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Statistical Regimes Across Constrainedness Regions*

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Abstract. Much progress has been made in terms of boosting the effectiveness of backtrack style search methods. In addition, during the last decade, a much better understanding of problem hardness, typical case complexity, and backtrack search behavior has been obtained. One example of a recent insight into backtrack search concerns so-called heavy-tailed behavior in randomized versions of backtrack search. Such heavy-tails explain the large variations in runtime often observed in practice. However, heavy-tailed behavior does certainly not occur on all instances. This has led to a need for a more precise characterization of when heavy-tailedness does and when it does not occur in backtrack search. In this paper, we provide such a characterization. We identify different statistical regimes of the tail of the runtime distributions of randomized backtrack search methods and show how they are correlated with the "sophistication" of the search procedure combined with the inherent hardness of the instances. We also show that the runtime distribution regime is highly correlated with the distribution of the depth of inconsistent subtrees discovered during the search. In particular, we show that an exponential distribution of the depth of inconsistent subtrees combined with a search space that grows exponentially with the depth of the inconsistent subtrees implies heavy-tailed behavior.

1 Introduction

Significant advances have been made in recent years in the design of search engines for constraint satisfaction problems (CSP), including Boolean satisfiability problems (SAT). For complete solvers, the basic underlying solution strategy is backtrack search enhanced by a series of increasingly sophisticated techniques, such as non-chronological backtracking, fast pruning and propagation methods, nogood (or clause) learning, and more recently randomization and restarts. For

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example, in areas such as planning and finite model-checking, we are now able to solve large CSP's with up to a million variables and several million constraints.

The study of problem structure of combinatorial search problems has also provided tremendous insights in our understanding of the interplay between structure, search algorithms, and more generally, typical case complexity. For example, the work on phase transition phenomena in combinatorial search has led to a better characterization of search cost, beyond the worst-case notion of NP-completeness. While the notion of NP-completeness captures the computational cost of the very hardest possible instances of a given problem, in practice, one may not encounter many instances that are quite that hard. In general, CSP problems exhibit an "easy-hard-easy" pattern of search cost, depending on the constrainedness of the problem [1]. The computational hardest instances appear to lie at the phase transition region, the area in which instances change from being almost all solvable to being almost all unsolvable. The discover of "exceptionally hard instances" reveals an interesting phenomenon : such instances seem to defy the "easy-hard-easy" pattern, they occur in the under-constrained area, but they seem to be considerably harder than other similar instances and even harder than instances from the critically constrained area. This phenomenon was first identified by Hogg and Williams in graph coloring and by Gent and Walsh in satisfiability problems [2, 3]. However, it was shown later that such instances are not inherently difficult; for example, by renaming the variables such instances can often be easily solved [4, 5]. Therefore, the "hardness" of exceptionally hard instances does not reside purely in the instances, but rather in the combination of the instance with the details of the search method. Smith and Grant provide a detailed analysis of the occurrence of exceptionally hard instances for backtrack search, by considering a deterministic backtrack search procedure on ensembles of instances with the same parameter setting (see e.g., [6]).

Recently, researchers have noted that for a proper understanding of search behavior one has to study full runtime distributions [3, 7–10]. In our work we have focused on the study of randomized backtrack search algorithms [8]. By studying the runtime distribution produced by a randomized algorithm on a *single* instance, we can analyze the variance caused *solely* by the algorithm, and therefore separate the algorithmic variance from the variance between different instances drawn from an underlying distributions. We have shown previously that the runtime distributions of randomized backtrack search procedures can exhibit extremely large variance, even when solving *the same instance over and over again.* This work on the study of the runtime distributions of randomized backtrack search algorithms further clarified that the source of extreme variance observed in exceptional hard instances was not due to the inherent hardness of the instances: A randomized version of a search procedure on such instances in general solves the instance easily, even though it has a non-negligible probability of taking very long runs to solve the instance, considerably longer than all the other runs combined. Such extreme fluctuations in the runtime of backtrack search algorithms are nicely captured by so-called heavy-tailed distributions, distributions that are characterized by extremely long tails with some infinite moments [3, 8]. The decay of the tails of heavy-tailed distributions follows a power law — much slower than the decay of standard distributions, such as the normal or the exponential distribution, that have tails that decay exponentially. Further insights into the empirical evidence of heavy-tailed phenomena of randomized backtrack search methods were provided by abstract models of backtrack search that show that, under certain conditions, such procedures provably exhibit heavy-tailed behavior [11, 12].

Main Results So far, evidence for heavy-tailed behavior of randomized backtrack search procedures on concrete instance models has been largely empirical. Moreover, it is clear that not all problem instances exhibit heavy-tailed behavior. The goal of this work is to provide a better characterization of *when* heavy-tailed behavior occurs, and *when it does not*, when using randomized backtrack search methods. We study the empirical runtime distributions of *randomized* backtrack search procedures across different constrainedness regions of random binary constraint satisfaction models.[1] In order to obtain the most accurate empirical runtime distributions, all our runs are performed without censorship (*i.e.*, we run our algorithms without a cutoff) over the largest possible size. Our study reveals dramatically different statistical regimes for randomized backtrack search algorithms across the different constrainedness regions of the CSP models. Figure 1 provides a preview of our results. The figure plots the runtime distributions (the survival function, *i.e.,* the probability of a run taking more than x backtracks) of a basic randomized backtrack search algorithm (no look-ahead and no look-back), using random variable and value selection, for different constrainedness regions of one of our CSP models (model E; instances with 17 variables and domain size 8). We observe two regions with dramatically different statistical regimes of the runtime distribution.

In the first regime (the bottom two curves in Fig. 1, $p \leq 0.07$), we see heavy-tailed behavior. This means that the runtime distributions decay slowly. In the log-log plot, we see linear behavior over several orders of magnitude. When we increase the constrainedness of our model (higher p), we encounter a different statistical regime in the runtime distributions, where the heavy-tails disappear. In this region, the instances become inherently hard for the backtrack search algorithm, all the runs become homogeneously long, and therefore the variance of the backtrack search algorithm decreases and the tails of its survival function decay rapidly (see top two curves in Fig. 1, with $p = 0.19$ and $p = 0.24$; tails decay exponentially).

[1] Hogg and Willimans (94) provided the first report of heavy-tailed behavior in the context of backtrack search. They considered a *deterministic* backtrack search procedure on different instances drawn from a given distribution. Our work is of different nature as we study heavy-tailed behavior of the runtime distribution of a given *randomized* backtrack search method on a particular problem instance, thereby isolating the variance in runtime due to different runs of the algorithm.

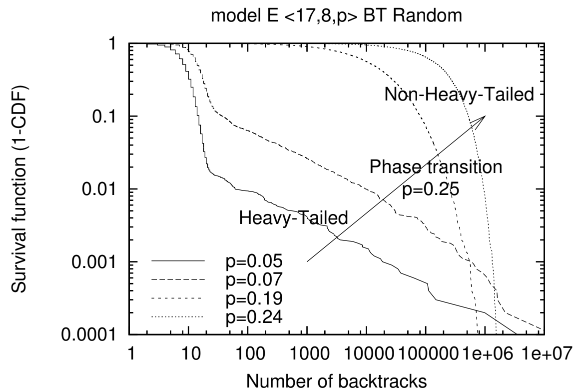

Fig. 1. Heavy-tailed (linear behavior) and non-heavy-tailed regime in the runtime of instances of model E $\langle 17, 8, p\rangle$. CDF stands for Cummulative Density Function.

A common intuitive understanding of the extreme variability of backtrack search is that on certain runs the search procedure may hit a very large inconsistent subtree that needs to be fully explored, causing "thrashing" behavior.

To confirm this intuition and in order to get further insights into the statistical behavior of our backtrack search method, we study the inconsistent sub-trees discovered by the algorithm during the search (see Figure 2).

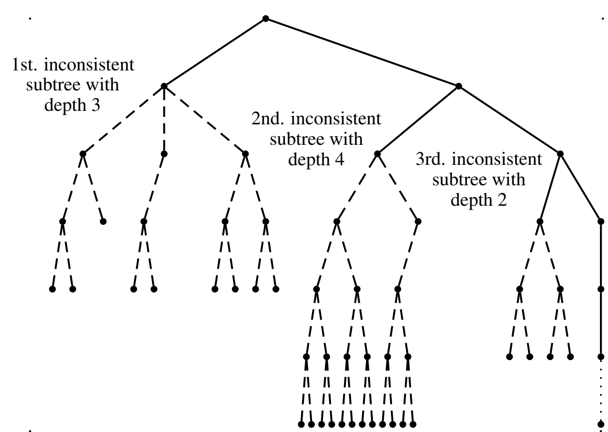

Fig. 2. Inconsistent subtrees in backtrack search.

The distribution of the depth of inconsistent trees is quite revealing: when the distribution of the depth of the inconsistent trees decreases exponentially (see Figure 3, bottom panel, $p = 0.07$) the runtime distribution of the backtrack search method has a power law decay (see Figure 3, top panel, $p = 0.07$). In other words, when the backtrack search heuristic has a good probability of finding relatively shallow inconsistent subtrees, and this probability decreases exponentially as the depth of the inconsistent subtrees increases, heavy-tailed behavior occurs. Contrast this behavior with the case in which the survival function of the runtime distribution of the backtrack search method is not heavy-tailed (see Figure 3, top panel, $p = 0.24$). In this case, the distribution of the depth of inconsistent trees no longer decreases exponentially (see Figure 3, bottom panel, $p = 0.24$).

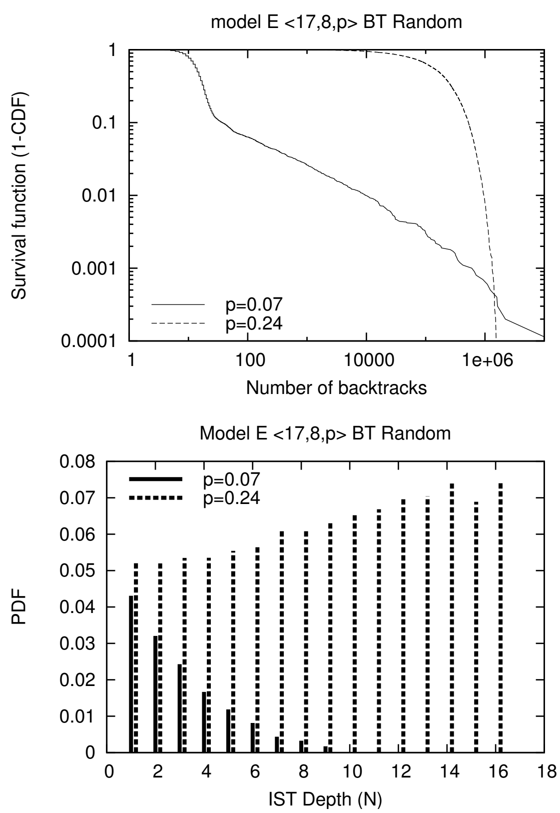

Fig. 3. Example of a heavy-tailed instance ($p = 0.07$) and a non-heavy-tailed instance ($p = 0.24$): (top) Survival function of runtime distribution, (bottom) probability density function of depth of inconsistent subtrees encountered during search. The subtree depth for $p = 0.07$ instance is exponentially distributed.

In essence, these results show that the distribution of inconsistent subproblems encountered during backtrack search is highly correlated with the tail behavior of the runtime distribution. We provide a formal analysis that links the exponential search tree depth distribution with heavy-tailed runtime profiles. As we will see below, the predictions of our model closely match our empirical data.

2 Definitions, Problem Instances, and Search Methods

Constraint Networks A finite binary *constraint network* $\mathcal{P} = (\mathcal{X}, \mathcal{D}, \mathcal{C})$ is defined as a set of n *variables* $\mathcal{X} = \{x_1, \ldots, x_n\}$, a set of *domains* $\mathcal{D} = \{D(x_1), \ldots, D(x_n)\}$, where $D(x_i)$ is the finite set of possible *values* for variable x_i, and a set $\mathcal{C}$ of binary *constraints* between pairs of variables. A constraint C_{ij} on the ordered set of variables (x_i, x_j) is a subset of the Cartesian product $D(x_i) \times D(x_j)$ that specifies the *allowed* combinations of values for the variables x_i and x_j. A *solution* of a constraint network is an instantiation of the variables such that all the constraints are satisfied. The constraint satisfaction problem (CSP) involves finding a solution for the constraint network or proving that none exists. We used a direct CSP encoding and also a Boolean satisfiability encoding (SAT) [13].

Random Problems The CSP research community has always made a great use of randomly generated constraint satisfaction problems for comparing different search techniques and studying their behavior. Several models for generating these random problems have been proposed over the years. The oldest one, which was the most commonly used until the middle 90's, is *model A*. A network generated by this model is characterized by four parameters $\langle N, D, p1, p2\rangle$, where N is the number of variables, D the size of the domains, p_1 the probability of having a constraint between two variables, and p_2, the probability that a pair of values is forbidden in a constraint. Notice that the variance in the type of problems generated with the same four parameters can be large, since the actual number of constraints for two problems with the same parameters can vary from one problem to another, and the actual number of forbidden tuples for two constraints inside the same problem can also be different. Model B does not have this variance. In *model B*, the four parameters are again $N, D, p1$, and $p2$, where N is the number of variables, and D the size of the domains. But now, p_1 is the proportion of binary constraints that are in the network (*i.e.*, there are exactly $c = \lfloor p_1 \cdot N \cdot (N-1)/2 \rfloor$ constraints), and p_2 is the proportion of forbidden tuples in a constraint (*i.e.*, there are exactly $t = \lfloor p_2 \cdot D^2 \rfloor$ forbidden tuples in each constraint). Problem classes in this model are denoted by $\langle N, D, c, t\rangle$. In [14] it was shown that model B (and model A as well) can be "flawed" when we increase N. Indeed, when N goes to infinity, we will almost surely have a *flawed* variable (that is, one variable which has all its values inconsistent with one of the constraints involving it). *Model E* was proposed to overcome this weakness. It is a three parameter model, $\langle N, D, p\rangle$, where N and D are the same as in the other models, and $\lfloor p \cdot D^2 \cdot N \cdot (N-1)/2 \rfloor$ forbidden pairs of values are selected with repetition out of the $D^2 \cdot N \cdot (N-1)/2$ possible pairs. There is a way of tackling the problem of flawed variables in model B. In [15] it is shown that by putting certain constraints on the relative values of N, D, p_1, and p_2, one can guarantee that model B is sound and scalable, for a range of values of the parameters. In our work, we only considered instances of model B that fall within such a range of values.

Search Trees A *search tree* is composed of *nodes* and *arcs*. A node u represents an ordered partial instantiation $I(u) = (x_{i_1} = v_{i_1}, \ldots, x_{i_k} = v_{i_k})$. A search tree is rooted at the particular node u_0 with $I(u_0) = \emptyset$. There is an arc from a node u to a node u_c if $I(u_c) = (I(u), x = v)$, x and v being a variable and one of its values. The node u_c is called a child of u and u a parent of u_c. Every node u in a tree T defines a *subtree* T_u that consists of all the nodes and arcs below u in T. The *depth* of a subtree T_u is the length of the longest path from u to any other node in T_u. An inconsistent subtree (IST) is a maximal subtree that does not contain any node u such that $I(u)$ is a solution. (See Fig. 2.) The maximum depth of an inconsistent subtree is referred to the "inconsistent subtree depth" (ISTD). We denote by $T(A, P)$ the search tree of a backtrack search algorithm A solving a particular problem P, which contains a node for each instantiation visited by A until a solution is reached or inconsistency of P is proved. Once assigned a partial instantiation $I(u) = (x_{i_1} = v_{i_1}, \ldots, x_{i_k} = v_{i_k})$ for node u, the algorithm will search for a partial instantiation of some of its children. In the case that there exists no instantiation which does not violate the constraints, algorithm A will take another value for variable x_{i_k}, and start again checking the children of this new node. In this situation, it is said that a *backtrack* happens. We use the number of wrong decisions or backtracks to measure the *search cost* of a given algorithm [16].[2]

Algorithms In the following, we will use different search procedures, that differ in the amount of propagation they perform, and in the order in which they generate instantiations. We used three levels of propagation: no propagation (backtracking, `BT`), removal of values directly inconsistent with the last instantiation performed (forward-checking, `FC`), and arc consistency propagation (maintaining arc consistency, `MAC`). We used three different heuristics for ordering variables: random selection of the next variable to instantiate (`random`), variables preordered by decreasing degree in the constraint graph (`deg`), and selection of the variable with smallest domain first, ties broken by decreasing degree (`dom+deg`) and always random value selection. For the SAT encodings we used the Davis-Putnam-Logemann-Loveland procedure. More specifically we used a simplified version of Satz [17], without its standard heuristic, and with static variable ordering, injecting some randomness in the value selection heuristics.

[2] In the rest of the paper sometimes we refer to the search cost as runtime. Even though there are some discrepancies between runtime and the search cost measured in number of wrong decisions or backtracks, such differences are not significant in terms of the tail regime of the distributions.

Heavy-tailed or Pareto-like Distributions As we discussed earlier, the runtime distributions of backtrack search methods are often characterized by very long tails or *heavy-tails* (HT). These are distributions that have so-called Pareto like decay of the tails. For a general Pareto distribution $F(x)$, the probability that a random variable is larger than a given value x, *i.e.*, its survival function, is:

$$1 - F(x) = P[X > x] \sim Cx^{-\alpha},\ x > 0,$$

where $\alpha > 0$ and $C > 0$ are constants. I.e., we have power-law decay in the tail of the distribution. These distributions have infinite variance when $1 < \alpha < 2$ and infinite mean and variance when $0 < \alpha \leq 1$. The log-log plot of the tail of the survival function $(1 - F(x))$ of a Pareto-like distribution shows linear behavior with slope determined by α.

3 Empirical Results

In the previous section, we defined our models and algorithms, as well as the concepts that are central in our study: the runtime distributions of our backtrack search methods and the associated distributions of the depth of the inconsistent subtrees found by the backtrack method. As we discussed in the introduction, our key findings are: (1) we observe different regimes in the behavior of these distributions as we move along different instance constrainedness regions; (2) when the depth of the inconsistent subtrees encountered during the search by the backtrack search method follows an exponential distribution, the corresponding backtrack search method search exhibits heavy-tailed behavior. In this section, we provide the empirical data upon which these findings are based.

We present results for the survival functions of the search cost (number of wrong decisions or number of backtracks) of our backtrack search algorithms. All the plots were computed with at least 10,000 independent executions of a randomized backtrack search procedure on a given (uniquely generated) problem satisfiable instance. For each parameter setting we considered over 20 instances. In order to obtain more accurate empirical runtime distributions, all our runs were performed without censorship, *i.e.*, we run our algorithms without any cutoff.[3] We also instrumented the code to obtain the information for the corresponding inconsistency sub-tree depth (ISTD) distributions.

Figure 4 (top) provides a detailed view of the heavy-tailed and non-heavy-tailed regions, as well as the progression from one region to the other. The figure displays the survival function (log-log scale) for running (pure) backtrack search with random variable and value selection on instances of Model E with 17 variables and a domain size of 8 for values of p (the constrainedness of the instances) ranging from $0.05 \leq p \leq 0.24$. We clearly identify the heavy-tailed region in

[3] For our data analysis, we needed purely uncensored data. We could therefore only consider relatively small problem instances. The results appear to generalize to larger instances.

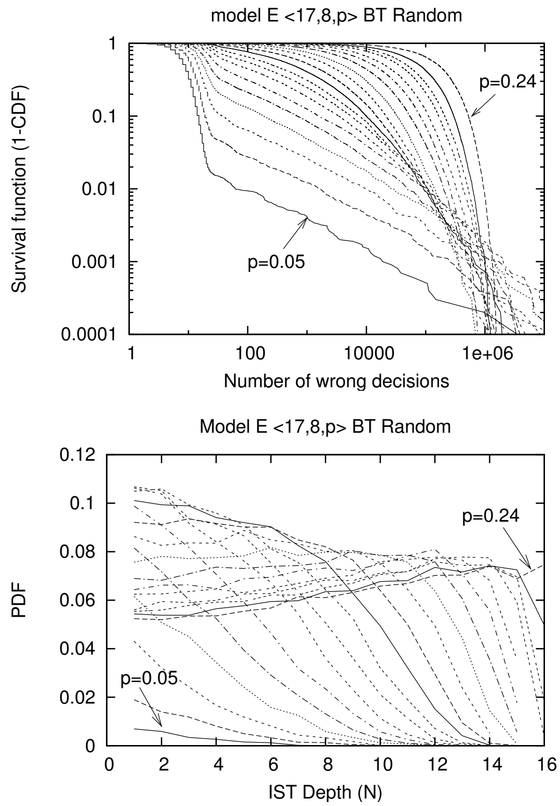

Fig. 4. The progression from heavy-tailed regime to non-heavy-tailed regime: (top) survival function of runtime distribution; (bottom) probability density function of the corresponding inconsistent sub-tree depth (ISTD) distribution.

which the log-log plot of the survival functions exhibits linear behavior, while in the non-heavy-tailed region the drop of the survival function is much faster than linear. The transition between regimes occurs around a constrainedness level of $p = 0.09$.

Figure 4 (bottom) depicts the probability density function of the corresponding inconsistent sub-tree depth (ISTD) distributions. The figure shows that while the ISTD distributions that correspond to the heavy-tailed region have an exponential behavior (below we show a good regression fit to the exponential distribution in this region), the ISTD distributions that correspond to the non-heavy-tailed region are quite different from the exponential distribution.

For all the backtrack search variants that we considered on instances of model E, including the DPLL procedure, we observed a pattern similar to that of figure 4. (See bottom panel of figure 6 for DPLL data.)

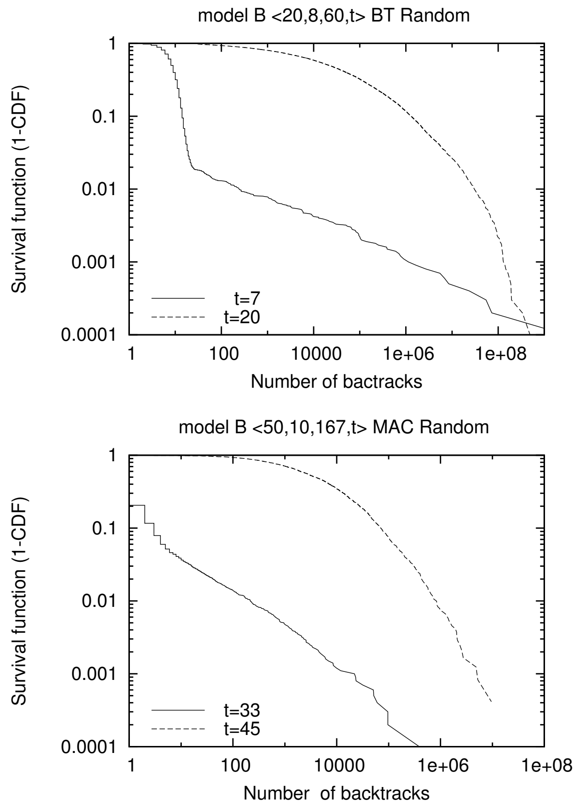

Fig. 5. Heavy-tailed and non-heavy-tailed regimes for instances of model B: (top) $\langle 20, 8, 60, t\rangle$, using `BT-random`, (bottom) $\langle 50, 10, 167, t\rangle$, using `MAC-random`.

We also observed a similar behavior — a transition from heavy-tailed region to non-heavy-tailed region with increased constrainedness — for instances of Model B, for different problem sizes and different search strategies. Figure 5 (top) shows the survival functions of runtime distributions of instances of model B $\langle 20, 8, 60, t\rangle$, for different levels of constrainedness, solved with `BT-random`. Fig.5 (bottom) shows the survival functions of runtime distributions of instances of model B $\langle 50, 10, 167, t\rangle$, for different levels of constrainedness, solved with `MAC-random`, a considerably more sophisticated search procedure. The top panel of Fig.6 gives the DPLL data. Again, the two different statistical regimes of the runtime distributions are quite clear.

To summarize our findings:

– For both models (B and E), for CSP and SAT encodings, for each backtrack search strategies, we clearly observe two different statistical regimes — a heavy-tailed and a non-heavy-tailed regime.

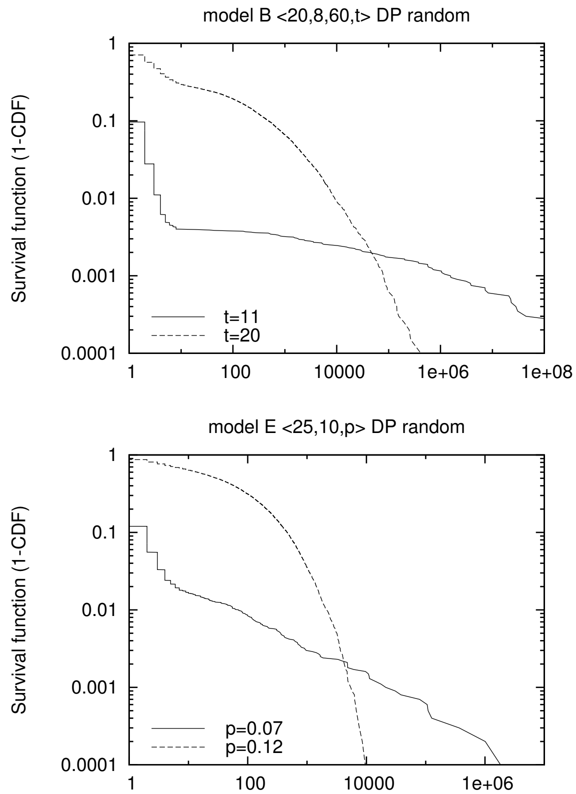

Fig. 6. Heavy-tailed and non-heavy-tailed regimes for instances of (top) model B $\langle 20, 8, 60, t\rangle$, using `DP-random` (`DPLL` procedure with static variable ordering and random value selection) and (bottom) model E $\langle 25, 10, p\rangle$ using `DP-random`.

- As constrainedness increases (p increases), we move from the heavy-tailed region to the non-heavy-tailed region.
- The transition point from heavy-tailed to non-heavy-tailed regime is dependent on the particular search procedure adopted. As a general observation, we note that as the efficiency (and, in general, propagation strength) of the search method increases, the extension of the heavy-tailed region increases and therefore the heavy-tailed threshold gets closer to the phase transition.
- Exponentially distributed inconsistent sub-tree depth (ISTD) combined with exponential growth of the search space as the tree depth increases implies heavy-tailed runtime distributions. We observe that as the ISTD distributions move away from the exponential distribution, the runtime distributions become non-heavy-tailed.

These results suggest that the existence of heavy-tailed behavior in the cost distributions depends on the efficiency of the search procedure as well as on the level of constrainedness of the problem. Increasing the algorithm efficiency tends to shift the heavy-tail threshold closer to the phase transition.

For both models, B and E, and for the different search strategies, we clearly observed that when the ISTD follows an exponential distribution, the corresponding distribution is heavy-tailed. We refer to the forthcoming long version of this paper for the probability density functions of the corresponding inconsistent sub-tree depth distributions (ISTD) of model B, and for data on the regression fits (see also below) for all curves.

4 Validation

Let X be the search cost of a given backtrack search procedure, $P_{istd}[N]$ be the probability of finding an inconsistent subtree of depth N during search, and $P[X > x|N]$ the probability of having a inconsistent search tree of size larger than x, given a tree of depth N. Assuming that the inconsistent search tree depth follows an exponential distribution in the tail and the search cost inside an inconsistent tree grows exponentially, then the cost distribution of a search method is lower bounded by a Pareto distribution. More formally:[4]

Theoretical Model

Assumptions:

- $P_{istd}[N]$ is exponentially distributed in the tail, i.e.,

$$P_{istd}[N] = B_1 e^{-B_2 N}, N > n_0 \quad (1)$$

  where B_1, B_2, and n_0 are constants.
- $P[X > x|N]$ is modeled as a complementary Heavyside function, $1 - H(x - k^N)$, where k is a constant and

$$H(x-a) = \begin{cases} 0, x < a \\ 1, x \geq a \end{cases}$$

Then, $P[X > x]$ is Pareto-like distributed

$$P[X > x] \approx \beta x^{-\alpha}$$

for $x > k^{n_0}$, where α and β are constants.

[4] See forthcoming extended version of the paper for further details. A similar analysis goes through using the geometric distribution, the discrete analogue of the exponential.

Derivation of result:

Note that $P[X > x]$ is lower bounded as follows

$$P[X > x] \geq \int_{N=0}^{\infty} P_{istd}[N]\, P[X > x|N] dN \tag{2}$$

This is a lower bound since we consider only one inconsistent tree contributing to the search cost, when in general there are more inconsistent trees. Given the assumptions above, Eq. (2) results

$$P[X > x] \geq \int_{N=0}^{\infty} P_{istd}[N]\, (1 - H(x - k^N))dN = \int_{N=\frac{\ln x}{\ln k}}^{\infty} P_{istd}[N]dN$$

Since $x > k^{n_0}$, we can use Eq.(1) for $P_{istd}[N]$, so Eq.(3) results in:

$$P[X > x] \geq \int_{N=\frac{\ln x}{\ln k}}^{\infty} B_1 e^{-B_2 N} dN = \frac{B_1}{B_2}\, e^{-B_2 \frac{\ln x}{\ln k}} = \beta x^{-\alpha}; \quad \alpha = \frac{B_2}{\ln k}; \quad \beta = \frac{B_1}{B_2}$$

In order to validate this model empirically we consider an instance of model B $\langle 20, 8, 60, 7\rangle$, running `BT-random`, the same instance plotted in Fig. 5(a), for which heavy-tailed behavior was observed ($t = 7$). The plots in Fig. 7 provide the regression data and fitted curves for the parameters B_1, B_2, and k, using $n_0 = 1$. The good quality of the linear regression fit suggests that our assumptions are very reasonable. Based on the estimated values for k, B_1, and B_2, we then compare the lower bound predicted using the formal analysis presented above with the empirical data. As we can see from Fig. 7, the theoretical model provides a good (tight) lower bound for the empirical data.

5 Conclusions and Future Work

We have studied the runtime distributions of complete backtrack search methods on instances of well-known random CSP binary models. Our results reveal different regimes in the runtime distributions of the backtrack search procedures and corresponding distributions of the depth of the inconsistent sub-trees. We see a changeover from heavy-tailed behavior to non-heavy-tailed behavior when we increase the constrainedness of the problem instances. The exact point of changeover depends on the sophistication of the search procedure, with more sophisticated solvers exhibiting a wider range of heavy-tailed behavior. In the non-heavy-tailed region, the instances become harder and harder for the backtrack search algorithm, and the runs become nearly homogeneously long. We have also shown that that there is a clear correlation between the the distributions of the depth of the inconsistent sub-trees encountered by the backtrack search method and the heavy-tailedness of the runtime distributions, with exponentially distributed sub-tree depths leading to heavy-tailed search. To further validate our findings, we compared our theoretical model, which models exponentially distributed subtrees in the search space, with our empirical data: the

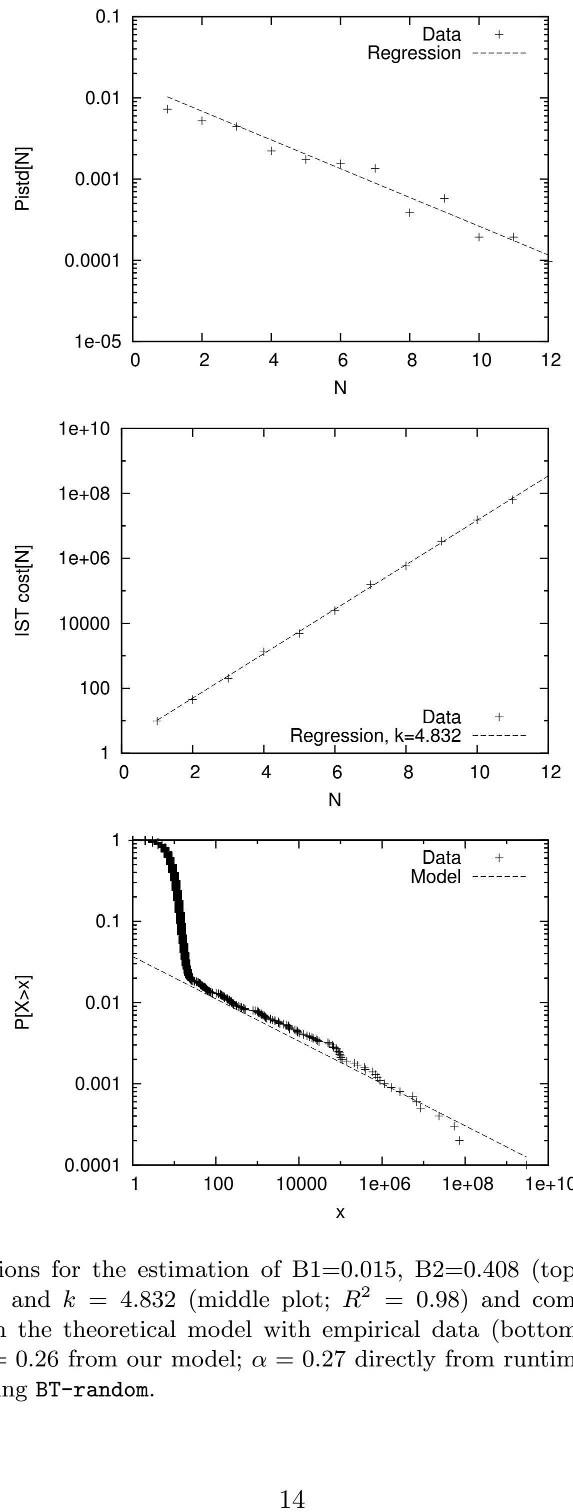

Fig. 7. Regressions for the estimation of B1=0.015, B2=0.408 (top plot; quality of fit $R^2 = 0.88$), and $k = 4.832$ (middle plot; $R^2 = 0.98$) and comparison of lower bound based on the theoretical model with empirical data (bottom plot). We have $\alpha = B_2/\ln(k) = 0.26$ from our model; $\alpha = 0.27$ directly from runtime data. Model B $\langle 20, 8, 60, 7 \rangle$, using `BT-random`.

theoretical model provides a good (tight) lower bound for the empirical data. Our findings about the distribution of inconsistent subtrees in backtrack search give, in effect, information about the inconsistent subproblems that are created during the search. We believe that these results can be exploited in the design of more efficient restart strategies and backtrack solvers.

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