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Jesús Marín
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SFI WORKING PAPER: 1998-11-108

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Macroevolutionary Algorithms: a New Optimization Method on Fitness Landscapes

Jesús Marín¹,² and Ricard V. Solé²,³

(1) Departament de Llenguatges i Sistemes Informàtics
Universitat Politècnica de Catalunya, Campus Nord, Mòdul C5
08034 Barcelona (Spain)
(2) Complex Systems Research Group
Departament of Physics, FEN, Campus Nord, Mòdul B4
08034 Barcelona (Spain)
(3) Santa Fe Institute
Hyde Park Road 1399, New Mexico 87501, USA

Abstract

In this paper we introduce a new approach to optimization problems based on a previous theoretical work on extinction patterns in macroevolution. We name them Macroevolutionary Algorithms (MA). Unlike population-level evolution, which is employed in standard genetic algorithms, evolution at the level of higher taxa is used as the underlying metaphor. The model exploits the presence of links between "species" which represent candidate solutions to the optimization problem. In order to test its effectiveness, we compare the performance of MAs versus genetic algorithms (GA) with tournament selection. The method is shown to be a good alternative to standard GAs, showing a fast monotonous search over the solution space even for very small population sizes. A mean field theoretical approach is presented, showing that the basic dynamics of MAs is close to an ecological model of multispecies competition.

Index Terms: Evolutionary computation, genetic algorithms, macroevolution, emergent computation.

Submitted to IEEE Transactions on Evolutionary Computation
1 Introduction

Evolutionary computation [2] comprises techniques that have been inspired in biological mechanisms of evolution to develop strategies for solving optimization problems [8]. The search takes place often on a rugged landscape which is a geometric representation of the optimality of all possible solutions [7]. Populations of individuals (candidate solution to a given problem) evolve using operators inspired in the theory of evolution by natural selection.

In genetic algorithms (GA) [4, 3, 7] populations are formed by a constant number of individuals $N$ described by $B$-bit sequences. From a given population at a given generation, the next generation is obtained by applying the selection operator followed by the crossover operator and the mutation operator. In standard GA, the selection operator chooses individuals with a probability proportional to its fitness, but this can sometimes lead to premature convergence. In this sense, the selection operator strongly constrains the convergence velocity of evolutionary algorithms. To avoid these problems, other operators as rank selection or tournament selection can be used [7]. Next, pairs of individuals are randomly combined with a crossover probability $p_c$ by randomly choosing the crossover point. Finally, each bit of each individual is mutated with a mutation probability $p_m$ [7].

As a result of their simplicity and flexibility, GA's can be applied to a large set of combinatorial optimization problems with a large space of candidate solutions, although the intrinsic metastability which characterizes their dynamics has been only recently understood in theoretical terms [14]. In optimization problems with several local extrema, the GA's are widely used because of its general purpose to find a good approximation. However, instead of the Darwinian, short-term evolutionary metaphor, a different time scale can be considered, the macroevolutionary one, where extinctions and diversification of species through internal interactions are at work. Large extinctions can generate coherent population responses very different from the slow, Darwinian dynamics of classical GA. Besides, the population of candidate solutions/species might be understood in terms of an ecological system with connections among different species, instead of just a number of independent entities with a given assigned fitness value.

In this paper, a simple model of macroevolution will be used as a starting point to solve global-extremization problems. Our method will be called macroevolutionary algorithm (MA) and it will be compared with GA through some statistical measures obtained from numerical experiments with seven standard multivalued functions. A theoretical approach to a specific (though relevant) case will be considered in order to understand the dynamics of this system. It will be shown that the basic mechanism involves competition among fitness peaks with an eventual symmetry.
breaking process if two peaks are identical or very close in fitness.

2 Model of Macroevolution

The biological model of macroevolution (MM) \([10,11]\) allows to simulate the dynamics of species extinction and diversification for large time scales \([11,12]\). The model used in our study is a network ecosystem where the dynamics is based only on the relation between species. The links between units/species are essential to determine the new state (alive or extinct) of each species at each generation. We can define the state of species \(i\) in the generation \(t\) as

\[
S_i(t) = \begin{cases} 
1 & \text{if state is "alive"} \\
0 & \text{if state is "extinct"}
\end{cases} (1)
\]

Moreover, the model considers that time is discretized in “generations” and that each generation is constituted by a set of \(P\) species where \(P\) is constant. The relationship between species is represented by a connectivity matrix \(W\), where each item \(W_{i,j}(t) \ (i,j \in \{1, \ldots, P\})\) measures the influence of species \(j\) on species \(i\) at \(t\) with a continuous value within the interval \([-1, +1]\) (in ecology, this influence is interpreted as the trophic relation between species). At the end of each generation, all extinct species will be replaced by the species. Briefly, each generation in the biological model consists on a set of steps (the rules) which will be translated to the MA model (see below):

1. **Random variation:** for each species \(i\), a connection \(W_{i,j}(t)\) is randomly chosen, and a new random value between -1 and 1 is assigned.

2. **Extinction:** the relation of each species with the rest of the population determines its survival coefficient \(h\) defined as

\[
h_i(t) = \sum_{j=1}^{P} W_{i,j}(t) (2)
\]

where \(t\) is the generation number. The species state in the next generation is synchronously updated:

\[
S_i(t + 1) = \begin{cases} 
1 & (\text{alive}) \text{ if } h_i(t) \geq 0 \\
0 & (\text{extinct}) \text{ otherwise}
\end{cases} (3)
\]

This step allows for the selection and extinction of species.
3. **Diversification**: we colonize vacant sites freed by extinct species with surviving species. Specifically, a colonizer \( c \) will be randomly chosen from the set of survivors. For all vacant sites (i.e., those such that \( S_k(t) = 0 \)) the new connections will be updated in this way:

\[
W_{k,j} = W_{c,j} + \eta_{k,j} \\
W_{j,k} = W_{j,c} + \eta_{j,k}
\]

where \( \eta \) is a small random variation and \( S_k(t+1) = 1 \).

This model was shown to reproduce most of the statistical features of macroevolution [11,12] and it provided a natural source for the decoupling between microevolution (i.e., those processes modeled by genetic algorithms involving selection and continuous adaptation) and macroevolution (i.e., those processes involving extinction and diversification) [12]. Because of the essentially different nature of this approximation, we could ask which kind of outcome would be expected from the application of this model to optimization problems. As we will see, the macroevolution model allows to construct a simple but powerful method of optimization which is able to outperform GAs in several relevant examples.

### 3 Macroevolutionary Algorithm

In this section we show how to map the previous model of extinction into a model of optimization. The new model will be called **macroevolutionary algorithm** (MA). Let us define the \( d \)-dimensional fitness function \( f \) as a multidimensional function that we want to maximize. Our objective is to find the best values for the \( d \)-dimensional vectors of our problem under consideration. Thus our individuals/species are now \( S_i \equiv p \in \Omega \subset \mathbb{R}^d \), i.e., \( d \)-dimensional objects constrained to a subspace \( \Omega \). In this context \( p \) will be a good approximation if \( \forall q : f(q) \leq f(p) + \epsilon \) where \( p \) and \( q \) are individuals and \( \epsilon > 0 \) is a given error threshold.

In this way each individual in MA is described by a \( d \)-input vector with fitness \( f \). The domains for these inputs describe the search space where our fitness function is nothing but a (more or less) rugged landscape.

As with GA, MA use a constant population size of \( P \) individuals evolving in time by successive updates of the given operators. The main idea is that our system will choose, through network interactions, which are the individuals to be eliminated so as to guarantee exploration by new individuals and exploitation of better solutions by further generations. To this purpose, it is essential to correctly establish a relationship between individuals. This is described by the following criteria:
(a) each individual gathers information about the rest of the population through the strength and sign of its couplings $W_{ij}$. Individuals with higher inputs $h_i$ will be favoured. Additionally, they must be able to outcompete other less-fit solutions.

(b) Some information concerning how close are two solutions in $\Omega$ is required (although this particular aspect is not strictly necessary). Close neighbors will typically share similar $f$-values and will cooperate. In this context, we can define the connection $W_{ij}$ as:

$$W_{ij} = \frac{f(p_i) - f(p_j)}{|p_i - p_j|}$$

where $p_i = (p_i^1, ..., p_i^d)$ are the input parameters of the $i$-th individual. The numerator is a consequence of our first criterion, while the second criterion is introduced in the denominator as a normalization factor that weights the relative distance among solutions.

Now we can define the most important ingredients that will be used in building the set of operators to be applied each generation:

1. **Selection operator:** it allows to calculate the surviving individuals through their relations, i.e. as a sum of penalties and benefits. The state of a given individual $S_i$ will be given by:

$$S_i(t + 1) = \begin{cases} 1 & \text{if } \sum_{j=1}^{N} W_{ij}(t) \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

where $t$ is generation number and $W_{ij} = W(p_i, p_j)$ is calculated according to (5). In the following this rule will be indicated as $S_i(t + 1) = \theta(h_i(t))$ where $\theta(z) = 1$ if $z \geq 0$ and zero otherwise. Additionally, if the distance $D_{ij}$ between two solutions is zero then we set $W_{ij}(D_{ij} = 0) = 0$.

2. **Colonization operator:** it allows to fill vacant sites freed by extinct individuals (that is, those such that $S_i = 0$). This operator is applied to each extinct individual in two ways. With a probability $\tau$, a totally new solution $p_n \in \Omega$ will be generated. Otherwise exploitation of surviving solutions takes place through colonization. For a given extinct solution $p_i$, we choose one of the surviving solutions, say $p_b$. Now the extinct solution will be "attracted" towards $p_b$.

Mathematically, a possible (but not unique) choice for this colonization of extinct solutions reads:

$$p_i(t + 1) = \begin{cases} p_b(t) + \rho \lambda (p_b(t) - p_i(t)) & \text{if } \xi > \tau \\ p_n & \text{if } \xi \leq \tau \end{cases}$$
where $\xi \in [0,1]$ is a random number, $\lambda \in [-1, +1]$ (both with uniform distribution) and $\rho$ and $\tau$ are given constants of our algorithm. So we can see that $\rho$ describes a maximum radius around surviving solutions and $\tau$ acts as a temperature.

Although all essential rules defining the MA have been presented, several improvements and additional rules have been explored. In particular, we can decrease $\tau$ with time as in simulated annealing [5,9,15] to get a good convergence. In this context, the "temperature" $\tau$, when lowered, provides a decrease in randomness which favours the exploitation around the best individual found. In order to lower $\tau$ in each generation, we can use a given decreasing function. In our analysis, we have used a linear relation:

$$\tau(t; G) = 1 - \frac{t}{G}$$

where $G$ is number of generations. The results of using this linear annealing procedure do not strongly differ from other choices of $\tau(t)$.

4 Mean-field theory

In this section we will introduce a qualitative approximation to the basic MA behavior, which is based on a competition process among the largest peaks, eventually followed by a symmetry-breaking phenomenon when the peaks are very similar.

To make our argument clear, let us assume the simplest case with two peaks with fitness $f_k^*, f_r^*$, located at two given points $p_k$ and $p_r$. For simplicity we will assume that $0 \leq f_k^*, f_r^* \leq 1$. A given number of solutions will be clustered around these peaks. Let us call $\Gamma_k$ and $\Gamma_r$ the sets of solutions around each peak, i.e. we will assume that if $p_a, p_b \in \Gamma_k$, then $f(p_a) \approx f(p_b) \approx f_k^*$. Let $D_{rk}$ the distance between these peaks, and let us assume that $f_k^* - f_r^* = \eta \geq 0$. Let $N^k(t)$ and $N^r(t)$ the number of solutions at each peak at a given step $t$.

The two operators act on each population around each peak. We can describe the time evolution of our system in terms of two steps:

$$N^k(t + 1) = D_{\mu, r} [E_{W_{ij}}(N^k(t))]$$

where $E$ and $D$ indicate extinction and diversification operators, respectively. Let us first introduce the extinction step. For the $\Gamma_k$ population we have:

$$N^k(t + 1/2) = E_{W_{ij}}(N^k(t)) = \sum_{i \in \Gamma_k} \theta(G_{ij}(p_i, p_j))$$
where we use the notation $G_\mu(p_i, p_j) = \sum_j W_{ij}$. So the final expression for the $\Gamma_k$ population is:

$$N_k(t + 1/2) = \sum_{i \in \Gamma_k} \theta \left[ \sum_{j \in \Gamma_k} \frac{\epsilon_{ij}}{\delta(\rho)} + \sum_{j \in \Gamma_r} G_\mu(p_i, p_j) \right]$$  \hfill (11)

And an equivalent expression can be derived for the second peak:

$$N^r(t + 1/2) = \sum_{i \in \Gamma_r} \theta \left[ \sum_{j \in \Gamma_r} \frac{\epsilon_{ij}}{\delta(\rho)} + \sum_{j \in \Gamma_k} G_\mu(p_i, p_j) \right]$$  \hfill (12)

where both populations have been explicitly separated. Here $\epsilon_{ij}$ indicates the distance between solutions in the same $z$-cluster. In our approximation, we assume that the $\Gamma_k$ set is formed by a closely related set of solutions, which are close inside a domain of size $\mu(\Gamma_k)$ and radius $\delta(\rho)$. This radius clearly depends in some simple way on rule (2). Here we just assume that $\delta$ is small (after the clustering process).

There are two terms in the previous equation which involve interactions among solutions in the same cluster and interactions among solutions of both clusters. We can assume that the first term is small compared with the cross-interaction term (i.e. we take $\epsilon_{ij} \approx 0$. This approximation will of course depend on the specific properties of the landscape but is reasonable in terms of our previous assumptions. Here we also assume that the number of random solutions generated by rule (2) (which will depend on $\tau$) is small and so we can approximate $N_k + N^r \approx P$.

A mean-field set of equations (i.e. a first approximation ignoring correlations) can be derived, first for the extinction operator. The basic equation for $N_k$ is:

$$N_k(t + 1/2) = N_k(1 - P[\theta(z) < 0])$$  \hfill (13)

and an equivalent expression for $N^r(t + 1/2)$. Now we can use the following (mean field) approximation:

$$\left\langle \theta(G_\mu(p_i, p_j)) \right\rangle_{\Gamma_z} \approx \frac{N^z(t)}{D_{r_k}} g_z(\eta)$$  \hfill (14)

where $z \equiv k, r$. The function $g_z(\eta)$ involves the specific response of each population to the difference in fitness between peaks and $D_{r_k}$ stands for the distance among maxima.
Figure 1: Vector field in the \((N^k, N^r)\)-space for the mean-field theory of the two-peak MA problem, as defined by equations (11-12). Here we use \(\eta = 0.5, \xi = 0.01, P = 1, D = 1, \tau = 0.01\). The system flows towards a single attractor \((P, 0)\) which is globally stable.

The following couple of nonlinear discrete maps is obtained:

\[
N^k(t + 1/2) = N^k(t) \left[1 - g_k(\eta) \frac{N^r(t)}{PD_{rk}}\right] \tag{15}
\]

\[
N^r(t + 1/2) = N^r(t) \left[1 - g_r(\eta) \frac{N^k(t)}{PD_{rk}}\right] \tag{16}
\]

Let us note that, strictly speaking, an additional equation for the \(N^n(t)\)-population (the one formed by randomly generated solutions) should also be included. Here we assume that it is very small and typically formed by low-fit individuals. The functions \(g_k(\eta)\) must fulfill some basic requirements. Several choices are possible (and all of them lead to the same basic results). The simplest one is: \(g_k(\eta) = \eta(f^*_k - \eta)\) and \(g_r(\eta) = \eta f^*_k\). The first \(g_k\)-function tells us that the \(\Gamma_r\)-population will have a negative effect on \(\Gamma_k\) proportionally to its fitness but also to the difference between peaks. As this difference increases, it is less likely for the smaller peak to have some harmful effect on \(\Gamma_k\). For simplicity, since all the dynamics depends on the difference between peaks, we will use \(f^*_k = 1\).
The next step in our analysis involves diversification. Following our previous approximations, it is not difficult to show that the equations for this second step read:

\[
N^k(t+1) = N^k(t + 1/2) + \Psi_k(P - N^k(t + 1/2) - N^r(t + 1/2))
\]

(17)

\[
N^r(t+1) = N^r(t + 1/2) + \Psi_r(P - N^r(t + 1/2) - N^r(t + 1/2))
\]

(18)

where the coefficients \(\Psi_z\) involve both the colonization of \(\Omega\) by the survivors towards the \(\Gamma_k\) domain, as well as the generation of new, random solutions. It is not difficult (although tedious) to show that these coefficients are: \(\Psi_k = \eta(1 - \tau) + \xi_k\tau\), \(\Psi_r = \eta(1 - \eta)(1 - \tau) + \xi_r\tau\). The second term in these quantities indicate the likelihood that a random solution falls into one of the \(\Gamma\) sets. Explicitly, \(\xi_z \equiv \mu(\Gamma_z) / \mu(\Omega)\), where \(\mu(z)\) is the measure (i.e. hypervolume) of each set.

After some algebra, using equations (15-18) and the continuous approximation \(N^z(t+1) - N^z(t) \approx dN^k/dt\), the full equations for the MA mean field dynamics are obtained:

\[
\frac{dN^k}{dt} = \Psi_k(P - N^r) + N^k(\Psi_k(\beta(2 - \eta)N^r - 1) - \beta(1 - \eta)N^r)
\]

(19)

\[
\frac{dN^r}{dt} = \Psi_r(P - N^k) + N^r(\Psi_r(\beta(2 - \eta)N^k - 1) - \beta(1 - \eta)N^k)
\]

(20)

where \(\beta = \eta / PD_{rk}\).

This dynamical system can be studied in terms of standard stability analysis [1]. It can be easily shown that the only fixed points here are \((P, 0)\) and \((0, P)\). It is worth mentioning that our model involves a competition process with is different from a standard Lotka-Volterra (LV) model of two-species competition [6]. The LV model is defined by two nonlinear differential equations \(dx/dt = \mu_1y(P - x - \beta_1y)\) and \(dy/dt = \mu_2y(P - y - \beta_2x)\), where \(x, y\) are the population sizes, \(\mu\) is the growth rate of each one and \(\beta_i > 0\) the competition coefficients. The LV model also involves the two so-called exclusion points \((P, 0)\) and \((0, P)\) but also two additional ones, \((0, 0)\) and \((x^* > 0, y^* > 0)\). The last one implies that coexistence among competitors can take place for some parameter combinations. In the model (19-20) no such coexistence can take place. This is important, as far as for optimization purposes no coexistence among different peaks is desired.

The Jacobi matrix \(J_{ij} = (\partial N^i/\partial N^j)\) for our model can be computed for the two fixed points and the eigenvalues are such that, for \(\eta > 0\), \(\lambda_\pm(P, 0) < 0\) and \(\lambda_\pm(0, P) > 0\), so a stable and an unstable node are associated to \((P, 0)\) and \((0, P)\) respectively. In fact it can be shown that \((P, 0)\) is globally stable, attracting all initial conditions towards \(\Gamma_r\) (figure 1).
Figure 2: Vector field in the $(N^k, N^r)$-space for the mean-field theory of the two-peak MA problem for the marginal problem $\eta = 0$ (two identical peaks). Here the system is described by a couple of linear equations (21-22) which lead to an infinite number of stable solutions, given by the line $N^r = 1 - N^k$ (see text).

A particular case is given by the $\eta=0$ case, where the same fitness is obtained for each peak. In terms of optimization, this is not a major problem, since we want to find the best solution. The vector field for this case is also shown in figure 2, where we can see that the trajectories converge to a full line given by $N^r = P - N^k$. This is what we could expect if we introduce $\eta = 0$ in the previous equations. This leads to a linear system of equations

\[
\frac{dN^k}{dt} = \xi_k \tau (P - N^r - N^k) 
\] (21)

\[
\frac{dN^r}{dt} = \xi_r \tau (P - N^r - N^k) 
\] (22)

which shows that, for the two-cluster problem with $N^n = 0$ the dynamics settles into a final state where a fraction of the population clusters around one peak and the other around the second. Numerical evidence shows, however, that this is not the case: symmetry-breaking (i. e. the choice among one of the two equal peaks) typically occurs: small fluctuations and the presence of random solutions eventually shifts the system towards one of the two peaks.
5 Numerical Results

A number of numerical experiments have been performed in order to study the behavior of MAs and their superiority in relation with standard genetic algorithms. Several functions have been used to this purpose, and are listed below\(^1\)

(1) Two 2-input (i.e. two-dimensional) functions (see figure 3) of the form

\[
f(x) = \sum_{i=1}^{m} \frac{a_i e^{e_i}}{e^{||x-P(i)||^2}}
\]  

(23)

The two specific examples are:
(a) A landscape \( f_1 \) with some local maxima of close heights where \( m = 10 \) and \( \bar{x} \in [0,100]^2 \) (see figure 1). The location of the maxima is given in the following table:

<table>
<thead>
<tr>
<th>( \bar{P}_i )</th>
<th>(35,85)</th>
<th>(75,75)</th>
<th>(25,30)</th>
<th>(45,45)</th>
<th>(80,55)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(65,55)</td>
<td>(25,65)</td>
<td>(85,15)</td>
<td>(90,90)</td>
<td>(70,10)</td>
<td></td>
</tr>
<tr>
<td>( a_i )</td>
<td>40</td>
<td>55</td>
<td>75</td>
<td>99</td>
<td>85</td>
</tr>
<tr>
<td>( e_i )</td>
<td>95</td>
<td>85</td>
<td>65</td>
<td>92</td>
<td>35</td>
</tr>
<tr>
<td>( \alpha_i )</td>
<td>35</td>
<td>30</td>
<td>45</td>
<td>55</td>
<td>60</td>
</tr>
<tr>
<td>( \beta_i )</td>
<td>20</td>
<td>70</td>
<td>40</td>
<td>40</td>
<td>55</td>
</tr>
</tbody>
</table>

(b) A landscape \( f_2 \) with infinite maxima around the global maximum where \( m = 2 \) and \( \bar{x} \in [0,100]^2 \) (figure 1, bottom). Now the table reads:

<table>
<thead>
<tr>
<th>( \bar{P}_i )</th>
<th>(50,50)</th>
<th>(50,50)</th>
<th>(50,50)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a_i )</td>
<td>750</td>
<td>-720</td>
<td>35</td>
</tr>
<tr>
<td>( e_i )</td>
<td>500</td>
<td>425</td>
<td>25</td>
</tr>
</tbody>
</table>

(2) In order to obtain a standard comparison with previous studies, we have also used several multivalued functions proposed in the contest held during the 1996 IEEE International Conference on Evolutionary Computation for real valued spaces containing five \( N \)-input functions:
(c) The sphere model where \( x_i \in [-5,5] \) with \( N = 10 \):

\[
f_3(\bar{x}) = -\sum_{i=1}^{N} (x_i - 1)^2
\]  

(24)

\(^1\)For all the numerical experiments, a Sun Ultra-1 workstations with SunOS operating system has been used
Figure 3: Landscape of two 2-input functions.
(d) Griewank’s function where $x_i \in [-600, 600]$ with $N = 10$:

$$f_4(\vec{x}) = -\frac{1}{4000} \sum_{i=1}^{N} (x_i - 100)^2 + \prod_{i=1}^{N} \cos \left( \frac{x_i - 100}{\sqrt{i}} \right) + 1 \quad (25)$$

(e) Shekel’s foxholes where $x_i \in [0, 10]$ with $N = 10$:

$$f_5(\vec{x}) = \sum_{i=1}^{N} \frac{1}{\|\vec{x} - A(i)\|^2 + c_i} \quad (26)$$

(f) Langerman’s function where $x_i \in [0, 10]$ with $N = 10$:

$$f_6(\vec{x}) = \sum_{i=1}^{N} c_i e^{\frac{1}{2}\|\vec{x} - A(i)\|^2} \cos(\pi \|\vec{x} - A(i)\|^2) \quad (27)$$

(g) Michalewicz’s function where $x_i \in [0, \pi]$ with $N = 10$:

$$f_7(\vec{x}) = \sum_{i=1}^{N} \sin(x_i) \sin^{20} \left( \frac{i x_i^2}{\pi} \right) \quad (28)$$

(h) Rotated Michalewicz’s function version where $x_i \in [0, \pi]$ with $N = 10$ and $\alpha = \frac{\pi}{4}$:

$$f_8(\vec{x}) = f_7(\text{Rotation}(\vec{x})) \quad (29)$$

where $\text{Rotation}$ means to perform $N - 1$ rotations of $\alpha$ radians centered at point $(\frac{\pi}{2}, \frac{\pi}{2}, \ldots, \frac{\pi}{2})$.

As a first approximation to numerically explore MAs behavior, we have represented (as points on the $\Omega$ domain) scores of local maxima and the population distribution at four different time steps for the 2-input functions $f_1$ and $f_2$ (see figures 4 and 5). The role of randomness is graphically shown with this 2D-representation: Initially, MA explores the input space looking for good individuals, which are clustered around local maxima (in the figures, stage with $t = 10$). Afterwards (see the plot at $t = 30$ and $t = 45$) competition between maxima takes place by attracting more individuals/solutions. Finally, at stage $t = 70$, it is expected that the global maximum wins because it captures all individuals.

In order to understand how the two parameters $\rho$ and $\tau$ influence MA behavior, three types of experiments were performed for $f_1$ and $f_2$ using equal population sizes for both functions ($P = 50$) over $G = 400$ generations and for $R = 50$ independent runs. Explicitly, we considered the following situations: (a) $\rho$ is varied using values in $[0, 1]$, while $\tau$ is fixed; (b) $\rho$ is varied using values in $[0, 1]$, and $\tau$ is varied using linear simulated annealing (according to (8)) and (c) $\tau$ is varied using values $[0, 1]$, while $\rho$ is
Figure 4: Four stages in the evolution of population applying MA to $f_1$ ($P = 50$, $G = 100$.) Each o indicates an individual represented in input space, $\Delta$ are local maxima.
Figure 5: Four stages in the evolution of population applying MA to \( f_2 \) \((P = 50, G = 100.)\) Each \( \circ \) indicates an individual represented in input space, \( \triangle \).
fixed. In order to quantify the differences, the following measures were used: (1) Mean of best fitness value reached; (2) Mean number of generations needed in order to reach a good fitness value ($98.0199$ for $f_1$, and $64.3500$ for $f_2$) and (3) Probability of success in reaching a good fitness value $f^*$, measured as the relative number of runs that have reached $f^*$.

The basic results of these experiments are summarized in figure 6. We can see that there is no well-defined optimum for neither $\tau$ nor $\rho$. Typically a wide range of parameter values gives similar results. These results allow us to reduce the number of parameters which should be tuned in our algorithm to just two: population size $P$ and number of generations $G$ to be calculated.

Actually, in most cases simulated annealing seems to be the best choice, being the specific $\rho$-value less important. For this reason, MA with linear simulated annealing will be used in our study. In all our simulations we will use $\rho = 0.5$. In figure (7) we compare MA with and without simulated annealing by measuring the mean fitness for all solutions in the population in each generation: for MA with simulated annealing (i.e. with reduced exploration in favour of exploitation) the mean tends monotonously to the optimum, while for $\tau$ constant, the population shows lower fitness values, close to GA results.

To further simplify the comparison between MA and GA, standard values of $p_c = 0.7$ and $p_m = 0.001$ for the genetic algorithm will be used (other reasonable choices gave equivalent statistical results). In the GA model, individuals are represented by a 32-bit sequence. Moreover, due to the fact that GA shows premature convergence for some functions, another selection operator, tournament selection [7] — (choosing the best of two random individuals with a probability of, say, 0.75) will be used.

A first comparison between GA and MA —with and without simulated annealing— is shown in figure (8) where single runs using the three methods are plotted. Here the left and right columns correspond to runs of the first and second examples of our list, respectively. These pictures shows that, while MA converges progressively with time, the GA tends to show considerable fluctuations.

In order to measure and compare their performance, several extensive simulation experiments were used (see figure 9) for $f_1$ and $f_2$ using different population sizes ($P \in [50, 400]$) over $G = 400$ generations and using $R = 50$ independent runs. The following measures were used:

(a) Mean of best fitness value reached after $R$ runs.
(b) Mean number of generations required to reach a good fitness value ($f^* = 98.0199$ for $f_1$, and $f^* = 64.3500$ for $f_2$).
(c) Probability of reaching a good fitness value.
(d) The time used (in clock ticks) to reach a good fitness value.

Many different simulation experiments were performed in order to compare the
Figure 6: Parameter behavior for the MA using $f_1$ (left) and $f_2$ (right). ($G = 400$, $P = 50$, $R = 50$.)
advantages of MA in relation with GA with tournament selection. The main results and conclusions from our simulations are:

1. Macroevolutionary algorithms reach higher fitness values than GAs for equal population sizes. The difference between both approaches decreases if \( P \) is large enough (simply due to fact that MA have already reached the optimum while GA continues exploring).

2. The probability of success in reaching a good fitness value along \( G \) generations in a typical run is higher in MA than in GA.

3. The time needed to reach the optimum using the same population size is lower in MA if the population size is small. But for large \( P \) (see figure 9), the time required in each iteration by MA can become larger than for GA (order \( P^2 \) vs \( P \)).

The asymptotic time difference is due to the selection operator, which is computationally more expensive. In standard GA, this operator chooses individuals with a probability proportional to their fitness in a time scale of order \( O(P \log P) \), but if tournament selection is used, it is only \( O(P) \). In contrast, MA involves a time scale of order \( O(P^2) \). For this reason, a comparison of these measures for both algorithms with equal populations \( P \) is not adequate. A possible alternative could be to apply a readjustment factor to \( P \) in terms of time cost. However the relevance of small values for \( P \) in the performance of MA makes the asymptotic comparison useless. However, if the distance between candidate solutions is removed from the definition of the couplings a considerable increase in MA performance is obtained, although
Figure 8: Best individual fitness in each generation for three runs using $f_1$ (left) and $f_2$ (right). ($G = 100$, $P = 100$ for GA and $P = 50$ for MA.)
Figure 9: Different measures according to population size for both Genetic and Macroevolutionary algorithms, for $f_1$ (left) and $f_2$ (right). ($P$ from 50 to 400 step 10, $G = 400$, $R = 50$.)
an extensive re-analysis of our results will be required in order to compare the two cases.

A different approximation can be used. We could be interested in faster but less accurate solutions, or in larger fitnesses but slower convergence. A good comparative criterion should allow us to explore this compromise between fitness values and the time needed to reach them. To this objective, several experiments have been performed —varying P and G for different sample sizes (R)— in which both the fitness of the best solution reached and time required are measured. These measures have been sorted and averaged over time, and the success probability calculated. The basic results of these simulations are summarized in the next table and in figures (10-12).

<table>
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These experiments shows that, for all the used test functions used —except Michalewicz's function f₇— the MA reaches better fitness values and has a higher success probability than GA. Michalewicz's function f₇ is a particular case where the geometric properties of the landscape favours GA. (However, a simple geometric transformation, like rotations of the function that keep the landscape shape, can strongly modify the GA performance).
Figure 10: Relation between fitness value reached, probability of success to reach a good fitness, and time required, applying GA and MA to $f_1$ (left) and $f_2$ (right).
Figure 11: Relation between fitness value reached and time needed, for GA and MA to $f_3$ to $f_5$ (from left to right, and top to bottom).
Figure 12: Relation between fitness value reached and time needed, applying GA and MA to $f_7$ (left) and $f_8$ (right).

6 Conclusions

In this paper we have introduced a novel optimization technique which we have called macroevolutionary algorithm. It is based in a simple procedure inspired in macroevolutionary responses of complex ecosystems to extinction events. In the original model extinctions removed some species and new ones were generated by diversification of the survivors. In the MA approach, the basic ecology-like structure is also preserved, but now applied to a set of candidate solutions to a given optimization problem on a fitness landscape. The survival of species/solutions is linked with the relative fitness as given by $f(x)$ in relation with all the other species. These differences define the strength of their couplings, weighted by their mutual distance in search space $\Omega$. If the total sum of input connections to a given species is positive, it survives. If negative, it disappears from the system. In this sense, the number of removed solutions is not fixed (as it happen to be the case for standard GA) but strongly dynamical. Sometimes, a large (mass-) extinction event takes place when a very good solution is found. The replacement process guarantees both the exploitation of the high-fit solutions as well as further, random exploration of other domains of the landscape. Because of the connection matrix, the whole population is able
to obtain a rather accurate map of the relative importance of the solutions being explored in the landscape.

There are two types of situations to be considered according to whether or not simulated annealing is used. The first case is appropriate when we want to find a good solution in a given number of generations and also guarantee that such solution is a local optimum within a given confidence. In this case, we should use the linear annealing to increase the exploitation over the last generations. In this way we guarantee that mass extinction will occur when all individuals have reached local optimum with. In the second case, when a constant value for $T$ is used, we keep the same exploration rate along time. This could be interesting when fitness is a time-varying function.

Moreover, other changes have been considered in the algorithm with no qualitative differences: (a) The colonizer $b$ can be chosen by the colonization operator with proportional fitness probability, instead of using just the best individual. Furthermore, we can add the possibility for each extinct individual to choose its own colonizer; (b) To use a different probability distribution (instead of the uniform one) to generate $\lambda$ in (7).

Numerical simulations have shown that MA typically outperform GA over a wide range of conditions. Together with a typically monotonous convergence, the interactions between individuals in MA (through the connection matrix $W_{ij}$) make exploration in input space much more satisfactory. Moreover, MA is being successfully applied to optimization problems that can be formulated in terms of an optimization function even if it is highly multi-modal or highly multi-dimensional. For example, MA can be successfully applied to learning in neural networks as a training algorithm and as a multi-dimensional scaling method. Following this approach, MA could be applied to combinational optimization problems, although the main difficulty is to express the problem in terms of relations between individuals. Further work should explore the efficiency of the MA in correlated/uncorrelated landscapes. The mean-field approximation to the simple two-peak problem shows that the best solution is always a global attractor of the dynamics. Due to (i) the antisymmetric nature of the connectivity matrix, (ii) the numerical observation that a peak-to-peak competition process takes place through the evolution and (iii) the monotonous change implicit in the competition dynamics, we conjecture that a general analytic treatment of MAs can be derived. A stochastic approach to this problem will be presented in a future paper [13].
Acknowledgments

The authors would like to thank Melanie Mitchell for useful comments and suggestions. Thanks also to Jordi Delgado, Ton Sales, Alberto García, and the members of Complex Systems Research Group in Barcelona. This work has been supported by a grant PB94-1195 and by the Santa Fe Institute (RVS).
References


