(To appear in AAAI-98)

Learning Evaluation Functions for Global Optimization and Boolean Satisfiability

Justin A. Boyan and Andrew W. Moore
Computer Science Department
Carnegie Mellon University
Pittsburgh, PA 15213
{jab,awm}@cs.cmu.edu

Abstract

This paper describes STAGE, a learning approach to automatically improving search performance on optimization problems. STAGE learns an evaluation function which predicts the outcome of a local search algorithm, such as hillclimbing or WALKSAT, as a function of state features along its search trajectories. The learned evaluation function is used to bias future search trajectories toward better optima. We present positive results on six large-scale optimization domains.

Introduction

VLSI design, engineering design, Boolean formula satisfaction, bin-packing, medical treatment planning and Bayes net structure finding are all examples of global optimization—the problem of finding the best possible configuration from a large space of possible configurations. Formally, a global optimization problem consists of a *state space* X and an *objective function* $\mathrm{Obj} : X \to \Re$. The goal is to find a state $x^* \in X$ which minimizes Obj. If X is large, then finding x^* is generally intractable unless the problem has a very specialized structure (e.g., a linear program). However, many general-purpose *local search* algorithms attempt to exploit Obj's structure to locate good approximate optima; for example, hillclimbing, simulated annealing, and tabu search. All of these work by imposing a neighborhood relation on the states of X and then searching the graph that results, guided by Obj.

Local search has been likened to "trying to find the top of Mount Everest in a thick fog while suffering from amnesia" (Russell & Norvig 1995, p.111). The climber considers each step by consulting an altimeter and deciding whether to take the step based on the change in altitude. But suppose the climber has access to not only an altimeter, but also additional senses and instruments—for example, the current x and y location, the slope of the ground underfoot, and whether or not the current location is on a trail. These additional "features" may enable the climber to make a more informed, more foresightful, evaluation of whether to take a step.

In real optimization domains, such additional state features are generally plentiful. Practitioners of local search algorithms often append additional terms to their objective function, and then spend considerable effort tweaking the coefficients. This excerpt, from a book on VLSI layout by simulated annealing (Wong, Leong, & Liu 1988), is typical:

> Clearly, the objective function to be minimized is the channel width w. However, w is too crude a measure of the quality of intermediate solutions. Instead, for any valid partition, the following cost function is used:
>
> $$C = w^2 + \lambda_p \cdot p^2 + \lambda_U \cdot U \qquad (1)$$

U measures the sparsity of the horizontal tracks, while p measures the longest path length in the current partition. In this application, the authors hand-tuned the coefficients of the extra state features p^2 and U, setting $\lambda_p = 0.5$ and $\lambda_U = 10$. (We will show that our algorithm learned to assign, counterintuitively, a *negative* value to λ_U, and achieved much better performance.) Similar examples of evaluation functions being manually configured and tuned for good performance can be found in, e.g., (Falkenauer & Delchambre 1992; Szykman & Cagan 1995).

The question we address is the following: can extra features of an optimization problem be incorporated automatically into improved evaluation functions, thereby guiding search to better solutions?

The STAGE Algorithm

STAGE analyzes sample trajectories and automatically constructs predictive evaluation functions. It then uses these new evaluation functions to guide further search. A preliminary version of STAGE, described in

(Boyan & Moore 1997), showed promising performance on VLSI layout. This paper describes an improved version of STAGE with superior results on VLSI layout and thorough results for five other global optimization domains. We also overview the theoretical foundations of STAGE, one consequence of which is an extension allowing STAGE to accelerate non-monotonic search procedures such as WALKSAT.

Learning to Predict

The performance of a local search algorithm depends on the state from which the search starts. We can express this dependence in a mapping from starting states x to expected search result:

$$V^\pi(x) \stackrel{\text{def}}{=} \text{expected best Obj value seen on a trajectory that starts from state } x \text{ and follows local search method } \pi \tag{2}$$

Here, π represents a local search method such as hillclimbing or simulated annealing. $V^\pi(x)$ evaluates x's *promise* as a starting state for π.

For example, consider minimizing the one-dimensional function $\text{Obj}(x) = (|x| - 10)\cos(2\pi x)$ over the domain $X = [-10, 10]$, as depicted in Figure 1. Assuming a neighborhood structure on this domain where tiny moves to the left or right are allowed, hillclimbing (greedy descent) search clearly leads to a suboptimal local minimum for all but the luckiest of starting points. However, the quality of the local minimum reached does correlate strongly with the starting position: $V^\pi(x) \approx |x| - 10$. Gathering data from only a few suboptimal trajectories, a function approximator can easily learn to predict that starting near $x = 0$ will lead to good performance.

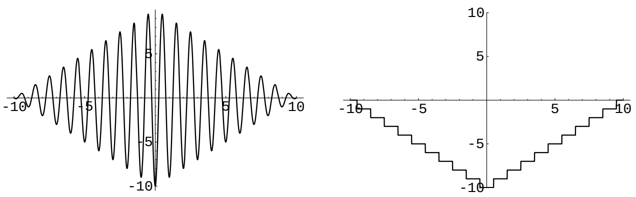


Figure 1: Left: $\text{Obj}(x)$ for a one-dimensional minimization domain. Right: the value function $V^\pi(x)$ which predicts hillclimbing's performance on that domain.

We approximate V^π using a function approximation model such as polynomial regression, where states x are encoded as real-valued feature vectors. As discussed above, these input features may encode any relevant properties of the state, including the original objective function $\text{Obj}(x)$ itself. We denote the mapping from states to features by $F : X \rightarrow \Re^D$, and our approximation of $V^\pi(x)$ by $\tilde{V}^\pi(F(x))$.

Training data for supervised learning of $\tilde{V}^\pi$ may be readily obtained by running π from different starting points. Moreover, if the algorithm π behaves as a Markov chain—i.e., the probability of moving from state x to x' is the same no matter when x is visited and what states were visited previously—then intermediate states of each simulated trajectory may also be considered alternate "starting points" for that search, and thus used as training data for $\tilde{V}^\pi$ as well. This insight enables us to get not one but perhaps hundreds of pieces of training data from each trajectory sampled. For the remainder of this paper, except in the section on WALKSAT, we will set π to be stochastic hillclimbing, rejecting equi-cost moves, terminating as soon as a fixed number (*patience*) of consecutive moves produces no improvement. This choice of π satisfies the Markov property. We will also always use simple linear or quadratic regression to fit $\tilde{V}^\pi$, since training these models incrementally is extremely efficient in time and memory (Boyan 1998).

Using the Predictions

The learned evaluation function $\tilde{V}^\pi(F(x))$ evaluates how promising x is as a starting point for algorithm π. To find the best starting point, we must optimize $\tilde{V}^\pi$ over X. We do this by applying stochastic hillclimbing with $\tilde{V}^\pi$ instead of Obj as the evaluation function.[1]

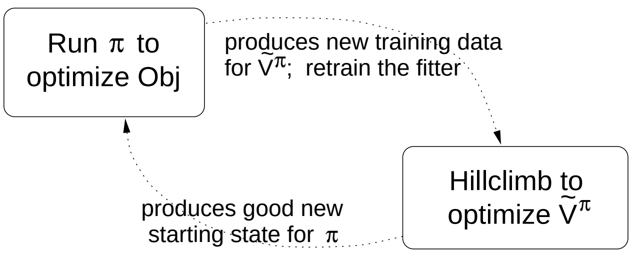


Figure 2: A diagram of the main loop of STAGE

The STAGE algorithm provides a framework for learning and exploiting $\tilde{V}^\pi$ on a single optimization instance. As illustrated in Figure 2, STAGE repeatedly alternates between two different stages of local search: running the original method π on Obj, and running hillclimbing on $\tilde{V}^\pi$ to find a promising new starting state for π. Thus, STAGE can be viewed as a *smart multi-restart* approach to local search.

[1]Note that even if $\tilde{V}^\pi$ is smooth with respect to the feature space—as it surely will be if we represent $\tilde{V}^\pi$ with a simple model like quadratic regression—it may still give rise to a complex cost surface with respect to the neighborhood structure on X. The existence of a state with a set of features similar to the current state's does not imply there is a step in state-space that will take us to that state.

STAGE effectively plots a single long trajectory through the state space, periodically switching between the original objective function $\text{Obj}(x)$ and the newly-learned evaluation function $\tilde{V}^\pi(x)$. The trajectory is only broken if the $\tilde{V}^\pi$ search phase accepts no moves, indicating that x is a local minimum of *both* evaluation functions. When this occurs, STAGE resets the search to a random starting state.

Illustrative Example

We will now work through a detailed illustrative example of STAGE in operation. Then we will provide results on six large, difficult, global optimization problems.

Our example comes from the practical, NP-complete domain of bin-packing (Coffman, Garey, & Johnson 1996). In bin-packing, we are given a *bin capacity* C and a list $L = (a_1, a_2, \dots a_n)$ of n *items*, each having a *size* $s(a_i) > 0$. The goal is to pack the items into as few bins as possible. Figure 3 depicts an example bin-packing instance with thirty items. Packed optimally, these items fill 9 bins exactly to capacity.

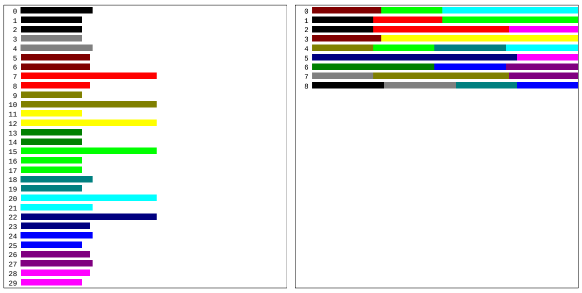


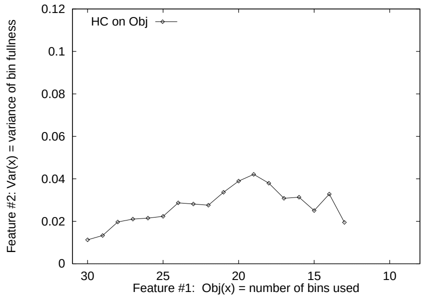
Figure 3: A small example bin-packing instance

To apply local search, we define a neighborhood operator which moves a single random item to a random new bin having sufficient spare capacity. STAGE predicts the outcome of stochastic hillclimbing using quadratic regression over two features of the state x:

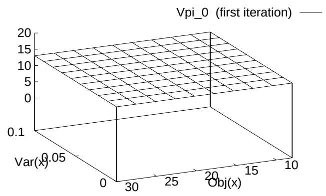
1. The actual objective function, Obj = # of bins used.
2. Var = the variance in fullness of the non-empty bins. This feature is similar to a cost function term introduced in (Falkenauer & Delchambre 1992).

Figure 4 depicts the first three iterations of a STAGE run on the example instance. On the first iteration (4a), STAGE hillclimbs from the starting state $(\text{Obj} = 30, \text{Var} = 0.011)$ to a local optimum $(\text{Obj} = 13, \text{Var} = 0.019)$. Training each of the 18 states of that trajectory to predict the outcome 13 results in the flat $\tilde{V}^\pi$ function shown in 4b. Hillclimbing on this flat $\tilde{V}^\pi$ accepts no moves, so STAGE resets to the initial state.

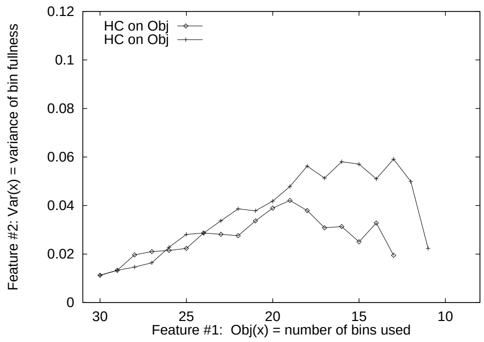
(4a)



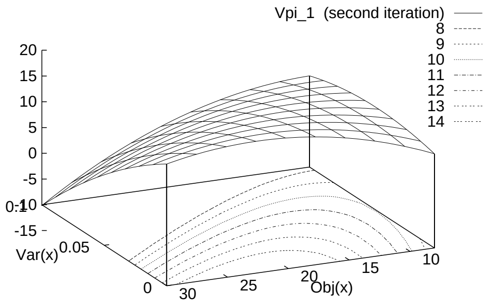
(4b)



(4c)



(4d)



(4e)

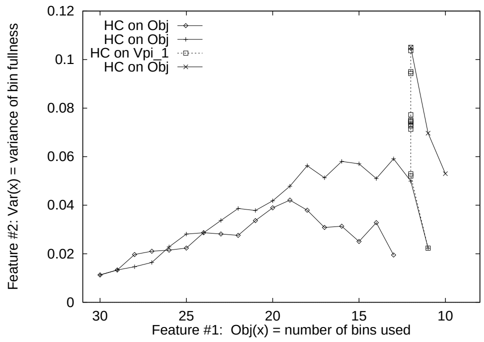


Figure 4: STAGE working on the bin-packing example

On the second iteration of STAGE (4c), the new stochastic hillclimbing trajectory happens to do better than the first, finishing at a local optimum (Obj $= 11$, Var $= 0.022$). Our training set is augmented with target values of 11 for all states on the new trajectory. The resulting quadratic $\tilde{V}^\pi$ already has significant structure (4d). Note how the contour lines of $\tilde{V}^\pi$, shown on the base of the surface plot, correspond to smoothed versions of the trajectories in our training set. Extrapolating, $\tilde{V}^\pi$ predicts that the the best starting points for hillclimbing are on arcs with higher Var(x).

STAGE hillclimbs on the learned $\tilde{V}^\pi$ to try to find a good starting point. The trajectory, shown as a dashed line in 4e, goes from (Obj $= 11$, Var $= 0.022$) up to (Obj $= 12$, Var $= 0.105$). Note that the search was willing to accept some harm to the true objective function during this stage. From the new starting state, hillclimbing on Obj does indeed lead to a yet better local optimum at (Obj $= 10$, Var $= 0.053$).

During further iterations, the approximation of $\tilde{V}^\pi$ is further refined. Continuing to alternate between hillclimbing on Obj and hillclimbing on $\tilde{V}^\pi$, STAGE manages to discover the global optimum at (Obj $= 9$, Var $= 0$) on iteration seven.

Results

Extensive experimental results are given in Table 1. For six problems with widely varying characteristics, we contrast the performance of STAGE with that of multi-start stochastic hillclimbing, simulated annealing, and domain-specific algorithms where applicable. The hillclimbing runs accepted equi-cost moves and restarted whenever *patience* consecutive moves produced no improvement. The simulated annealing runs made use of the successful "modified Lam" adaptive annealing schedule (Ochotta 1994, §4.5); its parameters were hand-tuned to perform well across the whole range of problems but not exhaustively optimized for each individual problem instance. On each instance, all algorithms were held to the same number M of total search moves considered, and run N times.

Bin-packing

The first set of results is from a 250-item benchmark bin-packing instance (u250_13, from (Falkenauer & Delchambre 1992)). Table 1 compares STAGE's performance with that of hillclimbing, simulated annealing, and *best-fit-randomized* (Coffman, Garey, & Johnson 1996), a bin-packing algorithm with good worst-case performance guarantees. STAGE significantly outperforms all of these. We obtained similar results for all 20 instances in the u250 suite (Boyan 1998).

Channel Routing

The problem of "Manhattan channel routing" is an important subtask of VLSI circuit design. Given two rows of labelled pins across a rectangular channel, we must connect like-labelled pins to one another by placing wire segments into vertical and horizontal tracks. Segments may cross but not otherwise overlap. The objective is to minimize the area of the channel's rectangular bounding box—or equivalently, to minimize the number of different horizontal tracks needed.

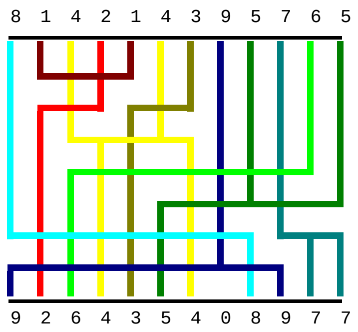


Figure 5: A small channel routing instance

We use the clever local search operators defined by Wong for this problem (Wong, Leong, & Liu 1988), but replace their contrived objective function C (see Equation 1 above) with the natural objective function $\mathrm{Obj}(x) =$ the channel width w. Wong's additional objective function terms, p and U, along with w itself, were given as the three input features to STAGE's function approximator.

Results on YK4, an instance with 140 vertical tracks, are given in Table 1. All methods were allowed to consider 500,000 moves per run. Experiment (A) shows that multi-restart hillclimbing finds quite poor solutions. Experiment (B) shows that simulated annealing, as used with the objective function of (Wong, Leong, & Liu 1988), does considerably better. Surprisingly, the annealer of Experiment (C) does better still. It seems that the "crude" evaluation function $\mathrm{Obj}(x) = w$ allows a long simulated annealing run to effectively random-walk along the ridge of all solutions of equal cost w, and given enough time it will fortuitously find a hole in the ridge. In fact, increasing hillclimbing's patience to ∞ (disabling restarts) worked nearly as well (D).

STAGE used simple linear and quadratic regression models for learning. The results (E,F) show that STAGE learned to optimize superbly, not only improving on the performance of hillclimbing as it was trained to do, but also finding better solutions on average than the best simulated annealing runs. This seems too good to be true; did STAGE really work according to its design?

We considered and eliminated two hypotheses:

1. *Since* STAGE *alternates between simple hillclimbing and another policy, perhaps it simply benefits from having more random exploration?* This is not the case: we tried the search policy of alternating hillclimbing with 50 steps of random walk, and its performance (G) was much worse than STAGE's.
2. *The function approximator may simply be smoothing Obj(x), which helps eliminate local minima and plateaus?* No: we tried a variant of STAGE which learned to smooth Obj(x) directly instead of learning $\tilde{V}^\pi$ (H); this also produced much less improvement than STAGE.

Bayes Network Structure-Finding

Given a data set, an important data mining task is to identify the Bayes net structure that best matches the data. We search the space of acyclic graph structures on A nodes, where A is the number of attributes in each data record. Following (Friedman & Yakhini 1996), we evaluate a network structure by a *minimum description length score* which trades off between fit accuracy and low model complexity. STAGE was given the following 7 features:

- mean & standard deviation of the conditional entropy score at each node
- mean & std. dev. of the number of parameters in each node's probability table
- mean & std. dev. of the number of parents of each node
- the number of "orphan nodes"

Results for a large dataset (ADULT2, 30162 records, 15 attributes) are shown in Table 1. All methods found comparably good solutions, although STAGE's performance was slightly better on average.

Radiotherapy Treatment Planning

Radiation therapy is a method of treating tumors. A linear accelerator which produces a radioactive beam is mounted on a rotating gantry, and the patient is placed so that the tumor is at the center of the beam's rotation. Depending on the exact equipment being used, the beam's intensity can be modulated in various ways as it rotates around the patient. A *radiotherapy treatment plan* specifies the beam's intensity at a fixed number of source angles.

A map of the relevant part of the patient's body, with the tumor and all important structures labelled, is available. Also known are good clinical forward models for calculating, from a treatment plan, the distribution of radiation that will be delivered to the patient's tissues. The optimization problem, then, is to produce a treatment plan which meets target radiation doses for the tumor while minimizing damage to sensitive nearby structures. The current practice is to use simulated annealing for this problem (Webb 1991).

Figure 6 illustrates a planar instance of the radiotherapy problem. The instance consists of an irregular-shaped tumor and four sensitive structures (the eyes, the brainstem, and the rest of the head). Given a treatment plan, the objective function is calculated by summing ten terms: an overdose penalty and an underdose penalty for each of the five structures. These ten subcomponents were the features for STAGE's learning.

Objective function evaluations are computationally expensive in this domain, so our experiments considered only 10,000 moves per run. Again, all algorithms performed comparably, but STAGE's solutions were best on average.

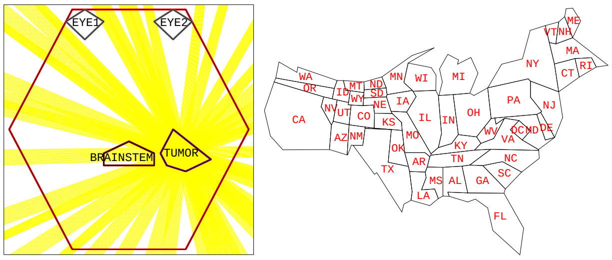


Figure 6: Left: a radiotherapy instance. Right: a cartogram in which each state's area is proportional to its electoral vote for U.S. President.

Cartogram Design

A "cartogram" is a map whose boundaries have been deformed so that population density is uniform over the entire map (Dorling 1994). We considered redrawing the map of the United States such that each state's area is proportional to its electoral vote. The goal is to best meet the new area targets while minimally distorting the states' shapes and borders.

We represented the map as a collection of 162 points in 2-space; each state is a polygon over a subset of those points. The search operator consisted of perturbing a random point slightly; perturbations that would cause two edges to cross were disallowed. The objective function was defined as

$$\text{Obj}(x) = \Delta\text{area} + \Delta\text{gape} + \Delta\text{orient} + \Delta\text{segfrac}$$

where Δarea penalizes states for missing their new area targets, and the other three terms penalize states shaped differently than in the true U.S. map. For STAGE, we represented each configuration by the four subcomponents of Obj. Learning a new evaluation

Problem Instance	Algorithm	Performance over N runs		
		mean	best	worst
Bin-packing (u250_13, opt=103) $M=10^5, N=100$	Hillclimbing, patience=250	109.38± 0.10	108	110
	Simulated annealing	108.19± 0.09	107	109
	Best-Fit Randomized	106.78± 0.08	106	107
	STAGE, quadratic regression	**104.77**± 0.09	**103**	**105**
Channel routing (YK4, opt=10) $M=5{\cdot}10^5, N=100$	(A) Hillclimbing, patience=250	22.35± 0.19	20	24
	(B) Simulated annealing, $\mathrm{Obj}(x) = w^2 + 0.5p^2 + 10U$	16.49± 0.16	14	19
	(C) Simulated annealing, $\mathrm{Obj}(x) = w$	14.32± 0.10	13	15
	(D) Hillclimbing, patience=∞	14.69± 0.12	13	16
	(E) STAGE, linear regression	**12.42**± 0.11	**11**	**14**
	(F) STAGE, quadratic regression	14.01± 0.77	**11**	31
	(G) Hillclimbing + random walk	17.26± 0.14	15	19
	(H) Modified STAGE—only smooth Obj	16.88± 0.22	14	19
Bayes net (ADULT2) $M=10^5, N=100$	Hillclimbing, patience=200	440567± 52	439912	441171
	Simulated annealing	440924± 134	**439551**	444094
	STAGE, quadratic regression	**440432**± 57	439773	**441052**
Radiotherapy (5E) $M=10^4, N=200$	Hillclimbing, patience=200	18.822±0.030	**18.003**	19.294
	Simulated annealing	18.817±0.043	18.376	19.395
	STAGE, quadratic regression	**18.721**±0.029	18.294	**19.155**
Cartogram (US49) $M=10^6, N=100$	Hillclimbing, patience=200	0.174±0.002	0.152	0.195
	Simulated annealing	**0.037**±0.003	**0.031**	0.170
	STAGE, quadratic regression	0.056±0.003	0.038	**0.132**
Satisfiability (par32-1.cnf, opt=0) $M=10^8, N=100$	(J) WALKSAT, noise=0, cutoff=10^6, tries=100	15.22± 0.35	9	19
	(K) WALKSAT + $\delta_w = 0$ (hillclimbing)	690.52± 1.96	661	708
	(L) WALKSAT + $\delta_w = 10$	15.56± 0.33	11	19
	(M) STAGE(WALKSAT), quadratic regression	5.36± 0.33	**1**	9
	(N) STAGE(WALKSAT/Markov), linear regression	**4.43**± 0.28	2	**8**

Table 1: Comparative results on a variety of minimization domains. For each problem, all algorithms were allowed to consider the same fixed number of moves M. Each line reports the mean, 95% confidence interval of the mean, best, and worst solutions found by N independent runs of one algorithm on one problem. Best results are boldfaced.

function with quadratic regression over these features, STAGE produced a significant improvement over hillclimbing, but did not outperform simulated annealing.

Satisfiability

Finding a variable assignment which satisfies a large Boolean expression is a fundamental (indeed, the original) NP-complete problem. In recent years, surprisingly difficult formulas have been solved by WALKSAT (Selman, Kautz, & Cohen 1996), a simple local search method. WALKSAT, given a formula expressed in CNF (a conjunction of disjunctive clauses), conducts a random walk in assignment space which is biased toward minimizing

$$\mathrm{Obj}(x) = \#\text{ of clauses unsatisfied by assignment } x.$$

When $\mathrm{Obj}(x) = 0$, all clauses are satisfied and the formula is solved.

WALKSAT searches as follows. On each step, it first selects an unsatisfied clause at random; it will satisfy that clause by flipping one variable within it. To decide which one, it first evaluates how much overall improvement to Obj would result from flipping each variable. If the best such improvement is positive, it greedily flips a variable that attains that improvement. Otherwise, it flips a variable which worsens Obj: with probability (1-*noise*), a variable which harms Obj the least, and with probability *noise*, a variable at random from the clause. The best setting of *noise* is problem-dependent (McAllester, Kautz, & Selman 1997).

WALKSAT is so effective that it has rendered nearly obsolete an archive of several hundred benchmark problems collected for a DIMACS Challenge on satisfiability (Selman, Kautz, & Cohen 1996). Within that archive, only the largest "parity function learning" instances (nefariously constructed by Kearns, Schapire, Hirsh and Crawford) are known to be solvable in principle, yet not solvable by WALKSAT. We report here results of experiments on the instance par32-1.cnf, a formula consisting of 10277 clauses on 3176 variables. Each experiment was run 100 times and allowed to consider 10^8 bit flips per run.

Experiment J (see Table 1) shows results with the best hand-tuned parameter settings for WALKSAT. The best such run still left 9 clauses unsatisfied. We introduced an additional WALKSAT parameter δ_w, with the following effect: any flip that would worsen Obj by more than δ_w is rejected. Normal WALKSAT has $\delta_w = \infty$. At the other extreme, when $\delta_w = 0$, no harmful moves are accepted, resulting in an ineffective form of hillclimbing (K). However, using intermediate settings of δ_w—thereby prohibiting only the most destructive of WALKSAT's moves—seems not to harm performance (L), and in some cases improves it.

For STAGE's learning, a variety of potentially useful additional state features are available, e.g.:

- % of clauses currently unsatisfied (= Obj(x))
- % of clauses satisfied by exactly 1 variable
- % of clauses satisfied by exactly 2 variables
- % of variables set to their "naive" setting[2]

Can STAGE, by observing WALKSAT trajectories, learn to combine these features usefully, as it did by observing hillclimbing trajectories in other domains?

Theoretically, STAGE can learn from any procedure π that is proper (guaranteed to terminate) and Markovian. WALKSAT's normal termination mechanism, cutting off after a pre-specified number of steps, is not Markovian: it depends on an extraneous counter variable, not just the current assignment. Despite this technicality, STAGE with quadratic regression (M) very nearly completely solved the problem, satisfying all but 1 or 2 of the 10277 clauses on several runs. With a properly Markovian cutoff criterion for WALKSAT (terminating with probability 1/10000 after each step) and linear instead of quadratic regression (N), STAGE's improvement over plain WALKSAT was about the same. Results on four other 32-bit parity benchmark instances were similar. In these experiments, WALKSAT was run with *noise*=25 and δ_w=10; full details may be found in (Boyan 1998).

Future work will pursue this further. We believe that STAGE shows promise for hard satisfiability problems—perhaps for MAXSAT problems where near-miss solutions are useful.

Transfer

There is a computational cost to training a function approximator on $\tilde{V}^\pi$. Learning from a π-trajectory of length L, with least-squares linear regression over D features, costs STAGE $O(D^2L + D^3)$ per iteration; quadratic regression costs $O(D^4L + D^6)$. In the experiments of the previous section, these costs were minimal—typically, 0–10% of total execution time. However, STAGE's extra overhead would become significant if many more features or more sophisticated function approximators were used.

For some problems such cost is worth it in comparison to a non-learning method, because a better or equally good solution is obtained with overall less computation. But in those cases where we use more computation, the STAGE method may nevertheless be preferable if we are then asked to solve further similar problems (e.g., a new channel routing problem with different pin assignments). Then we can hope that the computation we invested in solving the first problem will pay off in the second, and future, problems because we will already have a $\tilde{V}^\pi$ estimate. We call this effect *transfer*; the extent to which it occurs is largely an empirical question.

To investigate the potential for transfer, we re-ran STAGE on a suite of eight problems from the channel routing literature. Table 2 summarizes the results and gives the coefficients of the linear evaluation function learned independently for each problem. To make the similarities easier to see in the table, we have normalized the coefficients so that their squares sum to one; note that the search behavior of an evaluation function is invariant under linear transformations.

Problem instance	lower bound	best STAGE	learned coefficients $< w, p, U >$
YK4	10	12	$< 0.71,\ 0.05, -0.70 >$
HYC1	8	8	$< 0.52,\ 0.83, -0.19 >$
HYC2	9	9	$< 0.71,\ 0.21, -0.67 >$
HYC3	11	12	$< 0.72,\ 0.30, -0.62 >$
HYC4	20	23	$< 0.71,\ 0.03, -0.71 >$
HYC5	35	38	$< 0.69,\ 0.14, -0.71 >$
HYC6	50	51	$< 0.70,\ 0.05, -0.71 >$
HYC7	39	42	$< 0.71,\ 0.13, -0.69 >$
HYC8	21	25	$< 0.71,\ 0.03, -0.70 >$

Table 2: STAGE results ($M = 10^5, N = 3$) on eight problems from (Chao & Harper 1996).

The similarities among the learned evaluation functions are striking. Like the hand-tuned cost function C of (Wong, Leong, & Liu 1988) (Equation 1), all but one of the STAGE-learned cost functions (HYC1) assigned a relatively large positive weight to feature w and a small positive weight to feature p. Unlike the hand-tuned C, all the STAGE runs assigned a *negative*

[2] Given a CNF formula F, the naive setting of variable x_i is defined to be 0 if $\neg x_i$ appears in more clauses of F than x_i, or 1 if x_i appears in more clauses than $\neg x_i$.

weight to feature U. The similarity of the learned functions suggests that transfer between problem instances would indeed be fruitful.

The assignment of a negative coefficient to U is surprising, because U measures the sparsity of the horizontal tracks. U correlates strongly positively with the objective function to be minimized; a term of $-U$ in the evaluation function ought to pull the search toward terrible solutions in which each subnet occupies its own track. However, the positive coefficient on w cancels out this bias, and in fact a proper balance between the two terms can be shown to bias search toward solutions with an *uneven* distribution of track sparsity levels. Although this characteristic is not itself the mark of a high-quality solution, it does help lead hillclimbing search to high-quality solutions. STAGE successfully discovered and exploited this predictive combination of features.

Discussion

Under what conditions will STAGE work? Intuitively, STAGE maps out the attracting basins of a domain's local minima. When there is a coherent structure among these attracting basins, STAGE can exploit it. Identifying such a coherent structure depends crucially on the user-selected state features, the domain's move operators, and the regression models considered. What this paper has shown is that for a wide variety of large-scale problems, with very simple choices of features and models, a useful structure can be identified and exploited.

A very relevant investigation by Boese et. al. (Boese, Kahng, & Muddu 1994) gives further reasons for optimism. They studied the set of local minima reached by independent runs of hillclimbing on a traveling salesman problem and a graph bisection problem. They found a "big valley" structure to the set of minima: the better the local minimum, the closer (in terms of a natural distance metric) it tended to be to other local minima. This led them to recommend a two-phase "adaptive multi-start" hillclimbing technique similar to STAGE. A similar heuristic, Chained Local Optimization (Martin & Otto 1994), also works by alternating between greedy search and a user-defined "kick" that moves the search into a nearby but different attracting basin. The main difference is that these authors hand-build a problem-specific routine for finding good new starting states, whereas STAGE uses machine learning to do the same.

Zhang and Dietterich have explored another way to use learning to improve combinatorial optimization: they learn a search strategy from scratch using online value iteration (Zhang 1996). By contrast, STAGE begins with an already-given search strategy and uses prediction to learn to improve on it. Zhang reported success in transferring learned search control knowledge from simple job-shop scheduling instances to more complex ones.

STAGE offers many directions for further exploration. Among those currently under investigation are: reinforcement learning methods for building $\tilde{V}^\pi$ more efficiently; algorithms for robust transfer of learned $\tilde{V}^\pi$ functions between instances; and direct meta-optimization methods for feature weighting.

Acknowledgments: The first author acknowledges the support of a NASA GSRP Fellowship.

References

Boese, K. D.; Kahng, A. B.; and Muddu, S. 1994. A new adaptive multi-start technique for combinatorial global optimizations. *Operations Research Letters* 16:101–113.

Boyan, J. A., and Moore, A. W. 1997. Using prediction to improve combinatorial optimization search. In *Proceedings of AISTATS-6*.

Boyan, J. A. 1998. *Learning Evaluation Functions for Global Optimization*. Ph.D. Dissertation, Carnegie Mellon University.

Chao, H.-Y., and Harper, M. P. 1996. An efficient lower bound algorithm for channel routing. *Integration: The VLSI Journal*.

Coffman, E. G.; Garey, M. R.; and Johnson, D. S. 1996. Approximation algorithms for bin packing: a survey. In Hochbaum, D., ed., *Approximation Algorithms for NP-Hard Problems*. PWS Publishing.

Dorling, D. 1994. Cartograms for visualizing human geography. In Hearnshaw, H. M., and Unwin, D. J., eds., *Visualization in Geographical Information Systems*. Wiley. 85–102.

Falkenauer, E., and Delchambre, A. 1992. A genetic algorithm for bin packing and line balancing. In *Proc. of the IEEE 1992 International Conference on Robotics and Automation*, 1186–1192.

Friedman, N., and Yakhini, Z. 1996. On the sample complexity of learning Bayesian networks. In *Proc. 12th Conference on Uncertainty in Artificial Intelligence*.

Martin, O. C., and Otto, S. W. 1994. Combining simulated annealing with local search heuristics. Technical Report CS/E 94-016, Oregon Graduate Institute Department of Computer Science and Engineering.

McAllester, D.; Kautz, H.; and Selman, B. 1997. Evidence for invariants in local search. In *Proceedings of AAAI-97*.

Ochotta, E. 1994. *Synthesis of High-Performance Analog Cells in ASTRX/OBLX*. Ph.D. Dissertation, Carnegie Mellon University Department of Electrical and Computer Engineering.

Russell, S., and Norvig, P. 1995. *Artificial Intelligence: A Modern Approach*. Prentice Hall.

Selman, B.; Kautz, H.; and Cohen, B. 1996. Local search strategies for satisfiability testing. In *Cliques, Coloring, and Satisfiability: Second DIMACS Implementation Challenge*. American Mathematical Society.

Szykman, S., and Cagan, J. 1995. A simulated annealing-based approach to three-dimensional component packing. *ASME Journal of Mechanical Design* 117.

Webb, S. 1991. Optimization by simulated annealing of three-dimensional conformal treatment planning for radiation fields defined by a multileaf collimator. *Phys. Med. Biol.* 36:1201–1226.

Wong, D. F.; Leong, H.; and Liu, C. 1988. *Simulated Annealing for VLSI Design*. Kluwer.

Zhang, W. 1996. *Reinforcement Learning for Job-Shop Scheduling*. Ph.D. Dissertation, Oregon State University.