Use of Evolutionary Algorithms and Simulated Annealing to Optimize a Herd Dynamics Model

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Abstract The systems analysis and modelling of agricultural enterprises remains a developing discipline, with many real-world applications. Different methodologies and approaches are available, with each having advantages and better performance when applied to particular types of problems. These are outlined with examples. For the optimization of higher-dimensional general models, studies show that only the more recent methods of evolutionary algorithms (such as genetic algorithms) and simulated annealing (including its extension to simulated quenching) can be recommended. An economic case study using a large and difficult beef herd dynamics model, over a ten-year horizon, reveals that the superior searching capabilities of genetic algorithms generally resulted in this method identifying better solutions than simulated annealing, and achieving these using less computing time.

1. INTRODUCTION

The application of systems methodology and simulation modelling to agricultural areas is a growing discipline. Typically, an agricultural system (ranging, for example, from national industry systems down to whole or sub-farm enterprises) is modelled mathematically to arrive at a valid representation of the system under study. This model can then be investigated far more thoroughly, efficient and quickly than can the original system. In particular, the effects of the various input parameters of the system (such as a farm's management options) on relevant outputs (eg, economic gross margin) can be trialed, and the model used to identify the best strategies [Thornton and McGregor 1988]. As the size and complexity of the modelled enterprise grows, the task of identifying the system's economic optimum becomes increasingly more difficult. Even 20 years ago, the literature in this area of agricultural modelling was 'so vast as to preclude a comprehensive survey' [Day 1977], and since this time numerous textbooks and journals such as *Agricultural Systems* have continued reporting such studies.

Faced with this depth and diversity of applications, this paper focuses on the more difficult field of optimizing higher-dimensional models of these systems. The 'curse of dimensionality' causes most problems here - as the complexity and number of dimensions of these systems increase, so to a greater extent does the problem of finding the global optimum [Meadows and Robinson 1985]. These real-world problems typically present difficulties not evident in case studies on mathematical test functions. A simulation model cannot be differentiated to estimate the slope and curvature of the response surface. Also, these surfaces can range from smooth through to discontinuous, with the latter occurring when the system is over-utilized to the point where it 'crashes' (both biologically and economically). One frequent problem is the existence of multiple optima - high, low, or intermediate levels of management can all produce economic outcomes which may be locally optimal, but may or may not be comparable with each other. A successful optimization method needs to be able to search across the full range of all available options.

The following section outlines literature studies in the area of model optimization, identifying the more promising techniques. Sections 3 and 4 respectively introduce and solve the challenging case study of a herd dynamics model, and in section 5 general conclusions comparing methods are drawn.

2. OPTIMIZING MODELS OF AGRICULTURAL SYSTEMS

Applications of simulation modelling to agricultural systems can be divided into two main types. The first covers the broad field of mathematical programming, including linear, integer, quadratic and nonlinear programming methods. Here, the system under investigation is represented by a framework of mathematical equations and constraints which are conducive to solution, by a range of mathematical methods. These have been used for large-scale allocation studies [Pratt et al. 1986], the scheduling of irrigation applications [Botes et al. 1996], and the optimization of spatial and temporal harvesting schedules in forestry systems [Roise 1990], [Lockwood and Moore 1993]. However, the complex and heterogenous nature of many real-world systems can require more modelling detail than allowed by these methods [Fu 1994], and they have trouble dealing with nonlinear behaviour and interactions between variables

[Gabbert et al. 1991]. A horticultural allocation problem using linear and dynamic programming [Annevelink 1992] was found to be too computationally intensive for practical use, and a genetic algorithm was preferred. Mathematical programming methods are also prone to converging to local optima (rather than the targeted global optimum), as found with nonlinear programming of groundwater remediation strategies [Kuo et al. 1992], and sequential quadratic programming of chemical engineering processes [Messine et al. 1996].

The second class of optimization methods involves the separate steps of system simulation, followed by model optimization. For many systems, this 'simulate and search' process is more flexible and realistic than mathematical programming [Botes et al. 1996]. The simulation phase allows the development and refinement of the model until a realistic fit with the real world is achieved, and enhancements may be incorporated as necessary. When finished, the simulation model becomes an optimization problem. For simpler models, complete evaluation or factorial designs can be used to identify the optimum [Mayer et al. 1994], however this becomes infeasible with even moderately-sized problems. Given that many management decisions (eg., irrigation, fertilizer, supplements) may be required to within the nearest 2% of their full range, a small 6-dimensional problem can have a total of around 10^{10} discrete combinations of management options. This defines the search-space of the problem. Given its likely size, targeted and efficient optimization routines are required. Random search techniques do not fit this description, and perform poorly by comparison [Corona et al. 1987], [Syswerda 1991]. The more modern and efficient algorithms are rapidly gaining acceptance. For example, of the 21 papers in the 'Metaheuristics in Combinatorial Optimization' issue of the *Annals of Operations Research* [Laporte and Osman 1997], tabu search was used on 8, 6 applied simulated annealing, and 5 used genetic algorithms. The general methods used in the practical optimization of models include -

Gradient-type Methods - These include hill-climbing, conjugate-gradient, quasi-Newton, and a range of other algorithm types. In general, they operate by estimating the gradient and curvature of the response surface at the current point, and then jumping to the estimated location of the optimum for the next iteration [Fletcher 1987]. Originally developed to track the optimum of smooth, unimodal functions, these methods have serious shortcomings when applied to real-world systems. They do not adapt well to variable, fractal, or discontinuous surfaces [Polyak 1987]. However, a major problem is their inability to escape from the basins of attraction around local optima. Once in such a region, these methods tend to converge to the local optimum, rather than searching more widely and finding the global optimum. On a dairy farm model with 14 interacting dimensions, the quasi-Newton algorithm repeatedly converged to local optima, often far inferior (economically) to the best solution found [Mayer et al. 1991]. In the optimization of forestry schemes, Powell's method of conjugate directions was used successfully on problems with up to 200 separate stands [Roise 1990], and this was suggested as the approximate maximum size solvable by this method.

Direct Search Methods - These somewhat dated methods use only the model values in a geometric search pattern. Direct search algorithms include the simplex [Nelder and Mead 1965] and its extensions (such as the complex algorithm), and some more recent adaptations [Torczon 1991]. Generally viewed as inferior to other methods [Fletcher 1987], in practice they have proved valuable in the solution of real-world engineering systems [Karr 1991]. On a dairying model, the simplex performed better than a gradient method [Mayer et al. 1991], although it was subsequently found to be inferior to the more modern optimization algorithms [Mayer et al. 1996]. The simplex was also used to optimize irrigation scheduling for a crop growth model [Botes et al. 1996], in preference to linear programming.

Evolutionary Algorithms - This field of methods includes genetic algorithms [Davis 1991] which were developed throughout the 1980s, the more recent evolutionary strategies [Bäck and Schwefel 1993] and evolutionary programming, and their combined developments and hybrids, such as the breeder genetic algorithm [Mühlenbein and Schlierkamp-Voosen 1994]. All these methods are based on the processes of natural selection, with the input options of the modelled system mathematically defined as 'genes' [Davis 1991]. The 'fittest' (most profitable) trial solutions are selected for cross-breeding and mutation, to eventually produce the optimal combination of traits. Genetic algorithms tend to use a binary representation of genes, and include crossover as one of the key operations. On the other hand, evolutionary strategies use real-number representation, and rely primarily on mutation strategies to produce better 'offspring'. Keane [1996] conducted a comparative study of these two classes using difficult test functions, having high dimensionality, multiple optima, and discontinuities. Results indicated similar performance between the evolutionary algorithms tested, with all being superior to simulated annealing, which was also tested. Evolutionary algorithms have been applied to a wide range of real-world problems [South et al. 1993]. A genetic algorithm was used to solve a horticultural allocation problem which had proved intractable under mathematical programming [Annevelink 1992]. It was also successful in the calibration of catchment runoff parameters [Wang 1991], where the more traditional methods (gradient and direct search) failed. On a dairy farming model, genetic algorithms converged to the global optimum in 10 % of the runs, with an overall average performance of 99.7 % of the global optimum [Mayer et al. 1996].

Simulated Annealing - This algorithm models the annealing (cooling) process in metallurgy, where metals gradually settle into a minimal-energy state [Kirkpatrick et al. 1983]. By allowing steps to less successful solutions in the search space, it has the important property of being able to escape from regions around local optima. Whilst there is no guarantee that the global optimum will ultimately be identified [Ingber 1993], simulated annealing usually achieves this by searching slowly and thoroughly.

A number of improvements have been made to the original method [Ingber 1989], [Ingber 1996b] with a view to improving the rate of convergence. Its 'greedy' extension to simulated quenching [Ingber 1996b], whereby the rate of cooling is increased, has in some practical applications proved successful, but is yet to be widely tested. Simulated annealing identified the global optimum of a groundwater model, whilst gradient methods repeatedly converged to local optima [Kuo et al. 1992]. In models of forestry scheduling, systems with up to 27,500 stands of trees were solved by simulated annealing [Lockwood and Moore 1993], which is far larger than the limit suggested in gradient method studies above. On a dairy farming model, simulated annealing identified the global optimum in all runs [Mayer et al. 1996], whilst the direct-search and hill-climbing methods performing poorly.

Tabu Search - This method is more a metastrategy which can be used with other optimization methods [Cvijovic and Klinowski 1995]. This approach marks previously-visited locations of the search-space as being 'tabu', and thus forces the search away and into new regions [Glover et al. 1993]. This generally allows the method to escape from areas around local optima. Tabu search has seen wide use in the field of combinatorial optimization, including spatial and temporal scheduling, sequencing, patterning, and planning studies. Usually combined with hill-climbing methods, tabu search has also been used with simulated annealing [Fox 1993], [Osman 1993] and genetic algorithms [Fox 1993]. However, whilst these types of problems may have large numbers of nodes or items to allocate, they typically only have a low degree of dimensionality. Given simulation models with a higher number of independent dimensions, it is too easy for the search method to 'slide' into alternate dimensions and stay near a local minima. The curse of dimensionality again applies - to force the method away from even small basins of attraction, excessively long tabu lists must be maintained. For this reason, tabu search has rarely been used on higher-dimensional models. It was shown to be unsuccessful when used in combination with simulated quenching [Mayer et al. 1995], actually resulting in an increase in time to convergence.

Comparative Performance - On mathematical test functions, which tend to be smooth and of lower dimensionality (less than 10), results are varied - examples are reported where each of the above classes of methods appear superior to others. The more recent techniques of genetic algorithms, simulated annealing and simulated quenching tend to outperform the others in models of real-world systems, including agricultural models [Mayer et al. 1995], [Mayer et al. 1996]. For simulation models with up to 10 dimensions, simulated annealing appears superior to genetic algorithms [Bramlette and Cusic 1989], [Bramlette and Bouchard 1991]. At 16 dimensions they perform similarly [Mayer et al. 1995], [Mayer et al. 1996], with still a slight edge to simulated annealing. In models with 20 to 30 dimensions, genetic algorithms appear more successful [Powell et al. 1991], [Syswerda 1991], with this result also holding on a test function of 30 dimensions [Ingber and Rosen 1992].

3. HERD DYNAMICS PROBLEM

The model used to test simulated annealing and genetic algorithms was DYNAMA, a PC-based commercial herd dynamics package [Holmes 1995]. This simulates the outcomes of decisions made by beef property managers - in particular, the effects over time of changes in calving rates, purchasing decisions, selling ages and rates, and culling policies. Under the full set, there are 40 independent options to be trialed, resulting in a 40-dimensional search-space. A 'restricted' problem can also be formulated, where half these are set to supposedly near-optimal values, giving 20 dimensions. In practice these management decisions tend to be highly dependent on each other, resulting in a high degree of interaction in the outcomes. Thus, this is a challenging problem for optimization methods, in terms of both size and complexity of the response surface.

The single-property nature of DYNAMA was extended spatially by translating its definitions and relationships into a Fortran-77 version on networked Sun workstations, and test runs verified against the original package. For each of the 14 regions defined in the Northern Australian Beef Producers' Survey [O'Rourke et al. 1992], typical farm structures (in terms of size, variable and fixed costs, animal prices, age and sex balances of the animals, and mortality and conception rates) were estimated to best match the survey and other available data. The Brigalow region, which had the largest number of survey respondents (619), was used as the test case, taking the 'average farm set-up' from this region. The outcome value to be optimized was taken as the discounted before-tax net income over a 10-year horizon. To correctly evaluate the effect of herd improvements, the discounted closing value of the herd was added to this, and the opening value subtracted. All input parameters being optimized were constrained to biologically-determined limits, eg., annual sales of each cohort of animals must be between 0 and 100 % inclusive. To remove any scale-dependencies amongst the variables [Fletcher 1987], all input parameters were then re-scaled in the range 0-1, and the outcome value scaled to around one at the global optimum. The overall stocking pressure and annual management options were set to be constant over time, hence only the best 'steady-state' solution was estimated. Simulations

Table 1. Average performance (% of global optimum) of genetic algorithm evaluations

Selection Criteria	Score-based		Ranks-based	
Mutation Rate	0.001	0.01	0.001	0.01
Average optimum identified (%)	99.999	99.948	99.752	99.339

Table 2. Average performance (% of global optimum) of simulated annealing optimizations

Annealing Temperature	Quenching Factor 0.5	1 (= annealing)	2	5
1e-5	96.60	98.61	99.94	99.78
1e-7	99.72	99.63	99.98	96.34

of the best strategies for dynamic problems, such as going into, or coming out of, a drought remain to be investigated.

A range of 'free-ware' optimization algorithms are available on the Internet. The two C-codes we downloaded were selected because of their authors' reputations in the scientific literature. Version 13.8 of Adaptive Simulated Annealing [Ingber 1996a], and version 5.0 of GENESIS, a genetic algorithm [Grefenstette 1990] were cross-compiled with the object code of the herd dynamics routine. These were subjected to repeated runs using different random starting values. These runs provided both replicates for these stochastic methods, and tests of alternate values to the defaults for some of their operational parameters. The correct implementation of these programs was verified by checking the reported optimum against the original version.

4. RESULTS AND DISCUSSION

Restricted model (20 dimensions) - This problem had a search-space in practical terms of the order of 10^{50}. This is a daunting task, when one considers that even a million years of processing on our currently fastest Sun workstation would only result in around 10^{15} model evaluations. To effectively search this space, each method was allowed runs of up to two million individual model evaluations, which in some cases ran for two days. For the genetic algorithm, previous studies [South et al. 1993], [Mayer et al. 1996] suggested best results from use of floating-point representation, Grey coding, elitism, non-overlapping generations, and a cross-over rate of 0.6, these also being the defaults in GENESIS [Grefenstette 1990]. For the remaining three key operational parameters, a factorial structure (with different random starting values) was tested - 2 population sizes (30 and 50) by 2 mutation rates (0.001 and 0.01) by 2 selection criteria (rank-based and score-based). Based on these results, a double-precision genetic algorithm was run for twice as long, which identified an optimum of only 0.001 % better. Expressing all results as a percentage of this best value (now taken as the global optimum), these were subjected to factorial analysis of variance. This showed population size to have no effect, and Table 1 lists the average performance for combinations of the other factors.

Most of these genetic algorithm runs converged to the identified optimum comparatively early, at an average of 143 thousand model evaluations. This indicates that at this stage, most of the individuals in the populations are genetically similar, so no further progress can be made by cross-breeding. Advances are only possible via the random nature of mutation. Whilst the higher mutation rate (0.01) increased this probability, it also appeared to interfere with the efficiency of breeding, arriving at lower optima whilst taking 52 % longer to get there.

With simulated annealing, the enhancements and operational parameters suggested for large problems [Ingber 1996a] were adopted. Simulated quenching is also recommended for such systems, despite its increased probability of failure [Ingber 1996b]. In practice, quenching has proved successful [Mayer et al. 1995], with the best results achieved at quenching levels of around half the problem's dimensionality. However, initial runs on this problem using quenching factors of 20, 15 and 10 produced notably inferior results. From this, it was decided that slow, thorough annealing was required for this difficult problem, including also quenching at 0.5 to provide even slower cooling than true annealing (which occurs at a quenching factor of one). Annealing temperature is also a key parameter in controlling the cooling schedule, so in addition to the ASA default of 10^{-5}, a lower value (10^{-7}) was also trialed. For each combination of these parameters, three random replicates were run, with their average performance (as previously defined) listed in Table 2. The best individual run (at a temperature of 10^{-7} and quenching factor of one) did converge to the global optimum, but most results fell short of this. Three optimizations using a higher temperature (10^{-4}) averaged only 94 % of the this best value, so these ranges were discarded from further consideration.

Overall, the simulated annealing optimizations were slower to converge to their respective optima, with an average of 341 thousand model evaluations. This was related to the degree of quenching, with lower values averaging up to 607 thousand evaluations per optimization. Also notable was the overall low acceptance rate of 0.5 %, meaning the majority of model evaluations were rejected by the method.

Full model (40 dimensions) - By doubling the number of dimensions, the difficulty is increased enormously - the methods are now faced with a search-space of the

Table 3. Optimizations of 40-dimensional herd dynamics model

Method	Operational parameters	Optimum identified ($A ,000)	Model evaluations at optimum (,000)
Simulated annealing	temperature = 10^{-5}, annealing	116.19	594
	temperature = 10^{-5}, quenching (2)	130.89	363
	temperature = 10^{-7}, annealing	141.37	945
	temperature = 10^{-7}, quenching (2)	146.10	817
Genetic algorithm	score-based, mutation rate = 0.001	152.28	222
	score-based, mutation rate = 0.01	152.25	934
	ranks-based, mutation rate = 0.001	152.20	1,996
	ranks-based, mutation rate = 0.01	152.07	1,934

order of 10^{100}. Week-long optimization runs using up to 8 million model evaluations per run are required, and even these could be insufficient in that better values may have been found if longer runs were used. Results of single optimizations for the genetic algorithm, and the average of two random replicates for simulated annealing, are listed in Table 3.

It is evident from these tables that genetic algorithms are superior to simulated annealing on this problem, both in terms of optima found and speed of convergence. Whilst simulated annealing is thorough and safe on lower-dimensional problems, it does not appear to be able to adequately search the full space of larger models, and repeatedly converges to local optima as the temperature approaches 'freezing point' at the termination of each optimization. In contrast, the cross-mixing and searching nature of genetic algorithms consistently gives better results, especially when using score-based selection.

5. CONCLUSIONS

Whilst a range of methods exist for the optimization of multi-dimensional models, many will only work well in limited situations. For the more difficult real-world problems, a range of practical applications indicate the general superiority of genetic algorithms and simulated annealing or quenching over other methods. Between the former, genetic algorithms perform comparatively better as the number of dimensions of the problem increases.

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