with v_r having just been accepted by the Nelder-Mead algorithm. From this example, it can be observed that

$$\phi\left(\frac{1}{2}(v_0 + v_1)\right) > \phi\left(\frac{1}{2}(v_0 + v_r)\right) \tag{21}$$

thereby violating condition [14]. Thus, the sequence $\{\bar{v}^k\}$ is shown to be unacceptable, and only the sequences $\{v_0^k\}$ and $\{v_w^k\}$ can be considered viable alternatives. It is with these two sequences that the following convergence theorem was postulated by Woods (1985):[6]

[6] Woods' theorem was set in the context of a minimization problem. The theorem presented here has been set in the contest of maximization.

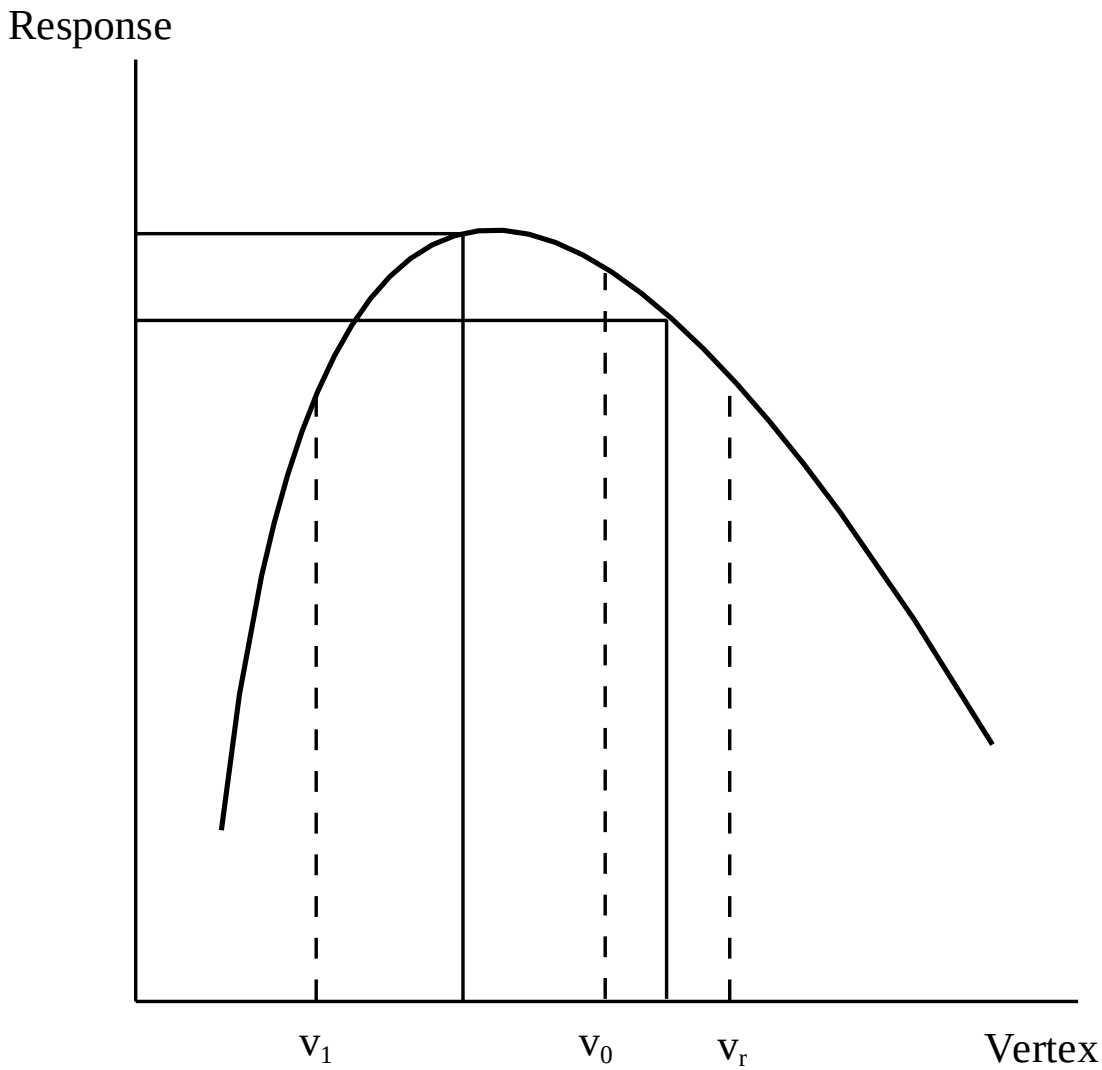

Figure 4. Demonstrating the inferiority of the centroid as a potential optimal solution. Given the initial simplex $<v_0, v_1>$, v_r would be accepted by the algorithm as a replacement vertex. However, it is obvious that $\phi\left[\frac{1}{2}\langle v_0 + v_1\rangle\right] > \phi\left[\frac{1}{2}\langle v_0 + v_r\rangle\right]$, demonstrating the inferiority of the sequence $\{\bar{v}^k\}$.

THEOREM: If the set $L\left(v_w^0\right) = \left\{v\colon\ \phi(v) \geq \phi\left(v_w^0\right)\right\}$ is bounded, where v_w^0 is the worst vertex of the initial simplex, then a subsequence of the sequence of simplexes converges to some $S^* = < v_0^*, v_1^*, \ldots, v_w^* >$. Additionally, let the Nelder-Mead algorithm be modified such that, at the kth iteration, the expansion step v_e^k is accepted only if

$$\phi\left(v_e^k\right) > \phi\left(v_r^k\right) > \phi\left(v_0^k\right) \tag{22}$$

and the reflection step v_r^k is accepted only if

$$\phi\left(v_r^k\right) > \max\left\{\phi\left(v_{w-1}^k\right),\ \phi\left(v_w^k\right)\left(1 + sign\left[\left(\phi\left(v_w^k\right)\right)\right]\epsilon\right)\right\} \tag{23}$$

for some $\epsilon > 0$ and $\phi\left(v_w^k\right) \neq 0$. If $\phi\left(v_w^k\right) = 0$, then v_r is accepted only if

$$\phi\left(v_r\right) > \epsilon > 0 \quad . \tag{24}$$

Then, for any $\epsilon > 0$ and strictly concave $\phi\colon\ \mathbb{R}^n \rightarrow \mathbb{R}^1$, each convergent subsequence of the sequence $\{S_k\}$ generated by the algorithm converges to some degenerate simplex $\hat{S}_i^* = < v_{0,i}^*, v_{0,i}^*, \ldots, v_{0,i}^* >$. Moreover, the function values at all limit points are equal, and the set of limit points is connected, so that the sequence either converges to a point, or else there are infinitely many limit points.

Furthermore, a corollary near the end of the above theorem's proof (see appendix) establishes that the Nelder-Mead algorithm will converge to a connected set of limit points even when the calculations are implemented on a finite precision, discrete computing machine.

The formal arguments for convergence hinge, to a large degree, on the concavity of the response function. In reality, however, few complex simulations will yield globally concave

response surfaces. In these cases, the above discussion would apply to locally concave regions and would establish convergence to a local optimizer. As a practical matter, the difficulties associated with non-global concavity can be overcome by initializing the algorithm over different regions of the feasible space and comparing the resulting optimizers. Studies suggest that the method is empirically better at finding the global optimum among many local optima than might be expected given the current status of convergence proofs (Barton 1987; Kim and Blake 1988).

ADVANTAGES AND DISADVANTAGES

What makes the Complex Method attractive is its adaptive features. In particular, a simplex is moved through solution space in such a way that allows it to reflect, extend, contract, and/or shrink to conform to the characteristics of the response surface. The simplex can elongate down long, inclined planes, change direction upon encountering a valley at an angle, or contract in the neighborhood of the optimum, with the aim of eventually including the optimum within the bounds of the simplex. This is in contrast to other external optimization procedures, most of which try to move along a line towards the optimum. The advantages of the method include:

1) Beginning at a point far from the optimum, the search approaches the neighborhood of the optimum rapidly compared to other techniques (Suk and Mitra 1972);
2) In general, a search results in only a small fraction of the feasible solution space being simulated, thereby conserving computing resources (Lee 1986);
3) A search can be easily modified to accommodate various special characteristic of the simulated system, including stochasticity (Lee 1986);
4) The approach is completely generalizable and can be used on both continuous and discrete simulations (Beveridge and Schechter 1970); and
5) The approach does not require an explicit expression of the objective or constraint functions.

Disadvantages of the Complex Method center on its potential to yield only locally optimal solutions, particularly when the response surface is very convoluted. However, in addition to the apparent robust characteristics of the optimizer (Barton 1987), research suggests that problems involving social welfare objectives, such as those often investigated with bioeconomic models, may inherently yield an extensive range of acceptable, near-optimal solutions within the feasible region (Chapman 1987; Rowse 1988).

EXAMPLE APPLICATION

As a demonstration of the Complex Method and its potential utility in agricultural economic research, consider the production model described in Kazmierczak et al. (1993). The authors examined the potential economic impacts of synergism between increased pesticide regulation and the ability of pest organisms to develop resistance to the control technology set. Concerns revolved around the possibility that regulatory withdrawal would lead to accelerated resistance development to the control chemicals remaining post-regulation, thereby inducing long-run declines in the flow of economic benefits from the perennial production system and increased use of pesticides. Given the time-dynamic nature of the problem and the intricacy of the pest/predator relationships in the system, an empirical biological model was needed to realistically track not only fluctuations in population levels and crop production, but also changes in the underlying genetic structure of the populations. While such models had been developed by entomologists, they generally consisted of complex computer simulations not easily summarized by a set of analytic equations (Tabashnik 1990). Simplification of the solution space was an alternative that has been used in a number of pest management studies, but this proved to be unsatisfactory given the desire for policy relevance. Thus, the requirements of the problem suggested the use of an external optimizer, such as the Complex method, which could be implemented through a number of specific steps:

1) *Initialization.* Generation of the initial simplex entailed the creation of a set of vertices, with each vertex composed of *w* elements representing a possible time-path of pest control actions that could be taken over a 25 year planning horizon. Considering re-entry and day-to-harvest restrictions, a baseline no-regulation scenario included 6 different control chemicals available for use in each of 20 time-steps per year. Thus, each *w* element of a vertex was defined as being the amount of a particular pesticide used in a specific time step, giving each vertex 3000 elements or controllable variables. The levels obtainable by each vertex element were bounded by labeled application rates, and ranged in discrete increments from zero use to 25 percent above the recommended application rate for each chemical in each time period. Given 3000 controllable variables, the initial simplex consisted of 3001 vertices uniformly distributed throughout the solution space.

2) *Ordering.* Each vertex defined in step (1) yielded a system response in terms of resistance- and/or regulation-induced changes in total economic surplus over 25 years. Given that each vertex evaluation required 30 seconds on a Pentium®/120mhz microcomputer, the entire simplex consumed approximately 25 hours of computation time, illustrating both the expense involved in evaluating the initial simplex and the relatively inexpensive evaluation of additional vertices generated in subsequent steps. The system responses were then used to arrange the vertices in descending order relative to the amount of surplus each generated, and the worst performing vertex was identified.

3) *Reflection and Expansion.* The generation of new and potentially superior time-paths of pest control proceeded by calculating the centroid, or the mean of the control actions taken in each specific time-step of a planning horizon across all vertices except the worst performer. This point was used to determine the reflection vector, which served to point the search away from a poorly performing region of the solution space and towards the general region

of all the other vertices. From this pointer, a new vertex was projected. Given the summation nature of the centroid, this calculation was stored and altered for subsequent reflections based on the entry and exit of vertices from the current simplex. Thus, the computational expense of reflection and expansion was minimal. Identifying the appropriate values for reflection and expansion coefficients was dependent on system scaling and required some experimentation, although optimum convergence speed and stability generally occur when the reflection coefficient is one-half the magnitude of the expansion coefficient (Lee 1986). Once projected, a potentially superior vertex was checked against constraint boundaries. Any vertex elements violating a constraint boundary were reset equal to the value of the constraint boundary. The system response was then generated for the newly projected pesticide use time-path and checked against explicit and implicit system constraints. A projected vertex was included in the simplex if all constraints were satisfied and the associated system response exceeded that of the next-to-worst vertex. After the simplex was reformed, stopping criteria (step 5) were checked and, if not satisfied, a new worst vertex was identified and the process began again at step 3.

4) *Retraction.* If the projected time-path of pest control actions elicited a system response that was no better than the response associated with the next-to-worst vertex, then the new vertex was retracted back towards the original inferior vertex until a better vertex was found. If a superior projected vertex was not identified during retraction, then the next-to-worst vertex was selected and the process restarted at step (3). If all the vertices were used as a point of reflection without finding a superior vertex, shrinkage would have been employed to reinitialize the simplex. This latter operation will not be used if the reflection and retraction coefficients are appropriately scaled.

5) *Search Termination.* Using the Nelder-Mead form of stopping criteria, the search was terminated when the simplex collapsed to a neighborhood defined in size as 5 percent of the mean of the system responses for all the vertices in the current simplex. Random searches were then conducted within the final simplex. If no superior pesticide use time-path was found, the best performing vertex of the final simplex was defined as the approximately optimal solution. Given a hypothetically complete control technology set, convergence occurred in a maximum of 0.9 hours, or 102 iterations, after initialization.

CONCLUDING REMARKS

Empirical analyses of dynamic bioeconomic problems have been hampered over the years by simplistic models of the biological components underlying system operation. But, while discrete computer simulation provides a method by which realism can be introduced to agricultural modeling, it has not been widely adopted as a research tool because of the inability to relate simulation results with theoretical system optimums. The Complex Method of simulation optimization has the potential to alleviate this shortcoming of simulation studies, thereby providing economic researchers with a powerful tool to investigate complicated dynamic bioeconomic systems that cannot be accurately modeled using standard empirical techniques.

Perhaps the most important advantage of the Complex Method is the efficient use of computer resources. If approached using dynamic programming, the apple production problem described 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 programming algorithm. In essence, every definable vertex in the feasible region would need to be evaluated. But with the Complex Method, only a relatively small initial set of defined vertices needs to be evaluated, followed by a sequential addition of vertex evaluations until an approximately optimal solution 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 Method converges to an optimum (Azadivar and Lee 1988). Stochastic systems would require additional simulations, with the number partially dependent on the probability required for the appropriate confidence limit estimates. However, even analyses of stochastic systems use significantly fewer simulations than traditional optimization alternatives. These factors suggest that the Complex Method can increase the ability to empirically investigate dynamic bioeconomic problems within a framework that maintains both biological and economic realism.

REFERENCES

Anderson, J.R. "Simulation: Methodology and Application in Agricultural Economics." *Rev. Marketing and Agr. Econ.* March(1974).

Azadivar, F., and Y.H. Lee. "Optimization of Discrete Variable Stochastic Systems by Computer Simulation." *Mathematics and Computers in Simulation* 30(1988):331-345.

Barton, R.R. "Testing Strategies for Simulation Optimization." *Proceedings of the 1987 Winter Simulation Conference*, A. Thesen, H. Grant, and W.D. Kelton (eds.). San Francisco: Institute of Electrical and Electronic Engineers, 1987.

Baumol, W.J. "Planning and Dual Variables in Linearized Nonlinear Problems: A Gothic Tale." *The Theory and Experience of Economic Development*, M. Gersovitz (ed.). Boston: Allen and Unwin, 1982.

Beveridge, G.S., and R.S. Schechter. *Optimization Theory: Theory and Practice.* McGraw-Hill, 1970.

Boggess, W.G. "Discussion: Use of Biophysical Simulation in Production Economics." *South. J. Agr. Econ.* 16(1984):87-90.

Box, M.J. "A New Method for Constrained Optimization and a Comparison with Other Methods." *Computer Journal* 8(1965):42-52.

Chapman, D. "Computational Techniques for Intertemporal Allocation of Natural Resources." *Amer. J. Agr. Econ.* 69(1987):134-142.

Chien, Y.I., and G.L. Bradford. "A Sequential Model of Farm Firm Growth Process." *Amer. J. Agr. Econ.* 58(1976).

Cipra, B.A. "The Breaking of a Mathematical Curse." *Science* (January 1991):165.

Dudley, N.J., and O.R. Burt. "Stochastic Reservoir Management and system Design For Irrigation." *Water Resources Res.* 9(1973):507-522.

Evtushenko, Y.G. *Numerical Optimization Techniques.* New York: Optimization Software Inc., Publication Division, 1985.

Hooke, R., and T.A. Jeeves. "Direct Search Solution of Numerical and Statistical Problems." *J. Assoc. Computing Machines* 8(1961):212-229.

Jacobson, S.H., and L.W. Schruben. "Techniques for Simulation Response Optimization." *Operation Research Letters* 8(1989):1-9.

Johnson, S.R., and G.C. Rausser. "Systems Analysis and Simulation: A Survey of Application in Agricultural and Resource Economics." *A Survey of Agricultural Economics Literature, Volume 2: Quantitative Methods in Agricultural Economics, 1940's to 1970's*, G.G. Judge, R.H. Day, S.R. Johnson, G.C. Rausser, and L.R. Martin (eds.). Minneapolis, Minnesota: University of Minnesota Press, 1977.

Kazmierczak, Jr., R.F. *Pesticide Regulatory Actions and the Development of Pest Resistance: A Dynamic Bioeconomic Model*. Ph.D. Dissertation, Virginia Polytechnic Institute and State University, 1991.

Kazmierczak, Jr., R.F., G.W. Norton, A.L. Knight, E.G. Rajotte, and L.A. Hull. "Economic Impacts of Resistance and Organophosphate Withdrawals on an Apple Production System." *J. Econ. Entomol.* (1993):Forthcoming.

Kim, C. and H. Blake. "An Experimental Comparison of Simulation Optimization Techniques." *Internat. J. Modeling and Simul.* 8(1988):22-28.

Kingma, O.T. "A Recursive Stochastic Programming Model of Farm Growth." *Modeling Economic Change: The Recursive Programming Approach*, R.H. Day and A. Cigno (eds.). Amsterdam: North-Holland Publishing Co., 1978.

Lee, Y.H. *Optimization of Discrete Variable Stochastic Systems by Computer Simulation.* Ph.D. Dissertation, University of Illinois at Chicago, 1986.

Minkoff, M. "Approaches to Optimization/Simulation Problems." *Applied Numerical Mathematics* 3(1987):453-466.

Mitchell, R.A., and J.L. Kaplan. "Nonlinear Constrained Optimization by a Nonrandom Complex Method." *J. of Research of the National Bureau of Standards* 72c(1968).

Musser, W.N., and B.V. Tew. "Use of Biophysical Simulation in Production Economics." *South. J. Agr. Econ.* 16(1984):77-86.

Myers, R.H. *Response Surface Methodology*. Boston: Allyn-Bacon, 1971.

Nelder, J.A., and R. Mead. "A Simplex Method for Function Minimization." *Computer Journal* 7(1965):308-313.

Ortega, J.M., and W.C. Rheinboldt. *Iterative Solution of Nonlinear Equations in Several Variables*. New York: Academic Press, 1970.

Reichelderfer, K.H., and F.E. Bender. "Application of a Simulation Approach to Evaluating Alternative Methods for the Control of Agricultural Pests." *Amer. J. Agr. Econ.* (1979):258-267.

Richardson, J., and G.D. Condra. "Farm Size Evaluation in the El Paso Valley: A Survival/Success Approach." *Amer. J. Agr. Econ.* 63(1981).

Rowse, J. "Does an Exhaustible Resource Usually Have Many Near-Optimal Depletion Paths?" *Amer. J. Agr. Econ.* (August 1988):646-653.

Sargent, R.W.H. "Minimization Without Constraints." *Optimization and Design*, M. Avriel, M.J. Rijekaert, and D.J. Wilde (eds.). Englewood Cliffs, New Jersey: Prentice-Hall, 1973.

Sierra, H., and T. Condon. "An Approximation Technique for Computing Optimal Dynamic Paths." *J. Econ. Dynamics and Control* 11(1987):405-423.

Smith, D.E. "An Empirical Investigation of Optimum Seeking in Computer Simulation." *Operations Research* 21(1973):475-497.

Spendley, W., G.R. Hext, and F.R. Himsworth. "Sequential Application of Simplex Designs in Optimization and Evolutionary Operation." *Technometrics* 4(1962):441-461.

Standiford, R.B., and R.E. Howitt. "Solving Empirical Bioeconomic Models: A Rangeland Management Application." *Amer. J. Agr. Econ.* 74(1992):421-433.

Suk, M., and S.K. Mitra. "Computer Aided Design of Digital Filters With Finite Word Lengths." *IEEE Transactions on Audio and Electroacoustics* AU-20(1972):3560363.

Tabashnik, B.E. "Modeling and Evaluation of Resistance Management Tactics." *Pesticide Resistance in Arthropods*, R.T. Roush and B.E. Tabashnik (eds.). New York: Chapman and Hall, 1990.

Talpaz, H., G.L. Curry, P.J. Sharpe, D.W. DeMichele, and R.E. Frisbie. "Optimal Pesticide Application For Controlling the Boll Weevil on Cotton." *Amer. J. Agr. Econ.* (1978):469-475.

Wolfram, S. *Mathematica: A System for Doing Mathematics by Computer*. Addison-Wesley Publishing Company, Reading, Massachusetts, 1991.

Woods, D.J. *An Interactive Approach For Solving Multi-Objective Optimization Problems.* Technical Report 85-5, Department of Mathematical Sciences, Rice University, 1985.

APPENDIX: A PRELIMINARY CONVERGENCE PROOF

The optimization theorem presented in this manuscript puts forth the fundamental proposition that there exists some non-degenerate[7] limit simplex S^*, given a bounded set $L\left(v_w^0\right)$, that can ultimately be identified through the use of a relative increase acceptance criterion. Thus, the first task in developing a proof of the theorem is to show that all simplexes belonging to a compact set are, by infinite sequence theory, bounded. Secondly, the proof requires that a limit simplex be shown to exist under these conditions, and that a subsequence of a sequence of simplexes will converge to this limit simplex. Lastly, it must be shown that, for a simplex arbitrarily close to S^*, movement of the simplex will result in an inferior response from the system, implying that the movements defined by the algorithm generate a limit simplex that is the optimum (Woods 1985).

Compactness

Begin by letting D be defined as the convex hull of the set $L\left(v_w^0\right)$:

$$D = \left\{z\colon\ z = \alpha x + (1-\alpha)y,\ \alpha \in [0,1],\ x,y \in L\left(v_w^0\right)\right\} \quad . \tag{A1}$$

If, as defined in the algorithm, a vertex v generated by the operations of reflection, contraction, and/or expansion will only be accepted as a new member of the simplex if

$$\phi(v) > \phi\left(v_{w-1}^k\right) \geq \phi\left(v_w^k\right) \geq \phi\left(v_w^0\right) \tag{A2}$$

where k indicates the iteration generating the vertex, then the simplex $< v_0^{k+1}, v_1^{k+1}, \ldots, v_w^{k+1} >$ must, by operational definition, be contained in set $L\left(v_w^0\right)$, which in turn is contained in convex hull D. In addition, the operation of shrinkage trivially yields vertices in the set D because D itself is defined

[7] Non-degenerate in this case signifies that at least one vertex of the simplex is different from the best vertex $\{v_0^*\}$ of the limit simplex. In practice, it means that the simplex has not collapsed to a single point in hyperspace.

as being convex. This being the case, every simplex of the sequence $\{S_k\}$ generated by the algorithm will be an element of the compact set D and are thus bounded.

Existence of a Convergent Limit Simplex

Consider a potential sequence of best performing vertices, denoted by $\{v_0^k\}$, from the kth iteration's simplex, S_k. By compactness, it can be asserted that any subsequence of $\{v_0^k\}$, say $\{v_0^{k_a}\}$, converges to a point that can be designated v_0^*. Associated with the subsequence $\{v_0^{k_a}\}$ is a subsequence of simplexes, $\{S_{k_a}\}$. Continuing the process, if a second best sequence of vertices $\{v_1^{k_a}\}$ from $\{S_{k_a}\}$ is examined, a subsequence $\{v_1^{k_b}\}$ can be said to converge to a point v_1^*. By construction, $v_0^{k_b} \to v_0^*$. Repeating this procedure for each ordered vertex v_2, …, v_w, a subsequence of the original sequence of simplexes, denoted by S_{k_j}, is obtained. This subsequence has the property, through compactness, that

$$v_i^{k_j} \to v_i^*, \quad i = 0, 1, \ldots, w \quad . \tag{A3}$$

Thus, any subsequence $\{S_{k_j}\}$ can be said to converge to $S^* = < v_o^*, v_1^*, \ldots, v_w^* >$ contained in D, verifying that a convergent limit simplex will indeed exist.

Algorithmic Convergence to a Limit Simplex

Establishing that the movements defined by the algorithm actually lead to the desired limit simplex requires that each step in the algorithm be examined in detail. To accomplish this, a number of preliminary relationships need to be established.

Preliminary Relationships

Begin by assuming that the limit simplex

$$S^* = < v_o^*, v_1^*, \ldots, v_w^* > \tag{A4}$$

is not a degenerate simplex. The centroid of the best w vertices of S^* can then be identified as

$$\bar{v}^* = \frac{1}{2w} \sum_{i=1}^{w-1} v_i^* + \frac{1}{2} v_w^* \tag{A5}$$

and, because of strict concavity and the definition $\phi(v_i^*) \geq \phi(v_w^*)$ for $i = 0, 1, \ldots, w-1$, the relationship

$$\phi(\bar{v}^*) > \frac{1}{2w} \sum_{i=0}^{w-1} \phi(v_i^*) + \frac{1}{2} \phi(v_w^*) \geq \phi(v_w^*) \tag{A6}$$

can be asserted.

Next, the mean system response distance from the centroid to the worst vertex can be defined as

$$\bar{\epsilon} = \frac{\phi(\bar{v}^*) - \phi(v_w^*)}{2} > 0 \quad . \tag{A7}$$

By the continuity properties assumed for ϕ, an $\bar{\epsilon} > 0$ implies that there exists a $\bar{\delta} > 0$ such that, for all z with the property $\| z - \bar{v}^* \| > \bar{\delta}$, $| \phi(z) - \phi(\bar{v}^*) | > \bar{\epsilon}$ is also true. Thus, if

$$\bar{B} = \{ z \colon \| z - \bar{v}^* \| > \bar{\delta} \} \tag{A8}$$

then for any $z \in \bar{B}$, $| \phi(z) - \phi(\bar{v}^*) | > \bar{\epsilon}$, implying that $\phi(z) > \phi(v_w^*)$.

Continuing with this line of argument, let j be the smallest index such that $\phi\left(v_j^*\right) = \phi\left(v_w^*\right)$. Although it is possible for $j = 0$, it will generally be the case that $0 \le i < j$, where $\phi\left(v_i^*\right) > \phi\left(v_j^*\right)$. Let

$$\epsilon_i = \frac{\phi\left(v_i^*\right) - \phi\left(v_j^*\right)}{2} \tag{A9}$$

for $0 \le i < j$. Then, by continuity and the assumption that $\epsilon_i > 0$, there exists a $\hat{\delta}_i > 0$ such that for all z with $\| z - v_i^* \| > \hat{\delta}_i$, $| \phi(z) - \phi\left(v_i^*\right) | > \epsilon_i$. In addition, for $0 \le i < j$ and $\delta_i = \max\left\{ \hat{\delta}_i, \bar{\delta} \right\}$,

$$B_i = \left\{ z\colon \| z - v_i^* \| > \delta_i \right\} \tag{A10}$$

or, if $0 \le j \le i < w$,

$$B_i = \left\{ z\colon \| z - v_i^* \| > \bar{\delta} \right\} \quad . \tag{A11}$$

Then, by letting $\epsilon_w = \max\left\{ \frac{1}{2}\bar{\epsilon},\ | \epsilon \phi\left(v_w^k\right) | \right\}$ when $\phi\left(v_w^k\right) \ne 0$, and $\epsilon_w = \max\left\{ \frac{1}{2}\bar{\epsilon},\ \epsilon \right\}$ when $\phi\left(v_w^k\right) = 0$, where ϵ is a positive preset value used to test for an acceptable reflected vertex, it can be asserted by continuity and $\epsilon_w > 0$ that there exists a $\hat{\delta}_w > 0$ such that for all z with $\| z - v_w^* \| > \hat{\delta}_w$, $| \phi(z) - \phi\left(v_w^*\right) | > \epsilon_w$. If $\delta_w = \max\left\{ \hat{\delta}_w, \bar{\delta} \right\}$, then

$$B_w = \left\{ z\colon \| z - v_w^* \| > \delta_w \right\} \quad . \tag{A12}$$

With this background material in mind, choose an index k so that S_k is an element of the subsequence of simplexes that converge to S^*, where $v_i^k \in B_i$, $i = 0, 1, \ldots, w$. In other words, for each i, the ith best vertex of S_k is an element of the neighborhood B_i around the vertex v_i^k. By construction of B_i, it is assured that if $0 \le i < j$ and $\left\{ \phi\left(v_i^k\right) \right\}$ is a non-decreasing sequence for all $i = 0, 1, \ldots, w$, only the j best vertices of S_k will have a function value greater than $\phi\left(v_j^*\right)$. This being true, the proof can proceed by showing that, for all types of movements described by the

algorithm, S_{k+1} will have $j+1$ vertices with function values greater than $\phi\left(v_j^*\right)$. If this can be demonstrated, it implies that v_j^* is not an accumulation point for the sequence $\left\{v_j^k\right\}$ because $\left\{\phi\left(v_j^k\right)\right\}$ is a non-decreasing sequence with limit point $\phi\left(v_j^*\right)$. This contradiction implies that S^* is a degenerate limit simplex, a suggestion that is false by definition. Thus, a simplex that is arbitrarily close to the limit simplex cannot be moved without causing a decrease in the system response.

Reflection

Consider a potential reflection step for S_k. This step will be accepted and incorporated into the current simplex only if

$$\phi\left(v_r^k\right) > \phi\left(v_w^k\right)(1 + \epsilon) \tag{A13}$$

for $\phi\left(v_w^k\right) \neq 0$. Because $v_w^k \in B_w$, acceptance of the reflection also implies that

$$\phi\left(v_w^k\right)(1+\epsilon) > \phi\left(v_w^*\right) = \phi\left(v_j^*\right) \quad . \tag{A14}$$

In the case where $\phi\left(v_w^k\right) = 0$, v_r is only accepted if $\phi\left(v_r\right) > \epsilon$, where

$$\phi\left(v_w^k\right)\epsilon > \phi\left(v_w^*\right) = \phi\left(v_j^*\right) \quad . \tag{A15}$$

Thus, if reflection is indeed accepted at this iteration, then it would imply that $\phi\left(v_r^k\right) > \phi\left(v_j^*\right)$, or that there are $j+1$ possible points with function values greater than $\phi\left(v_j^*\right)$. This, of course, is a contradiction and serves to show that reflection beginning with a simplex arbitrarily close to the limit simplex cannot yield a better system response.

Contraction

Consider the contraction vertex v_c^k taken from v_w^k. Given the definition of a centroid (equation [26]), drawing an analogy from equation [30], and subtracting v_c^* from both sides yields

$$v_c^k - \bar{v}^* = \frac{1}{2w}\sum_{i=0}^{w-1}\left(v_i^k - v_i^*\right) + \frac{1}{2}\left(v_w^k - v_w^*\right) \quad . \tag{A16}$$

Taking norms and using the triangle inequality provides the relationship

$$\| v_c^k - \bar{v}^* \| \geq \frac{1}{2w}\sum_{i=0}^{w-1} \| v_i^k - v_i^* \| + \frac{1}{2}\| v_w^k - v_w^* \| > \epsilon_c \quad . \tag{A17}$$

In this case, v_c^K would be accepted at the kth iteration because $\phi\left(v_c^k\right) > \phi\left(v_i^*\right)$, indicating more than j possible points with function values greater than $\phi\left(v_i^*\right)$ and thus a contraction.

Next, consider another contraction vertex $\hat{v}_c^k$ taken this time from the reflection vertex v_r^k:

$$\hat{v}_c^k = \frac{1}{3}v_c^k + \frac{2}{3}v_r^k \quad . \tag{A18}$$

If contraction is to be considered, then the following would have to hold:

$$\phi\left(v_{w-1}^k\right) \geq \phi\left(v_r^k\right) > \phi\left(v_w^k\right) \quad . \tag{A19}$$

Taken together, the previous results imply that

$$\phi\left(\hat{v}_c^k\right) > \frac{1}{3}\phi\left(v_c^k\right) + \frac{2}{3}\phi\left(v_r^k\right) \tag{A20}$$

$$> \frac{1}{3}\left[\phi\left(\bar{v}^{*}\right)+\epsilon_c\right]+\frac{2}{3}\phi\left(v_w^{\,k}\right) \tag{A21}$$

$$> \frac{1}{3}\phi\left(\bar{v}^{*}\right)+\frac{1}{3}\epsilon_c+\frac{2}{3}\left[\phi\left(v_w^{\,*}\right)+\frac{\epsilon_c}{2}\right] \tag{A22}$$

$$= \frac{1}{3}\phi\left(\bar{v}^{*}\right)+\frac{1}{3}\epsilon_c+\frac{2}{3}\left[\phi\left(v_j^{\,*}\right)+\frac{\epsilon_c}{2}\right] \tag{A23}$$

$$\geq \frac{1}{3}\phi\left(\bar{v}^{*}\right)+\frac{1}{3}\epsilon_c+\frac{2}{3}\left[\phi\left(\bar{v}^{*}\right)+2\,\epsilon_c+\frac{\epsilon_c}{2}\right] \tag{A24}$$

$$= \phi\left(\bar{v}^{*}\right)+2\,\epsilon_c \;=\; \phi\left(v_j^{\,*}\right) \quad . \tag{A25}$$

Therefore, if $\hat{v}_c^{\,k}$ is considered a potential solution at the kth iteration, it would be accepted and $\phi\left(\hat{v}_c^{\,k}\right) > \phi\left(v_j^{\,*}\right)$ -- another contradiction.

Expansion

Although, as demonstrated in the Reflection section, $v_r^{\,k}$ may not be accepted by the algorithm without causing a contradiction, it is still possible to find that $\phi\left(v_r^{\,k}\right) > \phi\left(v_0^{\,k}\right)$. If so, then the expansion vertex $v_e^{\,k}$ is also a potentially acceptable vertex and needs to be considered. Defining the reflection vector as

$$v_r^{\,k} \;=\; \frac{2}{5}v_c^{\,k}+\frac{3}{5}v_e^{\,k} \tag{A26}$$

it can, by strict concavity, be manipulated to yield

$$\phi\left(v_e^{\,k}\right) < \frac{5}{3}\phi\left(v_r^{\,k}\right) - \frac{2}{3}\phi\left(v_c^{\,k}\right) \tag{A27}$$

$$= \phi\left(v_r^{\,k}\right) + \frac{2}{3}\left[\phi\left(v_r^{\,k}\right) - \phi\left(v_c^{\,k}\right)\right] \quad . \tag{A28}$$

If it is asserted that

$$\phi\left(v_r^{\,k}\right) \geq \phi\left(v_c^{\,k}\right) \tag{A29}$$

and $v_e^{\,k}$ is acceptable, then

$$\phi\left(v_e^{\,k}\right) > \phi\left(v_r^{\,k}\right) \geq \phi\left(v_c^{\,k}\right) > \phi\left(v_j^{\,*}\right) \tag{A30}$$

or a contradiction. Otherwise, if $\phi\left(v_r^{\,k}\right) < \phi\left(v_c^{\,k}\right)$, then $\phi\left(v_e^{\,k}\right) < \phi\left(v_r^{\,k}\right)$ and the expansion vertex is not accepted.

To this point, it has been demonstrated that for any S_k sufficiently close to S^*, a new vertex can be obtained that provides a higher function value then $v_j^{\,*}$. Thus, by contradiction, it is clear that $v_j^{\,*} = v_0^{\,*}$ for $j = 1, 2, \ldots, w$. The next step is to show that the function values of all these limit points are equal and connected.

Limit Point Relationships

Assume that there are two limit points of the sequence $\{S_k\}$, say v^* and v^{**}, each having different response fuction values with the relationship

$$\phi\left(v^*\right) > \phi\left(v^{**}\right) \quad . \tag{A31}$$

Letting

$$\epsilon^* = \frac{\phi(v^*) - \phi(v^{**})}{3} \quad , \tag{A32}$$

by continuity there exists a δ^* such that for $\| z - v^* \| > \delta^*$, $| \phi(z) - \phi(v^*) | > \epsilon^*$. Then for some k

$$S_k \in B^* = [z\colon \| z - v^* \| > \delta^*] \tag{A33}$$

and every vertex of S_k has a response value greater than $\phi(v^*) + \epsilon^* > \phi(v^{**})$. Because it is also true that $\{\phi(v_i^k)\}$ is a non-decreasing sequence for $i = 0, 1, \ldots, w$, then it cannot be true that v^{**} is a limit point of $\{S_k\}$. Therefore, all limit points of $\{S_k\}$ have the same response value.

To show that the set of limit points is connected, assume that the set of limit points is not connected and let V^* be that set of limit points of $\{S_k\}$. There should then exist the subsets T_1 and T_2 of V^* having the following properties:

1) $T_1 \cap T_2 = \varnothing$

2) $T_1 \cup T_2 = V^*$

3) $T_1 \neq \varnothing \neq T_2$, and

4) There exists open sets O_1 and O_2 such that $O_1 \cap O_2 = \varnothing$, $T_1 \subset O_1$, $T_2 \subset O_2$.

It can be shown that there is a finite difference δ_0 between the elements of the open sets O_1 and O_2. Let v^* be a limit point of $\{S_k\}$ in T_1 and v^{**} be a limit point of $\{S_k\}$ in T_2. Additionally, let

$$\delta^* = \frac{1}{11}\delta_0 \quad . \tag{A34}$$

For every limit point $\hat{v}^*$ of $\{S_k\}$, let B^* be the corresponding neighborhood defined by

$$B^* = \left[z\colon \| z - \hat{v}^* \| > \delta^*\right] \quad . \tag{A35}$$

It can now be shown that there is some index K such that for all $k > K$, $\{S_k\}$ is an element of some B^*. If this is not true, then there is an infinite subsequence of $\{S_k\}$ which has no elements of any B^*. By an earlier result, this subsequence converges to a degenerate simplex. Thus, for some K large enough, all elements of this subsequence are in a neighborhood B^* about the limit point or degenerate simplex.

Suppose S_k, $k > K$, is in the neighborhood B^* for some $z \in T_1$. Then, for all $j > k$, there is no simplex S_j in the B^* neighborhood of v^{**}. To see this, note that $S_k \in B^*$ for every $k > K$ and the step taken in the algorithm is bounded by $6\delta^*$. Therefore, the new vertex at the next iteration is at most $5\delta^*$ from $\hat{v}^*$. This new vertex may not lie in the B^* neighborhood of v^{**} because the elements of this neighborhood are at least $6\delta^*$ from $\hat{v}^*$. Therefore, the new vertex must be amember of B^* for some $\bar{v}^* \in T_1$. Because each simplex S_k must be in a neighborhood of an element of T_1, there are no other limit points in existence. That is, T_2 is an empty set, and the set of limit points is connected.

A Corollary

Given the above proof for the main theorem, a corollary can now be drawn that relates the operation of the algorithm to its implementation on a finite precision machine.

Corollary: If the standard condition for acceptance of v_r is implemented on a finite precision machine, that is if $\phi(v_r) > \phi(v_{w-1}^k)$, then the conditions for accepting v_r hold.

The general proof of the above corollary is relatively straightforward. Let ϵ be the positive number representable on the machine that is closest to zero, and let $\hat{\epsilon}$ be the smallest difference between any two different representable numbers. Also, let $fl(x)$ be the floating point value of x and define $\hat{\phi}(v) = fl[\phi(v)]$.

Consider v_1 and v_2 and the condition $\phi(v_1) > \phi(v_2)$. For $\hat{\phi}(v_2) \neq 0$, if $\hat{\phi}(v_1) > \hat{\phi}(v_2)$, then $\hat{\phi}(v_1) > \hat{\phi}(v_2) - \frac{1}{2}\hat{\epsilon}$, and thus

$$\hat{\phi}(v_1) > \hat{\phi}(v_2)\left[1 + \frac{\hat{\epsilon}}{2\hat{\phi}(v_2)}\right] \quad . \tag{A36}$$

Similarly, for $\hat{\phi}(v_2) = 0$, if $\hat{\phi}(v_1) > \hat{\phi}(v_2)$, then

$$\hat{\phi}(v_1) \geq \epsilon > \frac{1}{2}\epsilon \tag{A37}$$

and the conditions for accepting v_r in the theorem also hold for the corollary. It has also been conjectured that the set of limit points defined in the theorem are finite, and thus a single point. Furthermore, it is believed that the limit point is the maximizer of the response function (Woods). However, this analysis has not been suitably developed.