Large-Scale Applications and Theory of Extremal Optimization

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1 Extremal Optimization (EO) Algorithm [1]

- Motivated by far-from-equilibrium dynamics [2]:
  - Emergent Structure (Self-Organized Criticality)
    - No tuning of control parameters.
    - Despite (or because of) large fluctuations.
    - Required: Definition of "fitness" λ_i
- How can we use it to optimize?
  - Extremal Driving (like Bak-Sneppen [3]):
    - Select and eliminate the "bad" λ_i .
    - Replace it at random.
    - Eventually, only "good" is left.

"Fitness" λ for various Problems:

•Spin Glasses (eg. MAX-CUT):

$\lambda_i = x_i \sum_j J_{i,j} x_j$

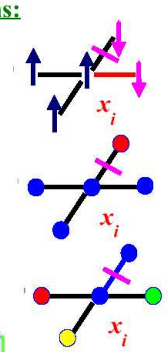
•Partitioning (eg. MIN-CUT):

λ_i = - (#-cut edges of x_i)

•Coloring (eg. Potts Anti-ferro):

λ_i = - (#-monochrome edges of x_i)

$Cost \propto H = -\sum_i \lambda_i$



>> "Extremal Optimization" (EO): <<

(1) Provide initial Configuration $S=(x_1,...,x_n)$,

(2) Determine "Fitness" λ_i for each Variable x_i,

(3) Rank all $i=\Pi(k)$ according to

$$\lambda_{\Pi(1)} \leq \lambda_{\Pi(2)} \leq \ldots \leq \lambda_{\Pi(n)}$$

(4) Select x_w w/ $w=\Pi(1)$, i.e. x_w has worst Fitness!

(5) Update x_w unconditionally,

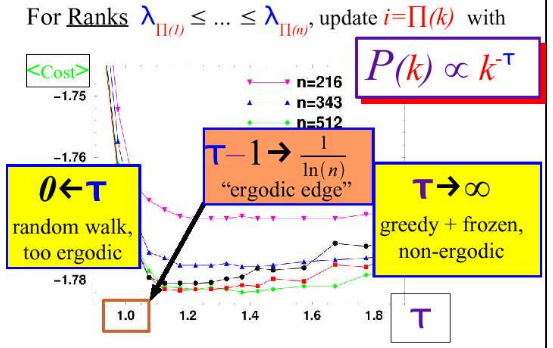
(6) For t_{max} times, Repeat at (2),

(7) Return: Best $C(S)$ found along the way!

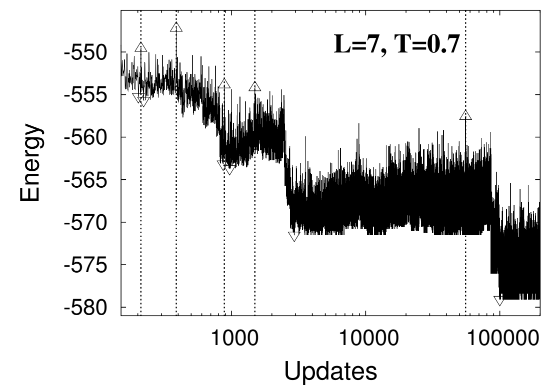
τ-EO - Searching at the "Ergodic Edge":

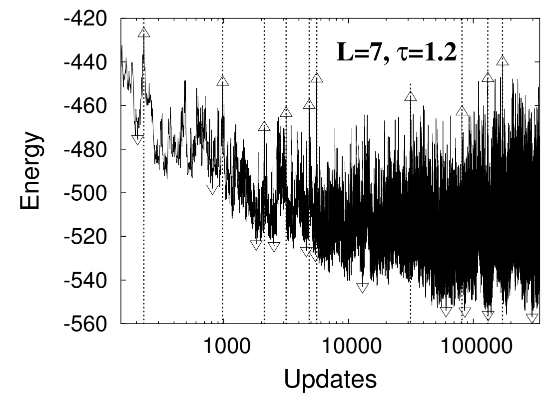
For Ranks $\lambda_{\Pi(1)} \leq \ldots \leq \lambda_{\Pi(n)}$, update $i=\Pi(k)$ with

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

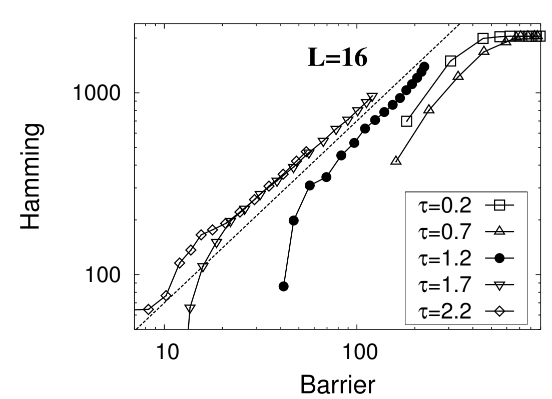


2 Extremal vs Metropolis Landscape Search





Plot of a typical run with a thermal search [4] at (above) and an extremal search [5] (below) for a $d = 3$ Gaussian spin glass of size $L = 7$. The fluctuating line marks the sequence of energies visited by the search. Energy records are marked by down-triangles, barrier records by up-triangles. The barrier records also demarcate the beginning and the end of a valley, so each time interval between two consecutive vertical lines constitutes a valley. Counting valleys starts (with $n_V = 0$) for updates $> N$ (where $N = 7^3 = 343$ here) to avoid transient behavior. While the absolute energy scale between both searches is not significant here (two distinct instances were used), the difference in range and shape of the fluctuations is remarkable.

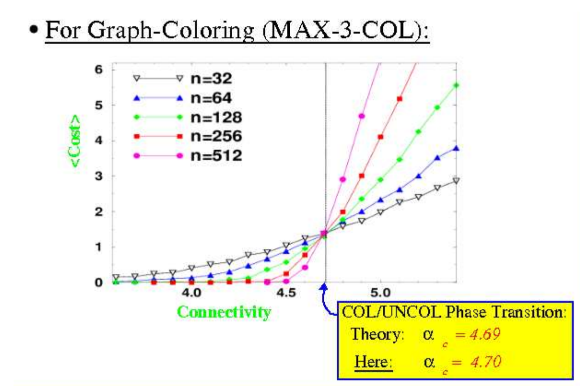


Plot of the Hamming distance between successive low-energy records as a function of the intervening barrier height. The relation for each value of τ appears to be in fact linear, even for $\tau < 1$ before the Hamming distances saturate. Linearity is exemplified by the dashed line of slope 1; the log-log scale was merely chosen for better visibility.

3 EO for MAX-3-Coloring [6]

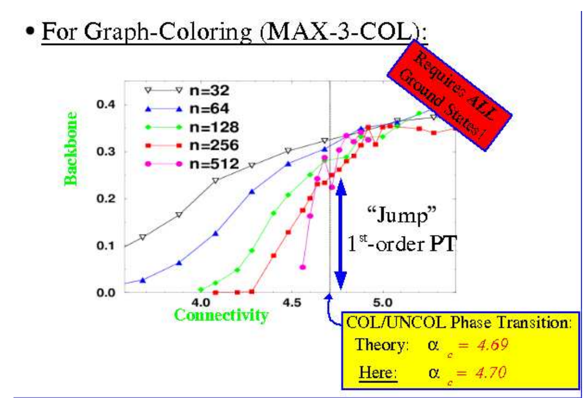
We investigate the phase transition of the 3-coloring problem on random graphs, using the extremal optimization heuristic. 3-coloring is among the hardest combinatorial optimization problems and is closely related to a 3-state anti-ferromagnetic Potts model. Like many other such optimization problems, it has been shown to exhibit a phase transition in its ground state behavior under variation of a system parameter: the graph's mean vertex degree. This phase transition is often associated with the instances of highest complexity. We use extremal optimization to measure the ground state cost and the "backbone", an order parameter related to ground state overlap, averaged over a large number of instances near the transition for random graphs of size n up to 512. For graphs up to this size, benchmarks show that extremal optimization reaches ground states and explores a sufficient number of them to give the correct backbone value after about $O(n^{3.5})$ update steps. Finite size scaling gives a critical mean degree value $\alpha_c = 4.703(28)$.

- For Graph-Coloring (MAX-3-COL):



Furthermore, the exploration of the degenerate ground states indicates that the backbone order parameter, measuring the constrainedness of the problem, exhibits a first-order phase transition.

- For Graph-Coloring (MAX-3-COL):



4 Jamming Model of EO [7]

Jamming Model for τ-EO :

Let: Only 3 states s for each x_i,

$$\lambda_i = -s, \quad s \in \{0,1,2\},$$

density of variables x_i in state s:

$$\rho_s(t) = \frac{1}{n} \left|\{i|\lambda_i = -s\}\right|,$$

Cost function:

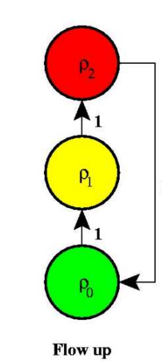
$$e(t) = \sum_{s=0}^{2} s\rho_s(t),$$

Annealed Flow Equation:

$$\rho_r(t+1) = \rho_r(t) + \sum_{s=0}^{2} T_{r,s} Q_s,$$

where

- $Q_s(\{\rho(t)\})$ = Prob. to update variable in state s,
- $T_{r,s}(\{\rho(t)\})$ = Flow of variables to state r, if variable in state s is updated.

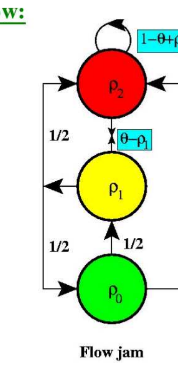


τ-EO Eq. for Jammed Flow:

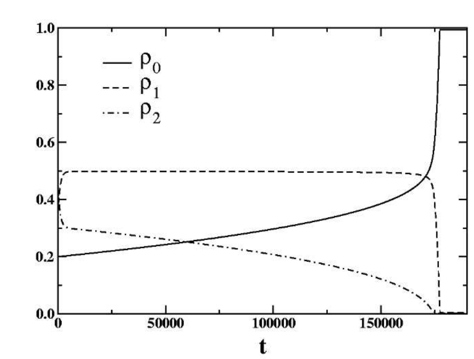
$$\dot\rho_0 = \frac{1}{n}\left[-Q_0 + \frac{1}{2}Q_1\right],$$
$$\dot\rho_1 = \frac{1}{n}\left[\frac{1}{2}Q_0 - Q_1 + (\theta - \rho_1)Q_2\right],$$
$$\dot\rho_2 = \frac{1}{n}\left[\frac{1}{2}Q_0 + \frac{1}{2}Q_1 - (\theta - \rho_1)Q_2\right],$$
$$1 = \rho_0 + \rho_1 + \rho_2.$$

For τ-EO:

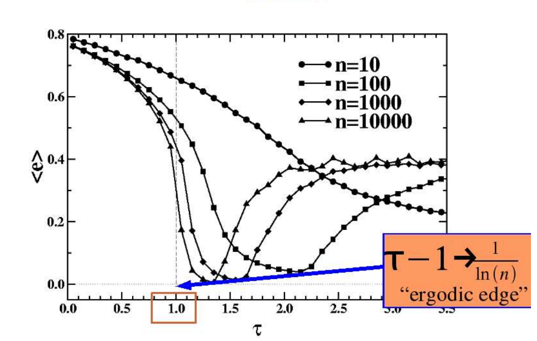
$$Q_2 = \int_{1/n}^{\rho_2} dx \, \frac{\tau - 1}{n^{\tau-1} - 1} x^{-\tau} = \frac{1}{1 - n^{\tau-1}}\left[\rho_2^{1-\tau} - n^{\tau-1}\right]$$
$$Q_1 = \frac{1}{1 - n^{\tau-1}}\left[(1-\rho_0)^{1-\tau} - \rho_2^{1-\tau}\right]$$
$$Q_0 = \frac{1}{1 - n^{\tau-1}}\left[1 - (1-\rho_0)^{1-\tau}\right]$$



τ-EO Evolution for Jammed Flow:



Optimal Choice for τ-EO:



References

[1] For a summary of recent results, see *New Optimization Algorithms in Physics*, eds. A. K. Hartmann and H. Rieger, (Wiley-VCH, Weinheim, 2004).

[2] S. Boettcher and A. G. Percus, *Optimization with Extremal Dynamics*, Phys. Rev. Lett. **86**, 5211 (2001).

[3] P. Bak and K. Sneppen, *Punctuated Equilibrium and Criticality in a simple Model of Evolution*, Phys. Rev. Lett. **71**, 4083-4086 (1993).

[4] J. Dall and P. Sibani, *Exploring Valleys of Aging Systems: The Spin Glass Case*, Eur. Phys. J. B **36**, 233-243 (2003).

[5] S. Boettcher and A. G. Percus, *Nature's Way of Optimizing*, Artificial Intelligence **119**, 275 (2000).

[6] S. Boettcher and A. G. Percus, *Extremal Optimization at the Phase Transition of the 3-Coloring Problem*, Phys. Rev. E **69** (to appear).

[7] S. Boettcher and M. Grigni, *Jamming Model for the Extremal Optimization Heuristic*, J. Phys. A. **35**, 1109 (2002).