EVOLUTIONARY DYNAMICS OF EXTREMAL OPTIMIZATION

Stefan Böttcher

Physics Department, Emory University, Atlanta, GA 30322, U.S.A.

- Keywords: Extremal Optimization, Self-Organized Criticality, Evolution Strategies, Co-evolution and Collective Behavior, Spin Glasses.
- Abstract: Motivated by noise-driven cellular automata models of self-organized criticality (SOC), a new paradigm for the treatment of hard combinatorial optimization problems is proposed. An extremal selection process preferentially advances variables in a poor local state. The ensuing dynamic process creates broad fluctuations to explore energy landscapes widely, with frequent returns to near-optimal configurations. This *Extremal Optimization* heuristic is evaluated theoretically and numerically.

1 INTRODUCTION

Physical processes have inspired many optimization heuristics. Most famously, variants of simulated annealing (Kirkpatrick et al., 1983) and genetic algorithms (Goldberg, 1989) are widely used tools for the exploration of many intractable optimization problems. But the breadth and complexity of important real-life problems leaves plenty of room for alternatives to verify or improve results. One truly alternative approach is the *extremal optimization* (EO) method (Boettcher and Percus, 2001b). Basically, EO focuses on eliminating only extremely bad features of a solution while replacing them at random. Good solutions emerge dynamically in an intermittent process that explores the configuration space widely. This method may share the evolutionary paradigm with genetic algorithms, but assigns fitnesses to individual variables within a single configuration. Hence, it conducts a local search of configuration space similar to simulated annealing. But it was intentionally conceived to leave behind the certainties (and limitations) of statistical equilibrium, which depends on a temperature schedule, instead handing control (almost) entirely to the update dynamics itself. In fact, as a few simple model problems reveal, the extremal update dynamics generically leads to a sharp transition between an ergodic and a non-ergodic ("jammed") search regime (Boettcher and Grigni, 2002). Adjusting its only free parameter to the "ergodic edge," as predicted by theory, indeed leads to optimal performance in numerical experiments.

Although our understanding of EO is only at its beginning, some quite useful applications have already been devised that have demonstrated its efficiency on a variety of combinatorial (Boettcher and Percus, 1999; Boettcher and Percus, 2001a; Boettcher and Percus, 2004; Hoos and Stützle, 2004) and physical optimization problems (Boettcher and Percus, 2001b; Boettcher, 2003; Boettcher, 2005; Boettcher, 2009). Comparative studies with simulated annealing (Boettcher and Percus, 2000; Boettcher and Percus, 1999; Boettcher, 1999) and other Metropolis based heuristics (Dall and Sibani, 2001; Wang and Okabe, 2003; Wang, 2003; Boettcher and Sibani, 2005; Boettcher and Frank, 2006) have established EO as a successful alternative for the study of NPhard problems and its use has spread throughout the sciences. EO has found a large number of applications by other researchers, e. g. for polymer confirmation studies (Shmygelska, 2007; Mang and Zeng, 2008), pattern recognition (Meshoul and Batouche, 2002b; Meshoul and Batouche, 2002a; Meshoul and Batouche, 2003), signal filtering (Yom-Tov et al., 2001; Svenson, 2004), transport problems (de Sousa et al., 2004b), molecular dynamics simulations (Zhou et al., 2005), artificial intelligence (Menai and Batouche, 2002; Menai and Batouche, 2003b; Menai and Batouche, 2003a), modeling of social networks (Duch and Arenas, 2005; Danon et al., 2005; Neda et al., 2006), and 3d-spin glasses (Dall and Sibani, 2001; Onody and de Castro, 2003). Also, extensions (Middleton, 2004; Iwamatsu and Okabe, 2004; de Sousa et al., 2003; de Sousa et al., 2004a) and rigorous performance guarantees (Heilmann et al., 2004; Hoffmann et al., 2004) have been established. In (Hartmann and Rieger, 2004b) a thorough description of EO and extensive comparisons with other heuristics (such as simulated annealing, genetic algorithms, tabu search, etc) is provided, addressed more at computer scientists.

Here, we will apply EO to a spin glass model on a 3-regular random graph to elucidate some of its *dynamic* features as an evolutionary algorithm. These properties prove quite generic, leaving local search with EO free of tunable parameters. We discuss the theoretical underpinning of its behavior, which is reminiscent of Kauffman's suggestion (Kauffman and Johnsen, 1991) that evolution progresses most rapidly near the "edge of chaos," in this case characterized by a critical transition between a diffusive and a jammed phase.

2 MOTIVATION: MEMORY AND AVALANCHES IN CO-EVOLUTION

The study of driven, dissipative dynamics has provided a plausible view of many self-organizing processes ubiquitous in Nature (Bak, 1996). Most famously, the Abelian sandpile model (Bak et al., 1987) has been used to describe the statistics of earthquakes (Bak, 1996). Another variant is the Bak-Sneppen model (BS) (Bak and Sneppen, 1993), in which variables are updated sequentially based on a global threshold condition. It provides an explanation for broadly distributed extinction events (Raup, 1986) and the "missing link" problem (Gould and Eldredge, 1977). Complexity in these SOC models *emerges* purely from the dynamics, *without* tuning of parameters, as long as driving is slow and ensuing avalanches are fast.

In the BS, "species" are located on the sites of a lattice, and have an associated "fitness" value between 0 and 1. At each time step, the one species with the smallest value (poorest degree of adaptation) is selected for a random update, having its fitness replaced by a new value drawn randomly from a flat distribution on the interval [0, 1]. But the change in fitness of one species impacts the fitness of interrelated species. Therefore, all of the species at neighboring lattice sites have their fitness replaced with new random numbers as well. After a sufficient number of steps, the system reaches a highly correlated state known as *self-organized criticality* (SOC) (Bak et al., 1987). In that state, almost all species have reached a fitness above a certain threshold. These species, however, possess *punctuated equilibrium* (Gould and Eldredge, 1977): only ones weakened neighbor can undermine ones own fitness. This co-evolutionary activity gives rise to chain reactions called "avalanches", large fluctuations that rearrange major parts of the system, making any configuration accessible.

We have derived an exact *delay* equation (Boettcher and Paczuski, 1996) describing the spatiotemporal complexity of BS. The evolution of activity P(r,t) after a perturbation at (r = 0, t = 0),

$$\partial_t P(r,t) = \nabla_r^2 P(r,t) + \int_{t'=0}^t dt' V(t-t') P(r,t'), \quad (1)$$

with the kernel $V(t) \sim t^{-\gamma}$, has the solution $P(r,t) \sim \exp\{-C(r^D/t)^{\frac{1}{D-1}}\}$ with $D = 2/(\gamma - 1)$. Thus, it is the *memory* of all previous events that determines the current activity.

Although co-evolution may not have optimization as its exclusive goal, it serves as a powerful paradigm. We have used it as motivation for a new approach to approximate hard optimization problems (Boettcher and Percus, 2000; Boettcher and Percus, 2001b; Hartmann and Rieger, 2004a). The heuristic we have introduced, called *extremal optimization* (EO), follows the spirit of the BS, updating those variables which have among the (extreme) "worst" values in a solution and replacing them by random values without ever explicitly improving them. The resulting heuristic explores the configuration space Ω widely with frequent returns to near-optimal solutions, *without* tuning of parameters.

3 EXTREMAL OPTIMIZATION FOR SPIN GLASS GROUND STATES

Disordered spin systems on sparse random graphs have been investigated as mean-field models of spin glasses or combinatorial optimization problems (Percus et al., 2006), since variables are long-range connected yet have a small number of neighbors. Particularly simple are α -regular random graphs, where each vertex possesses a fixed number α of bonds to randomly selected other vertices. One can assign a spin variable $x_i \in \{-1, +1\}$ to each vertex, and random couplings $J_{i,j}$, either Gaussian or ± 1 , to existing bonds between neighboring vertices *i* and *j*, leading to competing constraints and "frustration" (Fischer and Hertz, 1991). We want to minimize the energy of the system, which is the difference between violated bonds and satisfied bonds,

$$H = -\sum_{\{bonds\}} J_{i,j} x_i x_j.$$
⁽²⁾

EO performs a local search (Hoos and Stützle, 2004) on an existing configuration of *n* variables by changing preferentially those of poor *local* arrangement. For example, in case of the spin glass model in Eq. (2), $\lambda_i = x_i \sum_j J_{i,j} x_j$ assesses the local "fitness" of variable x_i , where $H = -\sum_i \lambda_i$ represents the overall energy (or cost) to be minimized. EO simply *ranks* variables,

$$\lambda_{\Pi(1)} \le \lambda_{\Pi(2)} \le \ldots \le \lambda_{\Pi(n)},\tag{3}$$

where $\Pi(k) = i$ is the index for the *k*th-ranked variable x_i . Basic EO always selects the (extremal) lowest rank, k = 1, for an update. Instead, τ -EO selects the *k*th-ranked variable according to a scale-free probability distribution

$$P(k) \propto k^{-\tau}.$$
 (4)

The selected variable is updated *unconditionally*, and its fitness and that of its neighboring variables are reevaluated. This update is repeated as long as desired, where the unconditional update ensures significant fluctuations with sufficient incentive to return to near-optimal solutions due to selection *against* variables with poor fitness, for the right choice of τ . Clearly, for finite τ , EO never "freezes" into a single configuration; it is able to return an extensive list of the best of the configurations visited (or simply their cost) instead (Boettcher and Percus, 2004).

For $\tau = 0$, this " τ -EO" algorithm is simply a random walk through configuration space. Conversely, for $\tau \rightarrow \infty$, the process approaches a deterministic local search, only updating the lowest-ranked variable, and is likely to reach a dead end. However, for finite values of τ the choice of a *scale-free* distribution for P(k) in Eq. (4) ensures that no rank gets excluded from further evolution, while maintaining a clear bias against variables with bad fitness. As Sec. 5 will demonstrate, fixing

$$\tau - 1 \sim 1/\ln(n) \tag{5}$$

provides a simple, parameter-free strategy, activating avalanches of adaptation (Boettcher and Percus, 2000; Boettcher and Percus, 2001b).

4 EO DYNAMICS

Understanding the Dynamics of EO has proven a useful endeavor (Boettcher and Grigni, 2002; Boettcher

and Frank, 2006). Such insights have lead to the implementation of τ -EO described in Sec. 3. Treating τ -EO as an evolutionary process allows us to elucidate its capabilities and to make further refinements. Using simulations, we have analyzed the dynamic pattern of the τ -EO heuristic. As described in Sec. 3, we have implemented τ -EO for the spin glass with Gaussian bonds on a set of instances of 3-regular graphs of sizes n = 256, 512, and 1024, and run each instance for $T_{\rm run} = 20n^3$ update steps. As a function of τ , we measured the ensemble average of the lowest-found energy density $\langle e \rangle = \langle H \rangle / n$, the firstreturn time distribution $R(\Delta t)$ of update activity to any specific spin, and auto-correlations C(t) between two configurations separated by a time t in a single run. In Fig. 1, we show the plot of $\langle e \rangle$, which confirms the picture found numerically (Boettcher and Percus, 2001b; Boettcher and Percus, 2001a) and theoretically (Boettcher and Grigni, 2002) for τ -EO. The transition at $\tau = 1$ in Eq. (5) will be investigate further below and theoretically in Sec. 5. The worsening behavior for large τ has been shown theoretically in (Boettcher and Grigni, 2002) to originate with the fact that in any *finite*-time application, $T_{run} < \infty$, τ -EO becomes less likely to escape local minima for increasing τ and *n*. The combination of the purely diffusive search below $\tau = 1$ and the "jammed" state for large τ leads to Eq. (5), consistent with Fig. 1 and experiments in (Boettcher and Percus, 2001a; Boettcher and Percus, 2001b).

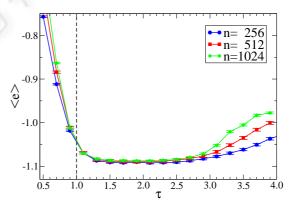


Figure 1: Plot of the average lowest energy density found with τ -EO over a fixed testbed of 3-regular graph instances of size *n* for varying τ . For $n \rightarrow \infty$, the results are near-optimal only in a narrowing range of τ just above $\tau = 1$. Below $\tau = 1$ results dramatically worsen, hinting at the phase transition in the search dynamics obtained in Sec. 5.

In Fig. 2 we show the first-return probability for select values of τ . It shows that τ -EO is a fractal renewal process for all $\tau > 1$, and for $\tau < 1$ it is a Poisson process: when variables are drawn according to

their "rank" k with probability P(k) in Eq. (3), one gets for the first-return time distribution

$$R(\Delta t) \sim -\frac{P(k)^3}{P'(k)} \sim \Delta t^{\frac{1}{\tau}-2}.$$
(6)

Neglecting correlations between variables, the number of updates of a variable of rank k is $\#(k) = T_{run}P(k)$. Then, the typical life-time is $\Delta t(k) \sim T_{run}/\#(k) = 1/P(k)$, which via $R(\Delta t)d\Delta t = P(k)dk$ immediately gives Eq. (6). The numerical results in Fig. 2 fit the prediction in Eq. (6) well. Note that the average life-time, and hence the memory preserved by each variable, *diverges* for all $\tau(> 1)$, limited only by T_{run} , a size-dependent cut-off, and is widest for $\tau \rightarrow 1^+$, where τ -EO performs optimal. This finding affirms the subtle relation between searching configuration space widely while preserving the memory of good solutions.

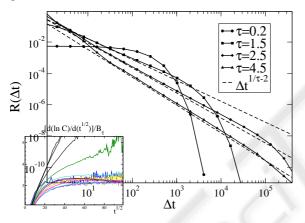


Figure 2: Plot of the first-return time distribution $R(\Delta t)$ for τ -EO for various τ and n = 256. Poissonian behavior for $\tau < 1$ develops into a power-law regime limited by a cut-off for $\tau > 1$. The power-law scaling closely follows Eq. (6) (dashed lines). Inset: Data collapse (except for $\tau \le 1$) of autocorrelations C(t) according to the stretched-exponential fit given in the text. From top to bottom, $\tau = 0.5, 0.7, \dots, 3.5$.

Interestingly, the auto-correlations between configurations shown in the inset of Fig. 2 appear to decay with a *stretched*-exponential tail, $C(t) \sim$ $\exp\{-B_{\tau}\sqrt{t}\}$ fitted with $B_{\tau} \approx 1.6 \exp\{-2.4\tau\}$, for all $\tau > 1$, characteristic of a super-cooled liquid (Fischer and Hertz, 1991) just *above* the glass transition temperature $T_g(>0$ in this model). While we have not been able to derive that result, it suggests that τ -EO, driven far from equilibrium, never "freezes" into a glassy ($T < T_g$) state, yet accesses T = 0 properties efficiently. Such correlations typically decay with an agonizingly anemic power-law (Fischer and Hertz, 1991) for local search of a complex energy landscape, entailing poor exploration and slow convergence.

5 THEORETICAL INVESTIGATIONS

Despite the general difficulty in predicting performance features for stochastic heuristics (Lundy and Mees, 1996; Aarts and van Laarhoven, 1987), we are able to theoretically extract a few non-trivial properties of τ -EO. We have studied a general model problem for which the asymptotic behavior of τ -EO can be solved exactly (Boettcher and Grigni, 2002; Boettcher and Frank, 2006). The model obtains Eq. (5) exactly in cases where the model develops a "jam" amongst its variables, a generic feature of frustrated systems.

To analyze the properties of the τ -EO update process, we have to access the fitness of individual variables. Our model (Boettcher and Grigni, 2002) consists of *n a priori* independent ("annealed") variables x_i , taking on one of, say, three fitness states, $\lambda_i = 0$, -1, or -2. At each point in time, respective fractions ρ_0 , ρ_1 , and ρ_2 of the variables occupy these states, where $\sum_{a} \rho_{a} = 1$. The optimal configuration is $\rho_{0} = 1$, $\rho_{1,2} = 0$ with a cost per variable of $C = -\sum_i \lambda_i / n =$ $\sum_{a=0}^{2} a \rho_a = 0$, according to Eq. (3). With this system, we can model the dynamics of a local search for hard problems by "designing" an interesting set of flow equations for $\rho(t)$ that can mimic a complex search space Ω with energetic and entropic barriers. In these flow equations, a transition matrix T_{ab} specifies what fraction of variables transitions in or out of a fitness state (a), given that a variable in a certain state (b) is updated. (This transition of a is conditioned by b, not necessarily between a and b!) The probabilities for the condition that a variable in ρ_b is updated, Q_b , can be derived *exactly* for local search,

$$\dot{\mathbf{p}}_a = \sum_b T_{ab} Q_b,\tag{7}$$

typically giving a highly non-linear dynamic system. For example, for τ -EO the vector **Q** depends exclusively on ρ , since for each update a variable is selected based only on its rank according to Eq. (5). When a rank $k(\leq n)$ has been chosen, a spin is randomly picked from state $0 \leq a \leq \alpha(= 2 \text{ here})$, if $k/n \leq \rho_{\alpha}$, from state $\alpha - 1$, if $\rho_{\alpha} < k/n \leq \rho_{\alpha} + \rho_{\alpha-1}$, and so on. We introduce a new, continuous variable x = k/n $(n \gg 1)$, and rewrite P(k) in Eq. (5) as

$$p(x) = \frac{\tau - 1}{n^{\tau - 1} - 1} x^{-\tau} \quad \left(\frac{1}{n} \le x \le 1\right), \tag{8}$$

where the maintenance of the low-*x* cut-off at 1/n will turn out to be crucial. Now, the average likelihood

that a spin in a given state is updated is given by

$$Q_{\alpha} = \int_{1/n}^{\rho_{\alpha}} p(x) dx = \frac{\rho_{\alpha}^{1-\tau} - n^{\tau-1}}{1 - n^{\tau-1}},$$

$$Q_{\alpha-1} = \int_{\rho_{\alpha}}^{\rho_{\alpha} + \rho_{\alpha-1}} p(x) dx$$

$$= \frac{(\rho_{\alpha-1} + \rho_{\alpha})^{1-\tau} - \rho_{\alpha}^{1-\tau}}{1 - n^{\tau-1}},$$

$$Q_{0} = \int_{1-\rho_{0}}^{1} p(x) dx = \frac{1 - (1 - \rho_{0})^{1-\tau}}{1 - n^{\tau-1}},$$
(9)

where in the last line the norm $\sum_i \rho_i = 1$ was used in both integration limits. These values of the *Q*'s completely describe the update preferences for τ -EO at arbitrary τ . In the case $\alpha = 2$, Eq. (10) gives

$$Q_0 = rac{1 - (1 -
ho_0)^{1 - au}}{1 - n^{ au - 1}}, \ Q_1 = rac{(
ho_1 +
ho_2)^{1 - au} -
ho_2^{1 - au}}{1 - n^{ au - 1}},$$

and $Q_2 = 1 - Q_0 - Q_1$. We can compare with *any* other local search heuristics, such as *simulated annealing* (SA) (Kirkpatrick et al., 1983) with temperature schedule $\beta = 1/T = \beta(t)$, where Metropolis-updates require (Boettcher and Grigni, 2002; Boettcher and Frank, 2006)

$$Q_a \propto \rho_a \min\left\{1, \exp\left[-\beta \sum_{b=0}^{\alpha} bT_{ba}\right]\right\},$$
 (10)

for $a = 0, 1, ..., \alpha$. Thus, with the *choice* of a specific model **T**, we could study any (dynamic or stationary) property of τ -EO as a function of τ and compare it to SA.

To demonstrate the use of these equations, we consider a (trivial) model with a constant matrix describing the transition of fractions of variables, $T_{ab} = [-\delta_{ab} + \delta_{(2+a \mod 3),b}]/n$, depicted on the left in Fig. 3. Here, variables in ρ_1 can only reach the lowest-energy state in ρ_0 by first jumping *up* in energy to ρ_2 . Using $\dot{\rho}_2 = -\dot{\rho}_0 - \dot{\rho}_1$, since $\rho_0 + \rho_1 + \rho_2 = 1$, Eq. (7) gives

$$\dot{\mathbf{p}}_0 = \frac{1}{n} \left(-Q_0 + Q_2 \right), \quad \dot{\mathbf{p}}_1 = \frac{1}{n} \left(Q_0 - Q_1 \right), \quad (11)$$

with **Q** in Eq. (10) for EO and for SA with

$$Q_0 = rac{
ho_0 e^{-eta}}{(1-e^{-eta})
ho_2 + e^{-eta}}, \ Q_1 = rac{
ho_1 e^{-eta}}{(1-e^{-eta})
ho_2 + e^{-eta}}.$$

The stationary solution, for $\dot{\rho} = 0$, yields $Q_0 = Q_1 = Q_2$, and gives for EO and SA:

$$\mathbf{EO}: \rho_0 = 1 - \left(\frac{n^{\tau - 1} + 2}{3}\right)^{\frac{1}{1 - \tau}}, \rho_2 = \left(\frac{2n^{\tau - 1} + 1}{3}\right)^{\frac{1}{1 - \tau}}$$

SA:
$$\rho_0 = \frac{1}{2 + e^{-\beta}}, \qquad \rho_2 = \frac{e^{-\beta}}{2 + e^{-\beta}}.$$
 (12)

and $\rho_1 = 1 - \rho_0 - \rho_2$. Therefore, SA reaches its best, albeit suboptimal, cost C = 1/2 > 0 at $\beta \to \infty$, due to the energetic barrier faced by the variables in ρ_1 . The result for EO is most remarkable (Boettcher and Grigni, 2002; Boettcher and Frank, 2006): For $n \to \infty$ at $\tau < 1$ EO remains suboptimal, but reaches the optimal cost *for all* $\tau > 1$! This transition at $\tau = 1$ separates an (ergodic) random walk phase with too much fluctuation, and a greedy-descent phase with too little fluctuation, which in real NP-hard problems would probably produce broken ergodicity (Bantilan and Palmer, 1981). This "ergodicity breaking" derives from the scale-free power-law in Eq. (5) (Boettcher and Percus, 2000).

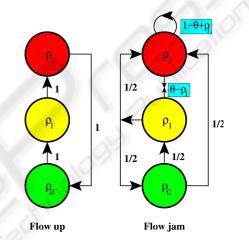


Figure 3: Plot of flow diagrams. In the diagram on the left, variables have to jump to higher energetic states first before they can attain the lowest state. The right diagram shows the model of a jam, where variables in the highest state can only traverse through the intermediate state to the lowest state, if the intermediate state moves its variables out of the way first to keep its density ρ_1 below the threshold θ .

Naturally, the range of phenomena found in a local search of NP-hard problems is not limited to energetic barriers. After all, so far we have only considered constant entries for $T_{i,j}$. In our next model we let **T** merely depend linearly on the ρ_i . Most of these cases reduce to the phenomena already discussed in the previous example. An entirely new effect arises in the case depicted on the right in Figure 3:

$$\dot{\rho}_{0} = \frac{1}{n} \left[-Q_{0} + \frac{1}{2}Q_{1} \right], \qquad (13)$$

$$\dot{\rho}_{1} = \frac{1}{n} \left[\frac{1}{2}Q_{0} - Q_{1} + (\theta - \rho_{1})Q_{2} \right].$$

Aside from the dependence of **T** on ρ_1 , we have also introduced the threshold parameter θ . The interesting regime is the case $0 < \theta < 1$, where further flow from state 2 into state 1 can be blocked for increasing ρ_1 , providing a negative feedback to the system. In effect, the model may exhibit a "jam" typical in glassy dynamics and in local search heuristics.

Eqs. (14) again have a unique fixed-point solution with $\tau = \infty$ being the most favorable value at which the minimal energy C = 0 is definitely reached. But it can be shown that the system has an ever harder time to reach that point, requiring typically $t = O(n^{\tau})$ update steps for a finite fraction of initial conditions. Thus, for a given finite computational time $t_{\rm max}$ the best results are obtained at some finite value of τ_{opt} . In that, this model provides a new feature – slow variables impeding the dynamics of faster ones (Palmer et al., 1984) - resembling the observed behavior for EO on real problems, e.g. the effect shown in Fig. 1. In particular, this model provides an analytically tractable picture for the relation between the value of τ_{opt} and the effective loss of ergodicity in the search conjectured in (Boettcher and Percus, 2000; Boettcher and Percus, 2001a).

For initial conditions that lead to a jam, $\rho_1(0) + \rho_2(0) > \theta$, we assume that

$$\rho_1(t) = \theta - \varepsilon(t) \tag{14}$$

with $\varepsilon \ll 1$ for $t \le t_{jam}$, where t_{jam} is the time at which ρ_2 becomes small and Eq. (14) *fails*. To determine t_{jam} , we apply Eq. (14) to the evolution equations in (14) and obtain after some calculation (Boettcher and Grigni, 2002)

$$t_{\rm jam} \sim n^{\tau},$$
 (15)

Further analysis shows that the average $\cot \langle C \rangle_{\tau}$ develops a minimum when $t_{\text{max}} \sim t_{\text{jam}}$ for $t_{\text{max}} > n$, so choosing $t_{\text{max}} = an$ leads directly to Eq. (5) for τ_{opt} . This sequence of minima in $\langle C \rangle(\tau)$ for increasing *n* is confirmed by the numerical simulations (with *a* = 100) shown in Fig. 1, with the correct *n*-dependence predicted by Eq. (5).

6 NUMERICAL RESULTS FOR EO

To gauge τ -EO's performance for larger 3*d*-lattices, we have run our implementation also on two instances, *toruspm*3-8-50 and *toruspm*3-15-50, with n = 512 and n = 3375, considered in the 7*th* DIMACS challenge for semi-definite problems¹. The best available bounds (thanks to F. Liers) established for the larger instance are $H_{\text{lower}} = -6138.02$ (from semidefinite programming) and $H_{\text{upper}} = -5831$ (from branch-and-cut). EO found $H_{\text{EO}} = -6049$ (or H/n = -1.7923), a significant improvement on the upper bound and already lower than $\lim_{n\to\infty} H/n \approx -1.786...$ found in (Boettcher and Percus, 2001b). Furthermore, we collected 10^5 such states, which roughly segregate into three clusters with a mutual Hamming distance of at least 100 distinct spins; though at best a small sample of the $\approx 10^{73}$ ground states expected (Hartmann, 2001)! For the smaller instance the bounds given are -922 and -912, while EO finds -916 (or H/n = -1.7891) and was terminated after finding 10^5 such states.

7 CONCLUSIONS

We have motivated the Extremal Optimization heuristic and reviewed briefly some of its previous applications. Using the example of Ising spin glasses, which is equivalent to combinatorial problems with constraint Boolean variables such as satisfiability or coloring, we have thoroughly described its implementation and analyzed its evolution, numerically and theoretically. The new paradigm of using the dynamics of extremal selection, i. e. merely eliminating the worst instead of freezing in the perceived good, is shown to yield a highly flexible and adaptive search routine that explores widely and builds up memory systematically. It is the dynamics more than any fine-tuning of parameters that determines its success. These results are largely independent of the specific implementation used here and beg for applications to other combinatorial problems in science and engineering.

ACKNOWLEDGEMENTS

I would like to thank M. Paczuski, A.G. Percus, and M. Grigni for their collaboration on many aspects of the work presented here. This work was supported under NSF grants DMR-0312510 and DMR-0812204 and the Emory University Research Committee.

REFERENCES

- Aarts, E. H. L. and van Laarhoven, P. J. M. (1987). Simulated Annealing: Theory and Applications. Reidel, Dordrecht.
- Bak, P. (1996). *How Nature works: The Science of Self-Organized Criticality.* Copernicus, New York.
- Bak, P. and Sneppen, K. (1993). Punctuated equilibrium and criticality in a simple model of evolution. *Phys. Rev. Lett.*, 71:4083–4086.

¹http://dimacs.rutgers.edu/Challenges/Seventh/

- Bak, P., Tang, C., and Wiesenfeld, K. (1987). Selforganized criticality: An explanation of the 1/f noise. *Phys. Rev. Lett.*, 59(4):381–384.
- Bantilan, F. T. and Palmer, R. G. (1981). Magnetic properties of a model spin glass and the failure of linear response theory. J. Phys. F: Metal Phys., 11:261–266.
- Boettcher, S. (1999). Extremal optimization and graph partitioning at the percolation threshold. *J. Math. Phys. A: Math. Gen.*, 32:5201–5211.
- Boettcher, S. (2003). Numerical results for ground states of mean-field spin glasses at low connectivities. *Phys. Rev. B*, 67:R060403.
- Boettcher, S. (2005). Extremal optimization for Sherrington-Kirkpatrick spin glasses. *Eur. Phys. J. B*, 46:501–505.
- Boettcher, S. (2009). Simulations of Energy Fluctuations in the Sherrington-Kirkpatrick Spin Glass. (submitted) arXiv:0906.1292.
- Boettcher, S. and Frank, M. (2006). Optimizing at the ergodic edge. *Physica A*, 367:220–230.
- Boettcher, S. and Grigni, M. (2002). Jamming model for the extremal optimization heuristic. *J. Phys. A: Math. Gen.*, 35:1109–1123.
- Boettcher, S. and Paczuski, M. (1996). Ultrametricity and memory in a solvable model of self-organized criticality. *Phys. Rev. E*, 54:1082.
- Boettcher, S. and Percus, A. G. (1999). Extremal optimization: Methods derived from co-evolution. In GECCO-99: Proceedings of the Genetic and Evolutionary Computation Conference, pages 825–832, Morgan Kaufmann, San Francisco.
- Boettcher, S. and Percus, A. G. (2000). Nature's way of optimizing. *Artificial Intelligence*, 119:275.
- Boettcher, S. and Percus, A. G. (2001a). Extremal optimization for graph partitioning. *Phys. Rev. E*, 64:026114.
- Boettcher, S. and Percus, A. G. (2001b). Optimization with extremal dynamics. *Phys. Rev. Lett.*, 86:5211–5214.
- Boettcher, S. and Percus, A. G. (2004). Extremal optimization at the phase transition of the 3-coloring problem. *Phys. Rev. E*, 69:066703.
- Boettcher, S. and Sibani, P. (2005). Comparing extremal and thermal explorations of energy landscapes. *Eur. Phys. J. B*, 44:317–326.
- Dall, J. and Sibani, P. (2001). Faster Monte Carlo Simulations at Low Temperatures: The Waiting Time Method. Computer Physics Communication, 141:260–267.
- Danon, L., Diaz-Guilera, A., Duch, J., and Arenas, A. (2005). Comparing community structure identification. J. Stat. Mech.-Theo. Exp., P09008.
- de Sousa, F. L., Ramos, F. M., Galski, R. L., and Muraoka, I. (2004a). Generalized extremal optimization: A new meta-heuristic inspired by a model of natural evolution. *Recent Developments in Biologically Inspired Computing*.

- de Sousa, F. L., Vlassov, V., and Ramos, F. M. (2003). Generalized Extremal Optimization for solving complex optimal design problems. *Lecture Notes in Computer Science*, 2723:375–376.
- de Sousa, F. L., Vlassov, V., and Ramos, F. M. (2004b). Heat pipe design through generalized extremal optimization. *Heat Transf. Eng.*, 25:34–45.
- Duch, J. and Arenas, A. (2005). Community detection in complex networks using Extremal Optimization. *Phys. Rev. E*, 72:027104.
- Fischer, K. H. and Hertz, J. A. (1991). *Spin Glasses*. Cambridge University Press, Cambridge.
- Goldberg, D. E. (1989). Genetic Algorithms in Search, Optimization, and Machine Learning. Addison-Wesley, Reading.
- Gould, S. and Eldredge, N. (1977). Punctuated equilibria: The tempo and mode of evolution reconsidered. *Pale-obiology*, 3:115–151.
- Hartmann, A. K. and Rieger, H., editors (2004a). New Optimization Algorithms in Physics. Springer, Berlin.
- Hartmann, A. K. (2001). Ground-state clusters of two-, three-, and four-dimensional $\pm J$ Ising spin glasses. *Phys. Rev. E*, 63.
- Hartmann, A. K. and Rieger, H. (2004b). *New Optimization Algorithms in Physics*. Wiley-VCH, Berlin.
- Heilmann, F., Hoffmann, K. H., and Salamon, P. (2004). Best possible probability distribution over Extremal Optimization ranks. *Europhys. Lett.*, 66:305–310.
- Hoffmann, K. H., Heilmann, F., and Salamon, P. (2004). Fitness threshold accepting over Extremal Optimization ranks. *Phys. Rev. E*, 70:046704.
- Hoos, H. H. and Stützle, T. (2004). *Stochastic Local Search: Foundations and Applications*. Morgan Kaufmann, San Francisco.
- Iwamatsu, M. and Okabe, Y. (2004). Basin hopping with occasional jumping. Chem. Phys. Lett., 399:396–400.
- Kauffman, S. A. and Johnsen, S. (1991). Coevolution to the edge of chaos: Coupled fitness landscapes, poised states, and coevolutionary avalanches. *J. Theor. Biol.*, 149:467–505.
- Kirkpatrick, S., Gelatt, C. D., and Vecchi, M. P. (1983). Optimization by simulated annealing. *Science*, 220:671– 680.
- Lundy, M. and Mees, A. (1996). Convergence of an Annealing Algorithm. *Math. Programming*, 34:111–124.
- Mang, N. G. and Zeng, C. (2008). Reference energy extremal optimization: A stochastic search algorithm applied to computational protein design. J. Comp. Chem., 29:1762–1771.
- Menai, M. E. and Batouche, M. (2002). Extremal Optimization for Max-SAT. In Proceedings of the International Conference on Artificial Intelligence (IC-AI), pages 954–958.
- Menai, M. E. and Batouche, M. (2003a). A Bose-Einstein Extremal Optimization method for solving real-world instances of maximum satisfiability. In *Proceedings* of the International Conference on Artificial Intelligence (IC-AI), pages 257–262.

- Menai, M. E. and Batouche, M. (2003b). Efficient initial solution to Extremal Optimization algorithm for weighted MAXSAT problem. *Lecture Notes in Computer Science*, 2718:592–603.
- Meshoul, S. and Batouche, M. (2002a). Ant colony system with extremal dynamics for point matching and pose estimation. In *16th International Conference on Pattern Recognition (ICPR'02)*, volume 3, page 30823.
- Meshoul, S. and Batouche, M. (2002b). Robust point correspondence for image registration using optimization with extremal dynamics. *Lecture Notes in Computer Science*, 2449:330–337.
- Meshoul, S. and Batouche, M. (2003). Combining Extremal Optimization with singular value decomposition for effective point matching. *Int. J. Pattern Rec. and AI*, 17:1111–1126.
- Middleton, A. A. (2004). Improved Extremal Optimization for the Ising spin glass. *Phys. Rev. E*, 69:055701(R).
- Neda, Z., Florian, R., Ravasz, M., Libal, A., and Györgyi, G. (2006). Phase transition in an optimal clusterization model. *Physica A.*, 362:357–368.
- Onody, R. N. and de Castro, P. A. (2003). Optimization and self-organized criticality in a magnetic system. *Physica A*, 322:247–255.
- Palmer, R. G., Stein, D. L., Abraham, E., and Anderson, P. W. (1984). Models of hierarchically constrained dynamics for glassy relaxation. *Phys. Rev. Lett.*, 53:958– 961.
- Percus, A., Istrate, G., and Moore, C. (2006). *Computational Complexity and Statistical Physics*. Oxford University Press, New York.
- Raup, M. (1986). Biological extinction in earth history. Science, 231:1528–1533.
- Shmygelska, A. (2007). An extremal optimization search method for the protein folding problem: the go-model example. In GECCO '07: Proceedings of the 2007 GECCO conference companion on Genetic and evolutionary computation, pages 2572–2579, New York, NY, USA. ACM.
- Svenson, P. (2004). Extremal Optimization for sensor report pre-processing. Proc. SPIE, 5429:162–171.
- Wang, J. (2003). Transition matrix Monte Carlo and flathistogram algorithm. In AIP Conf. Proc. 690: The Monte Carlo Method in the Physical Sciences, pages 344–348.
- Wang, J.-S. and Okabe, Y. (2003). Comparison of Extremal Optimization with flat-histogram dynamics for finding spin-glass ground states. J. Phys. Soc. Jpn., 72:1380.
- Yom-Tov, E., Grossman, A., and Inbar, G. F. (2001). Movement-related potentials during the performance of a motor task i: The effect of learning and force. *Biological Cybernatics*, 85:395–399.
- Zhou, T., Bai, W.-J., Cheng, L.-J., and Wang, B.-H. (2005). Continuous Extremal Optimization for Lennard-Jones clusters. *Phys. Rev. E*, 72:016702.