Divide to Coordinate: Coevolutionary Problem Solving

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Abstract

Optimization of systems with many conflicting constraints arises in numerous settings. Common optimization procedures seek to improve performance of the system as a whole. We show that coevolutionary problem solving, in which a system is partitioned into sub-systems each of which selfishly optimizes, can lead to enhanced performance as a collective emergent property. Optimally partitioned systems often lie near a transition from order to chaos.

1 Introduction

It is often assumed that coordination among subtasks or agents to optimize some overall performance criterion is best achieved by control procedures which ensure that any change is always for the benefit of overall performance. This belief underlies hierarchical command and control organizational structures in many venues, ranging from business, military, and political organizations to automated problem solving procedures [1]. Our purpose is to explore an alternative possibility: Coordination among subtasks to optimize very hard problems laden with conflicting constraints may often be better achieved by partitioning the overall problem into subtasks, subgroups of agents, or "patches". Thereafter, each patch selfishly seeks to optimize its own performance independently, regardless of the fact that its optimization may change the problems facing the remaining subtasks or patches. Despite the fact that the patches are now coevolving with one another while "no one is minding the whole store", enhanced overall performance arises as an emergent collective behavior of such systems - a case of an invisible hand at work. This enhanced performance of a partitioned problem is the meaning of our title, "Divide to Coordinate: Coevolutionary Problem Solving".

We explore these issues with respect to the optimization of a specific class of hard problems in which many variables, or degrees of freedom, are coupled subject to strongly conflicting constraints. Our problem setting is the NK model [2]. The NK model is a kind of spin-glass [3, 4], with a rugged, multivalleyed energy or cost surface. The aim of the optimization procedure is to find a low energy configuration of the system's variables.

Our fundamental questions are these: Are there hard NK landscape problems for which better solutions can be found by partitioning the overall problem into selfishly optimizing patches? If so, is there an optimal way to partition the problem? How is such an optimal partitioning related to the complexity of the problem to be optimized? What characterizes such a partitioning? We show below in the setting of the NK model, that such partitionings exist, lead to low energy configurations, depend upon the complexity of the overall problem, and are often characterized by creating a system poised near an order-disorder transition.

The second section introduces the NK model in a lattice setting and describes the patch partitionings we used. The third section describes the results of our numerical studies. The fourth section discusses the results and some potential directions for further work.

2 The model

The NK model of rugged fitness landscapes, or energy or cost surfaces, consists of a system with N "spins". The spins can be interpreted as Ising spins in a spin glass, as amino acids in a protein, as genes in a genotype, as traits in an organism, as components in an artifact, or even as actors in a game [2, 5, 6, 7]. In the case we consider here, each spin has two states, 1 and 0. Each spin makes an energy contribution to the the entire system which depends upon its own state, and the states of K other spins. The K other spins may be chosen in any way. In a spin glass setting, K reflects spin couplings. In a genetic context, the K spin couplings reflect epistatic effects from other genes on the fitness effects of a given allele of a given gene. In the setting of an artifact, the K spin couplings reflect the effects other components have on the functional contribution of each component. The number of other spins, K, that affect each spin ranges a minimum value of 0 to a maximum value of $K = N - 1$. In the problem setting we consider, the spins are located on a square lattice of 120×120 spins, with periodic boundary conditions. K took on the values of 4, 8, 12, and 24. Figure 1 shows the neighborhood on the square lattice that affects each spin for these values of K.

The NK model creates a complex energy, cost, or fitness surface. To do so, the "energy" or "fitness" contribution of each spin must be specified for each of the 2^{K+1} possible combinations of states of that spin and the K other spins which affect it. This "energy" or "fitness" is assigned, once and for all, at

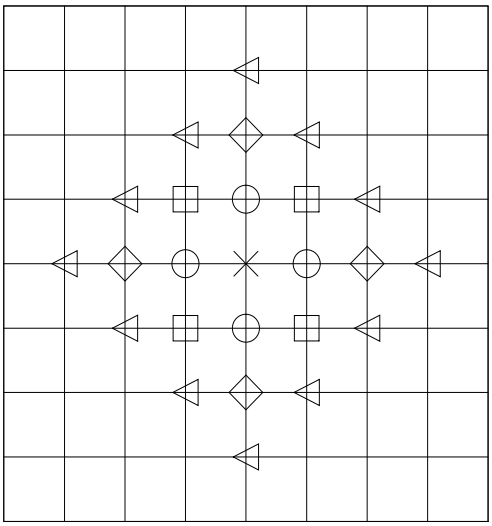


Figure 1: Neighborhoods for $K = 4$ (circles), $K = 8$ (circles and squares), $K = 12$ (circles, squares, and diamonds), and $K = 24$ (circles, squares, diamonds, and triangles).

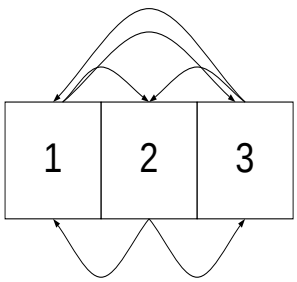
random from the uniform interval between 0.0 and 1.0, independently for each of the 2^{K+1} possible input configurations for each of the spins. The "energy" or "fitness" of the entire lattice for any given configuration of spin states is defined as the average of the energy or fitness contributions of the spins.

$$E\{s\} = \frac{1}{N}\sum_{i=1}^{N} E_i^{(K)}(s_i; s_{i_1}, \ldots, s_{i_K}) \tag{1}$$

The NK model creates an energy or fitness landscape on a discrete space. When each spin takes on only two states, 1 and 0, the configurations of the system can be arranged on the Boolean hypercube. Figures 2(a)-(c) show a small example with $N = 3$ spins, each with $K = 2$ inputs from the other spins. The 8 possible configurations are located at the corners of the Boolean cube, Figure 2(c). Each has an "energy", "cost", or "fitness". In the biological context one thinks of adaptation due to mutation and selection as climbing towards fitness peaks on the resulting fitness landscape, 2(c). In a physical setting, one thinks of a system as minimizing an energy towards minima on the energy surface. In an economic context one might think of minimizing cost on a cost surface.

The NK model is a general model creating a family of rugged fitness or energy surfaces. The ruggedness increases with K because the number of conflicting constraints in the system increases with K [2, 5]. In the limit of $K = N - 1$, the NK model is identical to Derrida's random energy spin glass model [2, 8, 9].

(a)



(b)

s_1	s_2	s_3	$E_1^{(2)}$	$E_2^{(2)}$	$E_3^{(2)}$	$E = \frac{1}{N}\sum_{i=1}^{N} E_i^{(2)}$
0	0	0	0.6	0.3	0.5	0.47
0	0	1	0.1	0.5	0.9	0.50
0	1	0	0.4	0.8	0.1	0.43
0	1	1	0.3	0.5	0.8	0.53
1	0	0	0.9	0.9	0.7	0.83
1	0	1	0.7	0.2	0.3	0.40
1	1	0	0.6	0.7	0.6	0.63
1	1	1	0.7	0.9	0.5	0.70

(c)

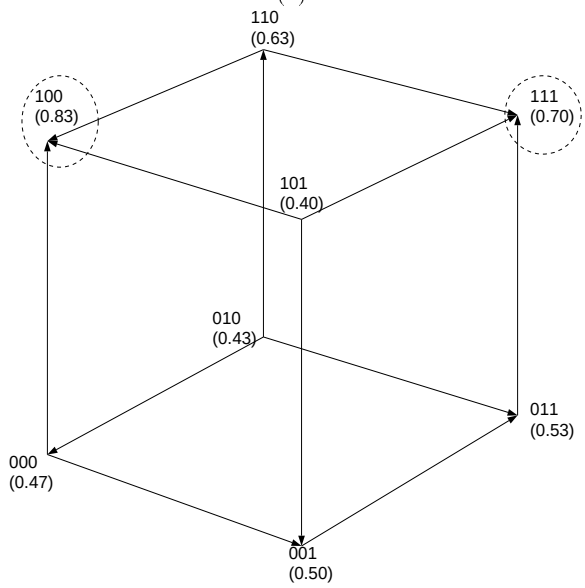


Figure 2: (a) Assignment of the $K = 2$ epistatic interactions for each of the $N = 3$ spins, (b) Random assignment of fitness values, (c) Fitness landscape on the Boolean cube indicating uphill directions.

2.1 Patches: partitioning the system into domains

Consider our 120×120 lattice. We seek low energy configurations over its energy or cost surface. One procedure, "Glauber dynamics" [10] is to pick an initial configuration of all the spins, then calculate the energy of the entire lattice. Thereafter, pick a spin at random, flip it, calculate the resulting energy of the entire lattice, and accept the flip move if the move lowers the energy of the entire lattice. If this procedure is carried out at zero temperature, so that only moves which decrease energy are accepted, the system will follow an "adaptive walk" through 1-flip neighboring spin configurations of successively lower energy to a nearby local minimum then freeze. Even were the local minimum a poor, high energy, minimum, the system would remain trapped forever.

Consider instead partitioning the 120×120 spin lattice into four patches, each 60×60 spins. The partitioning does not alter the couplings between the spins. However, the partitioning into patches is used to alter the criterion to accept a spin flip move: A randomly chosen spin is flipped. If the flip lowers the energy of the patch in which that spin resides, the move is accepted, even if it raises the energy of other patches due to the couplings across patch boundaries. Were the entire lattice frozen at a poor energy minimum, then for it to remain trapped after the lattice is broken into four patches, the poor minimum of the entire lattice would have to be a local minimum of each of the four patches independently. If not, one or more of the patches will no longer be frozen, and can move to new configurations. The division into patches allows the system to escape a poor local minimum and search its configuration space further. This observation leads to our central questions: As a function of landscape ruggedness, what is the optimal partitioning of an NK lattice to minimize energy? And what characterizes that optimal partitioning?

In order to explore these questions we partitioned the 120×120 square lattice, with $N = n^2 = 14\,400$ sites, into $p \times q$ uniform rectangular or square patches where both p and q divide $n = 120$ evenly. If the number of patches is $N_P = N/pq$, then Equation (1) can also be written as a sum over patches or subproblems:

$$E\{s\} = \frac{1}{N} \sum_{P=1}^{N_P} \sum_{i \in P} E_i^{(K)}(s_i; s_{i_1}, \ldots, s_{i_K}) \tag{2}$$

We investigate the behavior of Equation (2) for differing numbers of patches, N_P, and different patch geometries p and q.

Minimizing over the landscape defined by Equation (2) is accomplished by a modified Glauber dynamics. Starting from a random initial spin configuration a spin is flipped only if it lowers the energy of the patch it is in. A generation is defined as N trial flips. Three different updating techniques have been looked at:

- Random: At each moment a spin is chosen at random from the lattice and

flipped if it satisfies the criterion. Because the spin is chosen at random some patches may receive more updating than others.

- Fitter: For each patch we examine all possible single spin flips within the patch and randomly choose one which leads to lower energy. The patches are updated sequentially and not in parallel.

- Greedy: Like fitter we examine all possible single spin flips within the patch but we choose the flip which lowers the energy of the patch the most. Again the updating is sequential.

The simulations are run until we see convergence in the energy, typically 50 generations at most.

All results are the averages of 50 different, randomly generated landscapes at the given N and K. The error bars are $\pm$ one standard deviation over the 50 landscapes.

3 Results

3.1 Squares vs. other partitionings

A lattice might be broken into patches in many ways. Our purpose is not to find the optimal partitioning among all possible partitionings, but to investigate a small family of partitionings to assess the conditions under which division into subproblems enhances overall performance. For small patch areas squares outperformed rectangles. The energies of rectangles decreased as their perimeter to area ratio decreased towards that of squares. Therefore we have confined our analysis to squares in evaluating Equation (2). This gives a simple 1 parameter family of partitionings of the lattice into $p \times p$ squares, where $p \in \{1, 2, 3, 4, 5, 6, 8, 10, 12, 15, 20, 24, 30, 40, 60, 120\}$.

3.2 Optimal patch size

Optimal patch size, that which minimizes total lattice energy, depends upon the value of K, hence the ruggedness of the fitness or energy landscape. Our results show that when K is small and landscapes are relatively smooth, the optimal patch size is the entire 120×120 lattice. However, as K increases, hence conflicting constraints increase so that the landscape becomes more rugged and multivalleyed, we find that the system as a whole achieves lower energy if the lattice is broken into many patches of intermediate size. Figures 3-5 show the results for the random, fitter, and greedy dynamics on NK landscapes with $K = 4$. All three spin updating procedures give the lowest energy if the lattice is a single large patch, 120×120. However, in the case of the greedy updating

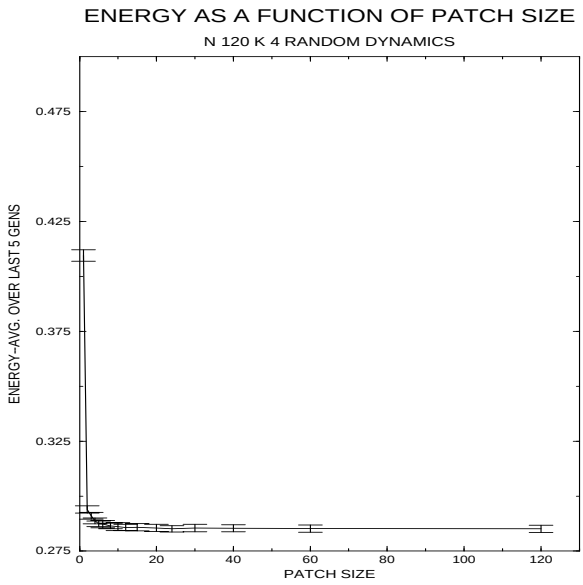


Figure 3: Energy of $K = 4$ landscape under random dynamics.

procedure, energy does not decrease monotonically as patch size increases, hinting at an interior minimum. While suggestive, this feature is within the error bars.

Figures 6-8 show the results for the three updating dynamics for $K = 8$ landscapes. Figures 9-11 show similar results for $K = 12$ landscapes. Figures 12-14 show similar results for $K = 24$ landscapes. A t-test of the significances of differences in energies for a number of cases is found in Table 1. These figures demonstrate that as K increases, an intermediate patch size, very much smaller than 120×120, minimizes total lattice energy. This result is statistically significant. Thus, breaking the total problem into patches each one of which is optimized "selfishly", despite the fact that that optimization may raise the energy of neighboring patches, helps achieve a significantly lower energy for the entire lattice.

For the $K = 8$ landscapes, Figures 6 and 7 show that the random and fitter dynamics lead to an optimum patch sizes when $p = 6$ and 5, rather than 120, hence patches with 36 and 25 spins rather than 14 400. On $K = 8$ landscapes, the greedy dynamics still finds the lowest energy for $p = 120$, but the hint of an interior optimum with p near 8 is clear.

For $K = 12$ landscapes, Figures 9-11 clearly show that the optimal patch size for all three spin updating procedures is very much smaller than $p = 120$. The optimal patch size is found at $p = 8$, hence 64 spins, for the random dynamics, $p = 6$ for the fitter dynamics, and $p = 5$ for the greedy dynamics.

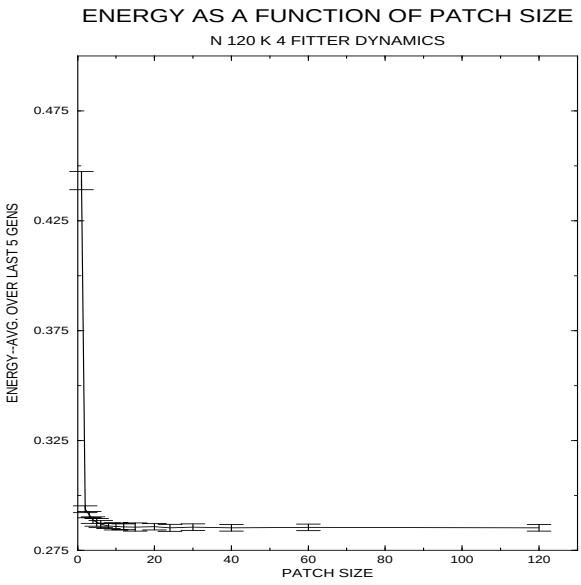


Figure 4: Energy of $K = 4$ landscape under fitter dynamics.

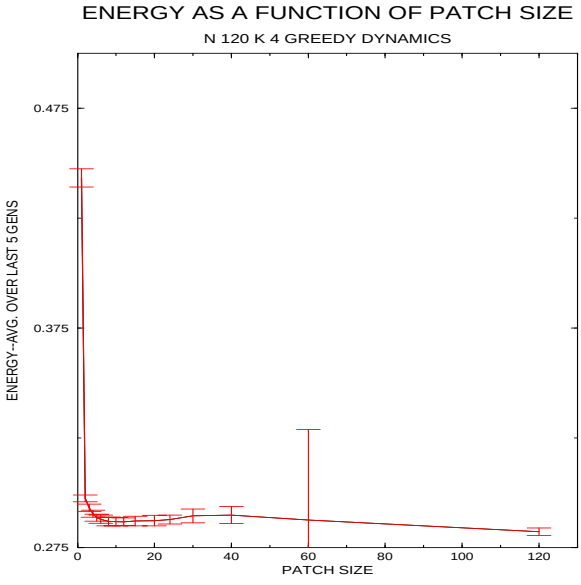


Figure 5: Energy of $K = 4$ landscape under greedy dynamics.

(a)

p	5	6	8	10	120
5		0.93 (0.35)	0.45 (0.65)	0.01 (0.99)	-5.00 (0.00)
6	-0.93 (0.35)		-0.50 (0.62)	-1.01 (0.32)	-6.71 (0.00)
8	-0.45 (0.65)	0.50 (0.62)		-0.49 (0.63)	-5.85 (0.00)
10	-0.01 (0.99)	1.01 (0.32)	0.49 (0.63)		-5.26 (0.00)
120	5.00 (0.00)	6.71 (0.00)	5.85 (0.00)	5.26 (0.00)	

(b)

p	5	6	8	10	120
5		59.09 (0.00)	56.84 (0.00)	56.25 (0.00)	42.78 (0.00)
6	-59.09 (0.00)		-4.26 (0.00)	-9.31 (0.00)	-31.28 (0.00)
8	-56.84 (0.00)	4.26 (0.00)		-4.84 (0.00)	-27.48 (0.00)
10	-56.25 (0.00)	9.31 (0.00)	4.84 (0.00)		-25.53 (0.00)
120	-42.78 (0.00)	31.28 (0.00)	27.48 (0.00)	25.53 (0.00)	

(c)

p	15	20	30	120
15		18.32 (0.00)	7.46 (0.00)	-11.39 (0.00)
20	-18.32 (0.00)		-13.89 (0.00)	-40.78 (0.00)
30	-7.46 (0.00)	13.89 (0.00)		-25.11 (0.00)
120	-11.39 (0.00)	40.78 (0.00)	25.11 (0.00)	

Table 1: Student's t-test showing showing energy differences (row − column) over the pooled standard deviation on (a) $K = 8$ landscape, (b) $K = 12$ landscape, and (c) $K = 24$ landscape under the fitter updating technique. The trailing number in brackets is the probability that the energy difference could be this large in magnitude by chance.

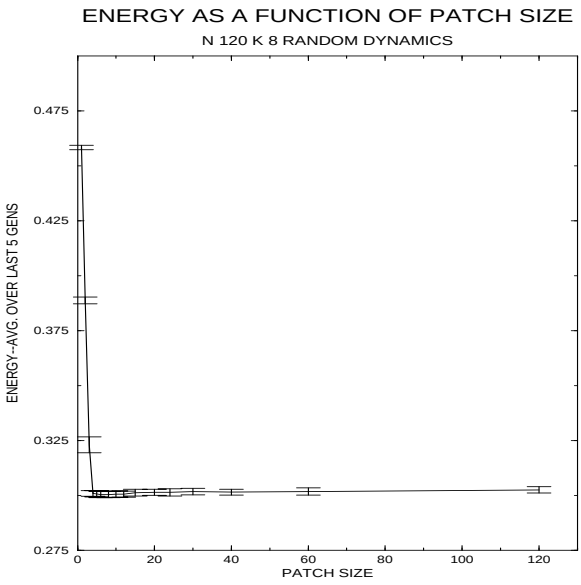


Figure 6: Energy of $K = 8$ landscape under random dynamics.

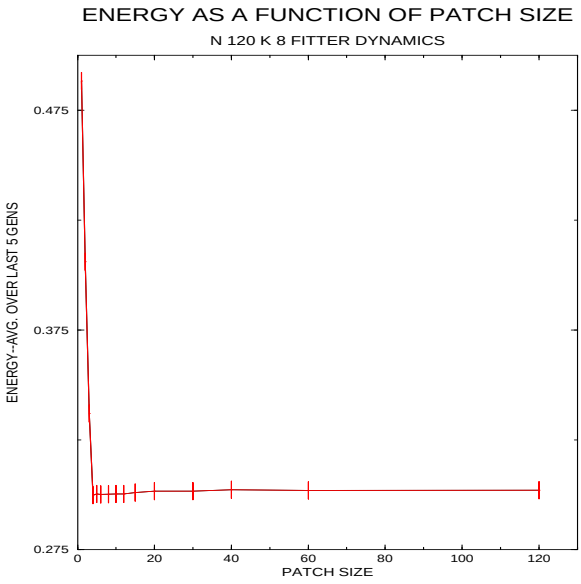


Figure 7: Energy of $K = 8$ landscape under fitter dynamics.

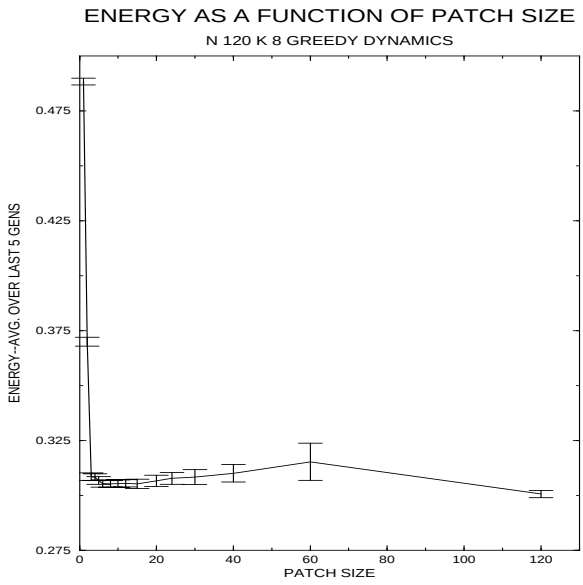


Figure 8: Energy of $K = 8$ landscape under greedy dynamics.

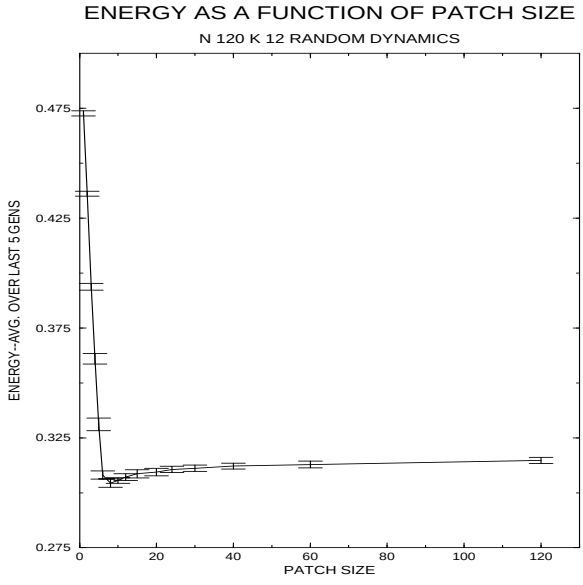


Figure 9: Energy of $K = 12$ landscape under random dynamics.

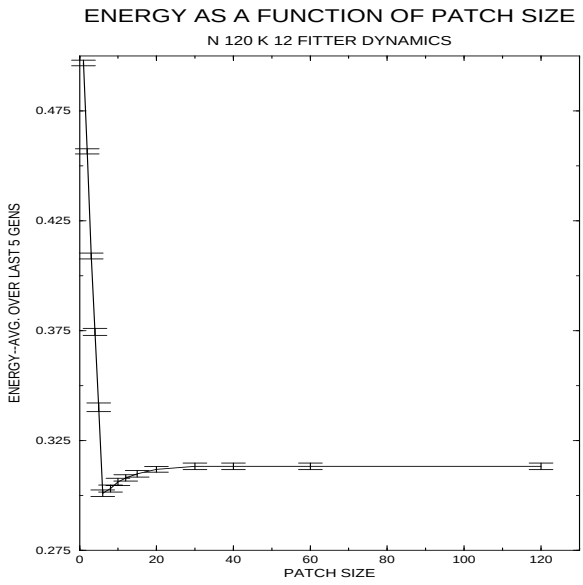


Figure 10: Energy of $K = 12$ landscape under fitter dynamics.

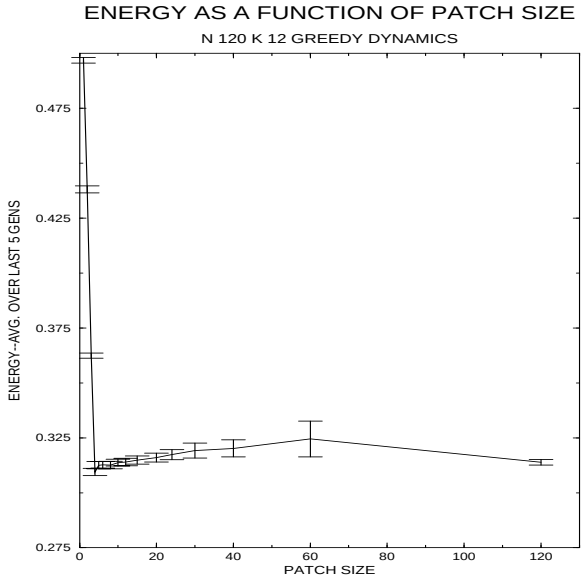


Figure 11: Energy of $K = 12$ landscape under greedy dynamics.

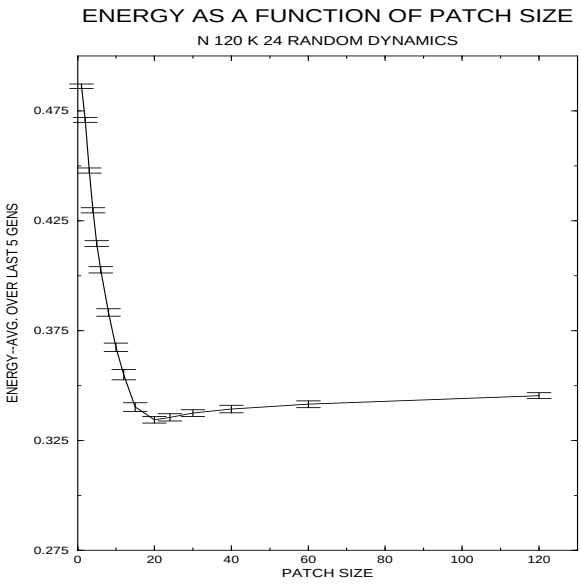


Figure 12: Energy of $K = 24$ landscape under random dynamics.

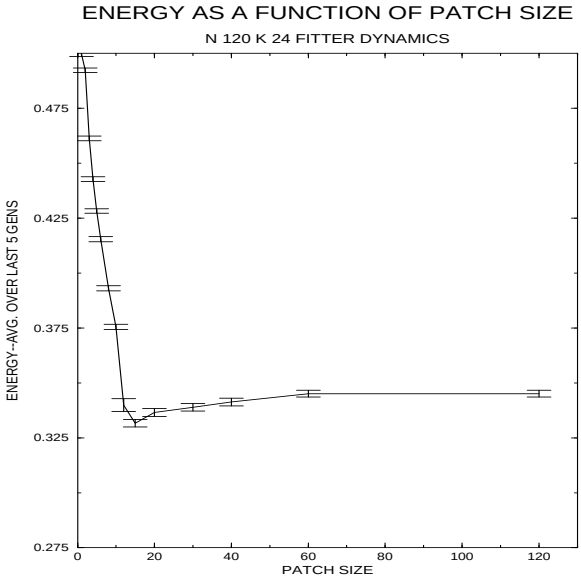


Figure 13: Energy of $K = 24$ landscape under fitter dynamics.

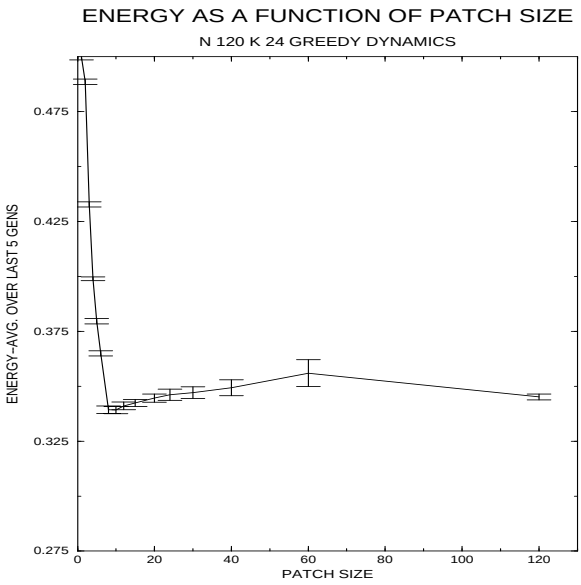


Figure 14: Energy of $K = 24$ landscape under greedy dynamics.

For $K = 24$ landscapes, Figures 12-14 show that the optimal patch size for random and fitter updating dynamics occurs at $p = 20$, corresponding to patches with 400 spins, while for greedy updating the optimum patch size is $p = 10$.

The size of the patch, $p \times p$, which minimizes energy is not simply related to the range of interaction defined by K. For example, on the $K = 24$ landscapes, the farthest range of interaction between spins is over a distance of 3 lattice constants, while the optimal patch size extends over 20 lattice constants. Conversely, on $K = 4$ landscapes, the maximum extent of spin interactions is 1 lattice constant, while the optimal patch size extends over the entire lattice, 120 lattice constants.

In order to test the effect of lattice size on optimal patch size, we have studied lattices for $K = 12$ landscapes with $N = n^2$ for $n = 24$, 40, 120, and 160. The results, shown in Figure 15, show little shifting in the position of the optimal patch size. Thus, for lattices as large and larger than 120×120, we believe that the optimal patch size will not change appreciably.

3.3 A phase transition in patched lattices

As a function of patch size and number, NK lattice systems can exhibit what might be called ordered dynamics, and what might be called chaotic dynamics. If the entire lattice is a single patch, 120×120, then any of our three spin

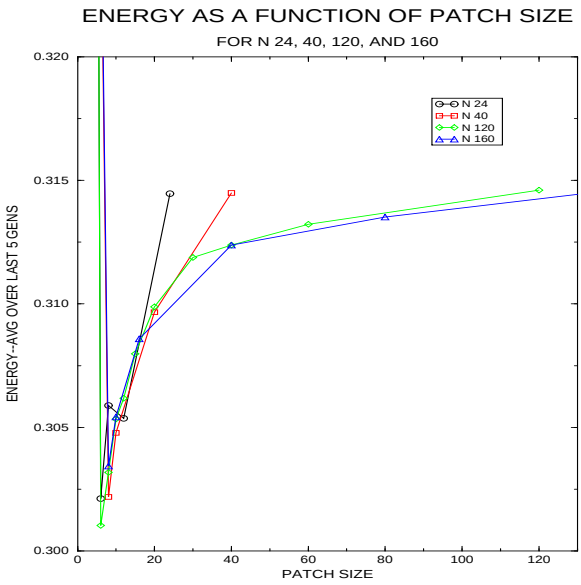


Figure 15: Scaling of optimal patch size with lattice dimension n for $K = 12$ landscapes under fitter updating.

updating procedures will lead the lattice from an initial spin configuration to some nearby local minimum on its energy surface. Once that local minimum is attained, no further spin flips will be accepted, for any such flip raises the energy of the total lattice. Thus, all spins are "frozen". This freezing defines what we will call an ordered regime.

If the lattice is broken into as many patches as possible, $p = 1$, such that each site is a separate patch, then the lattice corresponds to a Boolean network in which each spin is governed by a randomly chosen, then fixed, Boolean function of its K inputs [2]. Previous work [2, 11, 12], shows that on a square lattice, such Boolean networks are in a chaotic regime. Most spins continue to flip indefinitely in complex temporal patterns. Nearby initial configurations diverge over time [2, 13, 14, 15].

Since NK lattices, when broken into patches, can exhibit an ordered regime in the $p = 120$ limit, and a chaotic regime in the $p = 1$ limit, we might expect a qualitative change in behavior at some intermediate patch size. To investigate this issue, we allowed $K = 12$ lattices for different values of p to converge to their asymptotic low energy, then plotted the cumulative fraction of the 14 400 sites of the entire lattice which eventually flipped at least once thereafter. For patch sizes $p = 1$, 2, 3, 4, and 5, all sites eventually flip. Then suddenly, for patches sizes 6×6, or larger, the vast majority of spins freeze and never flip thereafter. The same sharp transition is found with random and greedy dynamics.

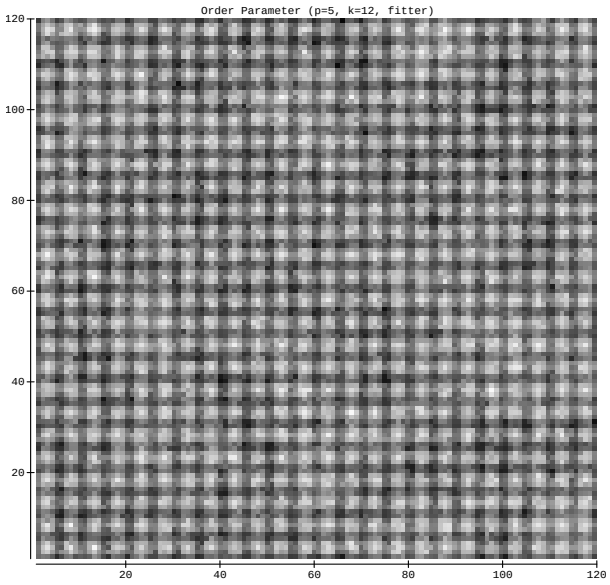


Figure 16: Order parameter for 5×5 patches on a $K = 12$ landscape.

A particularly dramatic view of this phase transition is shown in Figures 16 and 17. We examine the spatial structure of flipping behavior with an order parameter defined for each spin site: $\phi_i = 1 - 2 \langle \text{probability of site i flipping} \rangle_{\text{eq}}$, where the time average $\langle \ \rangle_{\text{eq}}$ is taken at equilibrium, or the asymptotic long time behavior. This order parameter is 1 if the spin is frozen and 0 if the spin is randomly flipping. Figure 16 shows this order parameter for a $K = 12$ landscape under fitter dynamics. Darker sites are flipping more often (lower values of the order parameter). The 5×5 patch sizes are clearly visible, for sites on the boundaries flip more often than central sites. This is due to perturbations across the boundaries.

In marked contrast, Figure 17 shows the same NK lattice, now broken into 6×6 patches. Suddenly, almost all spins are frozen. Only two pairs across two patch boundaries, continue to flip frequently.

3.4 The correlation of the energy minima with the phase transition

NK lattices, as a function of patch size, p, appear to undergo a phase transition from chaos to order as p is increased from 1 to 120. Patched lattices also can exhibit an optimal patch size which minimizes asymptotic energy. How are these two properties related?

Figure 18 shows, for each of the 50 landscapes chosen at a given K value,

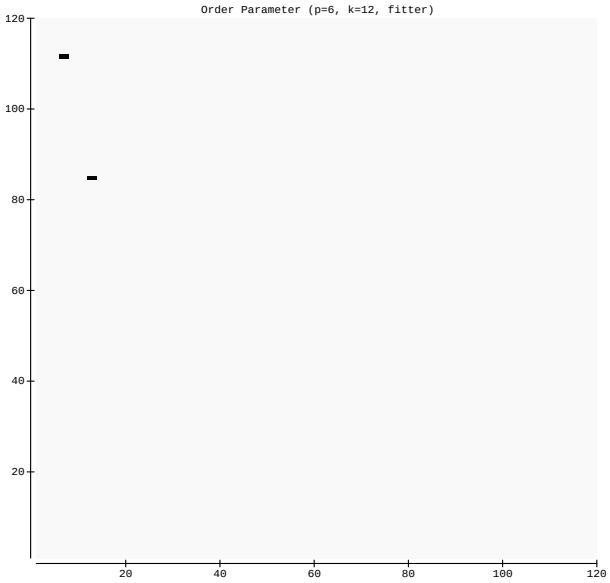


Figure 17: Order parameter for 6×6 patches on the same $K = 12$ landscape as in Figure 16.

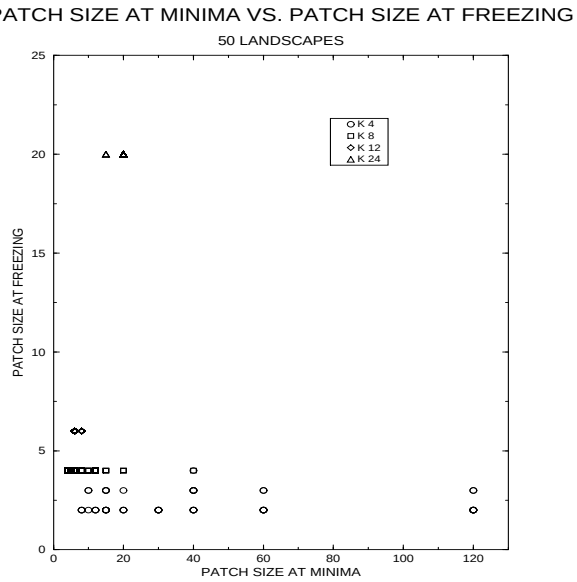


Figure 18: Correlation between patch size at the energy minima and the patch size at the freezing point for fitter dynamics.

	$K=4$	$K=8$	$K=12$	$K=24$
greedy	0	2	0	48
fitter	0	26	84	96
random	0	6	58	92

Table 2: Percentage of landscapes for which the patch size at the minimum energy equals the patch size at first freezing.

the patch size, p, at which freezing occurs, and also the patch size for that same landscape at which the energy minimum occurs. The correlation between freezing and energy minima is absent for $K = 4$, where the patches freeze at $p = 2$ and typically have an energy minimum at $p = 120$. The correlation is strongest at $K = 24$. Table 2 shows the percentage of the 50 landscapes for which the patch size at freezing equals the patch size which minimizes energy. The correlation depends upon the updating dynamics and K. It is highest at any K for the fitter dynamics and lowest for the greedy dynamics, and increases as K increases. When $K = 24$, the correlation is strong for all updating procedures. Thus, as K increases and landscapes become more rugged, the minimum energy at the optimal patch size, p, becomes more distinctly advantageous compared to other patch sizes, Figures 3-14, and at the same time, the optimal patch size more commonly is found very near the phase transition from order to chaos.

4 Discussion

Our results show that for a class of hard combinatorial optimization problems, enhanced solutions can often be found by partitioning the total problem into patches each of which then optimizes selfishly, ignoring the effects of its actions on neighboring patches. Such "patched" problems constitute coevolutionary problem solving. Enhanced solutions are found, not in spite of, but because of the patch boundaries. Such boundaries allow constraints from spins in other patches to be ignored by the spins in each patch. Ignoring constraints helps avoid trapping on poor local minima.

Coevolutionary problem solving is not useful on simple problems, but becomes progressively more so as landscapes become more rugged. Our results show that for sufficiently smooth landscapes, $K = 4$, the minimum energy is, in fact, achieved when any prospective spin flip must lower the total energy of the entire lattice. That is, the lowest energy is found when the entire lattice is a single large, 120×120, patch. Thus, our results show that the common assumption, that good optimization requires that any candidate change be good for overall system performance, extends to problems with some level of genuinely conflicting constraints.

When the level of conflicting constraints, captured by K, increases to 8 and beyond, our results show clearly that the 120×120 lattice system achieves lower

energy if the entire lattice is partitioned into "patches". The optimum patch size is very much smaller than the total size of the lattice, 14 400 spins, and ranges from about 36 spins for $K = 8$ landscapes to 400 spins for $K = 24$ landscapes. Importantly, as the overall problem becomes harder, that is, as K increases hence conflicting constraints increase, the advantage of the optimally "patched" lattice over the behavior of the lattice treated as a single large "patch", becomes more dramatic. Presumably, this increasing advantage reflects the increasing danger, as K increases, of trapping on very poor local minima when the entire lattice is treated as a single unit.

Our lattice system shows two broad regimes of behavior: A chaotic regime exists when the system is broken into many very small patches, and an ordered regime exists when the system is broken into a few large patches. In the chaotic regime every spin will ultimately flip. In the ordered regime almost all spins freeze into one or the other of the two states, 1 or 0 and never flip thereafter. A small number of isolated pairs of spins continue to flip. On each specific NK lattice, as patches are made larger and fewer, that lattice shifted abruptly from chaotic behavior to frozen behavior at a specific size and number of patches. Thus, these systems appear to undergo a phase transition from chaos to order as the sizes of patches increase.

A particularly interesting feature of our NK lattices is that the optimal energy tends to be found when the lattice is broken into patches such that the system is near the phase transition from order to chaos. This property is not present on $K = 4$ landscapes, but emerges increasingly clearly as K increases and landscapes become increasingly rugged.

Our results suggest a number of directions for future research. First, we do not know that our patch results extend to non-lattice NK systems, but expect that they do. Second, it would be deeply interesting to discover simple algorithms by which patches might selfishly evolve their membership and boundaries such that the system as a whole "spontaneously" achieved a very low energy. Third, our results have been obtained only for the NK family of landscapes. It will be important to extend them to other classes of complex problems with richly conflicting constraints.

While the above extensions await exploration, it may be worth considering possible implications of our main result. Contrary to intuition, optimization of systems with many conflicting constraints is often better achieved by partitioning the overall system into selfishly optimizing subsytems. Partitioning allows each subsystem to ignore constraints and avoids trapping on poor minima. Overall good performance arises as a collective emergent behavior of the interacting, coevolving subsystems. Here, in fact, is an invisible hand made visible. It is presumably no accident that organizations which have developed to solve hard problems with many conflicting constraints are typically divided into departments, profit centers, and other semi-independent sub-organizations. Indeed, abundant, if anecdotal, evidence suggests that monolithic hierarchical organizations in business, government, and elsewhere perform and adapt poorly. Calls

for decentralization and "flattening" of organizations are common [17]. The results demonstrated here may be an important theoretical foundation for useful decentralization. Coevolutionary problem solving may be a very general means by which human agents collectively solve hard social and practical problems.

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