12 Complexity of Search

- The “No Free Lunch” Theorem
- Combinatorial Phase Transitions
- Complexity of Local Search

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12.1 The “No Free Lunch” Theorem

- Wolpert & Macready 1997
- Basic content: All optimisation methods are equally good, when averaged over uniform distribution of objective functions.
- Alternative view: Any nontrivial optimisation method *must* be based on assumptions about the space of relevant objective functions. [However this is very difficult to make explicit and hardly any results in this direction exist.]
- Corollary: one cannot say, unqualified, that ACO methods are “better” than GA’s, or that Simulated Annealing is “better” than simple Iterated Local Search. [Moreover as of now there are *no* results characterising some nontrivial class of functions $\mathcal{F}$ on which some interesting method $\mathcal{A}$ would have an advantage over, say, random sampling of the search space.]

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The NFL theorem: definitions (1/4)

- Consider family $\mathcal{F}$ of all possible objective functions mapping finite search space $\mathcal{X}$ to finite value space $\mathcal{Y}$.
- A *sample d* from the search space is an ordered sequence of distinct points from $\mathcal{X}$, together with some associated cost values from $\mathcal{Y}$:

$$d = \{(d^x(1), d^y(1)), \dots, (d^x(m), d^y(m))\}.$$

  Here m is the *size* of the sample. A sample of size m is also denoted by d_m, and its projections to just the x- and y-values by d_m^x and d_m^y, respectively.
- The set of all samples of size m is thus $\mathcal{D}_m = (\mathcal{X} \times \mathcal{Y})^m$, and the set of all samples of arbitrary size is $\mathcal{D} = \cup_m \mathcal{D}_m$.

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The NFL theorem: definitions (2/4)

- An *algorithm* is any function a mapping samples to *new* points in the search space. Thus:

$$a : \mathcal{D} \to \mathcal{X}, \quad a(d) \notin d^x.$$

- *Note 1:* The assumption $a(d) \notin d^x$ is made to simplify the performance comparison of algorithms; i.e. one only takes into account *distinct* function evaluations. Not all algorithms naturally adhere to this constraint (e.g. SA, ILS), but without it analysis is difficult.
- *Note 2:* The algorithm may in general be stochastic, i.e. a given sample $d \in \mathcal{D}$ may determine only a *distribution* over the points $x \in \mathcal{X} - d^x$.

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The NFL theorem: definitions (3/4)

- A *performance measure* is any mapping Φ from cost value sequences to real numbers (e.g. minimum, maximum, average). Thus:

$$\Phi : \mathcal{Y}^* \to \mathbb{R},$$

where $\mathcal{Y}^* = \cup_m \mathcal{Y}^m$:

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The NFL theorem: definitions (4/4)

- Finally, denote by $P(d^y_m \mid f, m, a)$ the probability distribution of value samples of size m obtained by using a (generally stochastic) algorithm a to sample a (typically unknown) function $f \in \mathcal{F}$.
- More precisely, such a sample is obtained by starting from some a-dependent search point $d^x(1)$, querying f for the value $d^y(1) = f(d^x(1))$, using a to determine search point $d^x(2)$ based on $(d^x(1), d^y(1))$, etc., up to search point $d^x(m)$ and the associated value $d^y(m) = f(d^x(m))$. The value sample d^y_m is then obtained by projecting the full sample d_m to just the y-coordinates.

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The NFL theorem: statement

Theorem

[NFL] For any value sequence d^y_m and any two algorithms a_1 and a_2:

$$\sum_{f \in \mathcal{F}} P(d^y_m \mid f, m, a_1) = \sum_{f \in \mathcal{F}} P(d^y_m \mid f, m, a_2).$$

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The NFL theorem: corollaries

Corollary

[1] Assume the uniform distribution of functions over $\mathcal{F}$, $P(f) = 1/|\mathcal{F}| = |\mathcal{Y}|^{-|\mathcal{X}|}$. Then for any value sequence $d^y_m \in \mathcal{Y}^m$ and any two algorithms a_1 and a_2:

$$P(d^y_m \mid m, a_1) = P(d^y_m \mid m, a_2).$$

Corollary

[2] Assume the uniform distribution of functions over $\mathcal{F}$. Then the expected value of any performance measure Φ over value samples of size m,

$$E(\Phi(d^y_m) \mid m, a) = \sum_{d^y_m \in \mathcal{Y}^m} \Phi(d^y_m) P(d^y_m \mid m, a),$$

is independent of the algorithm a used.

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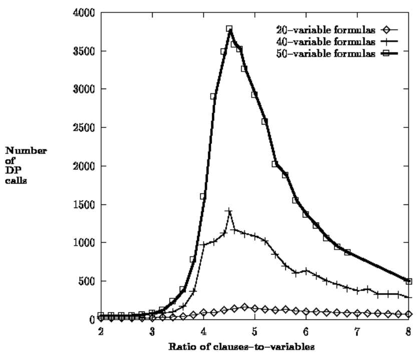
12.2 Combinatorial Phase Transitions

- “Where the Really Hard Problems Are” (Cheeseman et al. 1991)
- Many NP-complete problems can be solved in polynomial time “on average” or “with high probability” for reasonable-looking distributions of problem instances. E.g. Satisfiability in time $o(n^2)$ (Goldberg et al. 1982), Graph Colouring in time $o(n^2)$ (Grimmett & McDiarmid 1975, Turner 1984).
- Where, then, are the (presumably) exponentially hard instances of these problems located? Could one tell ahead of time whether a given instance is likely to be hard?
- Early studies: Yu & Anderson (1985), Hubermann & Hogg (1987), Cheeseman, Kanefsky & Taylor (1991), Mitchell, Selman & Levesque (1992), Kirkpatrick & Selman (1994), etc.

Hard instances for 3-SAT (1/4)

- Mitchell, Selman & Levesque, AAAI-92
- Experiments on the behaviour of the DPLL procedure on randomly generated 3-cnf Boolean formulas.
- Distribution of test formulas:
  - n = number of variables
  - $m = \alpha n$ randomly generated clauses of 3 literals, $2 \leq \alpha \leq 8$
- For sets of 500 formulas with $n = 20/40/50$ and various α, Mitchell et al. plotted the median number of recursive DPLL calls required for solution.

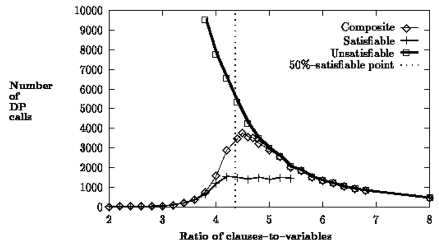
Hard instances for 3-SAT (2/4)



Results:

- A distinct peak in median running times at about clauses-to-variables ratio $\alpha \approx 4.5$.
- Peak gets more pronounced for increasing $n \Rightarrow$ well-defined “delta” distribution for infinite n?

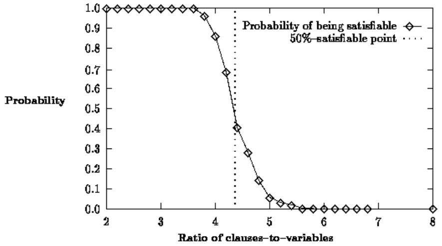
Hard instances for 3-SAT (3/4)



- The runtime peak seems to be located near the point where 50% of formulas are satisfiable.
- The peak seems to be caused by relatively short unsatisfiable formulas.

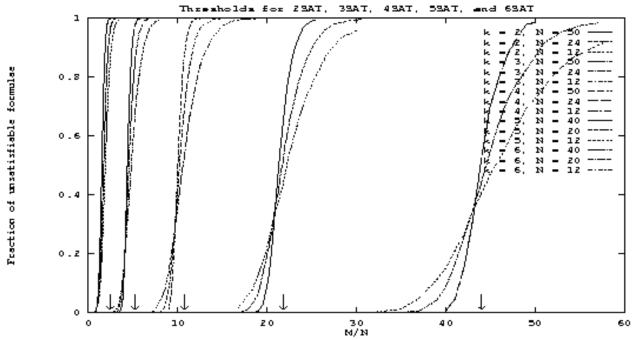
Question: Is the connection of the running time peak and the satifiability threshold a characteristic of the DPLL algorithm, or a (more or less) algorithm independent “universal” feature?

The satisfiability transition (1/2)



Mitchell et al. (1992): The "50% satisfiable" point or "satisfiability threshold" for 3-SAT seems to be located at $\alpha \approx 4.25$ for large n.

The satisfiability transition (2/2)



Kirkpatrick & Selman (1994):

- Similar experiments as above for k-SAT, $k = 2, \ldots, 6$, 10000 formulas per data point.
- The "satisfiability threshold" α_c shifts quickly to larger values of α for increasing k.

Statistical mechanics of k-SAT (1/4)

Kirkpatrick & Selman, *Science* 1994

A "spin glass" model of a k-cnf formula:

- variables x_i $\sim$ spins with states ± 1
- clauses c $\sim$ k-wise interactions between spins
- truth assignment σ $\sim$ state of spin system
- Hamiltonian $H(\sigma)$ $\sim$ number of clauses unsatisfied by σ
- α_c $\sim$ critical "interaction density" point for "phase transition" from "satisfiable phase" to "unsatisfiable phase"

Statistical mechanics of k-SAT (2/4)

Estimates of α_c for various values of k via "annealing approximation", "replica theory", and observation:

k	α_{ann}	α_{rep}	α_{obs}
2	2.41	1.38	1.0
3	5.19	4.25	4.17 ± 0.03
4	10.74	9.58	9.75 ± 0.05
5	21.83	20.6	20.9 ± 0.1
6	44.01	42.8	43.2 ± 0.2

Statistical mechanics of k-SAT (3/4)

The "annealing approximation" means simply assuming that the different clauses are satisfied independently. This leads to the following estimate:

- Probability that given clause c is satisfied by random σ: $p_k = 1 - 2^{-k}$.
- Probability that random σ satisfies all $m = \alpha n$ clauses assuming independence: $p_k^{\alpha n}$.
- E[number of satisfying assignments] $= 2^n p_k^{\alpha n} \triangleq S_k^n(\alpha)$.
- For large n, $S_k^n(\alpha)$ falls rapidly from 2^n to 0 near a critical value $\alpha = \alpha_c$. Where is α_c?
- One approach: solve for $S_k^n(\alpha) = 1$.

$$S_k^n(\alpha) = 1 \Leftrightarrow 2p_k^{\alpha} = 1$$

$$\Leftrightarrow \alpha = -\frac{1}{\log_2 p_k} = -\frac{\ln 2}{\ln(1-2^{-k})} \approx \frac{\ln 2}{2^{-k}} = (\ln 2) \cdot 2^k$$

Statistical mechanics of k-SAT (4/4)

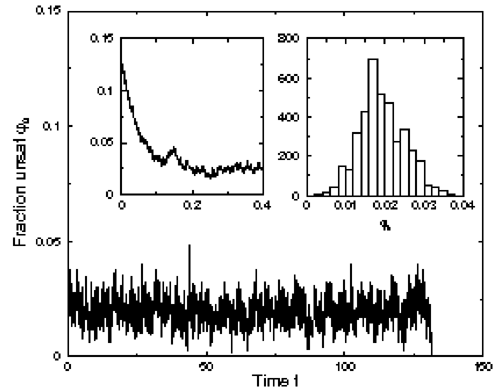
It is in fact known that:

- A sharp satisfiability threshold α_c exists for all $k \geq 2$ (Friedgut 1999).
- For $k = 2$, $\alpha_c = 1$ (Goerdt 1982, Chvátal & Reed 1982). Note that 2-SAT $\in$ P.
- For $k = 3$, $3.145 < \alpha_c < 4.506$ (lower bound due to Achlioptas 2000, upper bound to Dubois et al. 1999).
- Current best empirical estimate for $k = 3$: $\alpha_c \approx 4.267$ (Braunstein et al. 2002).
- For large k, $\alpha_c \sim (\ln 2) \cdot 2^k$ (Achlioptas & Moore 2002).

12.3 Complexity of Local Search

- Good experiences for 3-SAT in the satisfiable region $\alpha < \alpha_c$: e.g. GSAT (Selman et al. 1992), WalkSAT (Selman et al. 1996).
- *Focusing* the search on unsatisfied clauses seems to be an important technique: in the (unsystematic) experiments in Selman et al. (1996), WalkSAT (focused) outperforms NoisyGSAT (unfocused) by several orders of magnitude.

Dynamics of local search



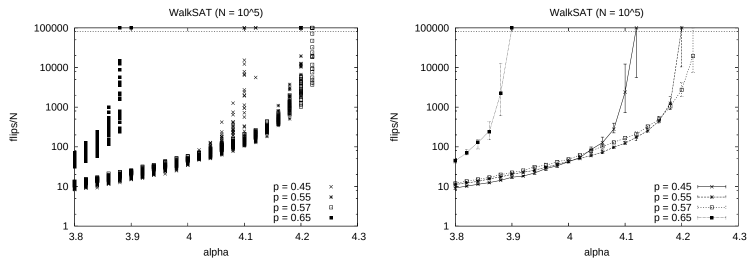
A WalkSAT run with $p = 1$ ("focused random walk") on a randomly generated 3-SAT instance, $\alpha = 3$, $n = 500$: evolution in the fraction of unsatisfied clauses (Semerjian & Monasson 2003).

Some recent results and conjectures

- Barthel, Hartmann & Weigt (2003), Semerjian & Monasson (2003): WalkSAT with $p = 1$ has a “dynamical phase transition” at $\alpha_{\mathrm{dyn}} \approx 2.7 - 2.8$. When $\alpha < \alpha_{\mathrm{dyn}}$, satisfying assignments are found in linear time per variable (i.e. in a total of cn “flips”), when $\alpha > \alpha_{\mathrm{dyn}}$ exponential time is required.
- Explanation: for $\alpha > \alpha_{\mathrm{dyn}}$ the search equilibrates at a nonzero energy level, and can only escape to a ground state through a large enough random fluctuation.
- Conjecture: all local search algorithms will have difficulties beyond the so called “clustering transition” at $\alpha \approx 3.92 - 3.93$ (Mézard, Monasson, Weigt et al.)

Some WalkSAT experiments

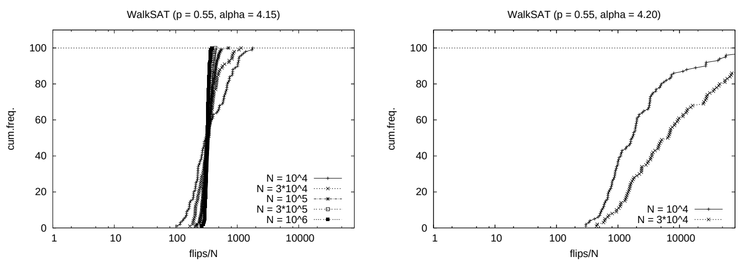
For $p > 1$, the α_{dyn} barrier for linear solution times can be broken (Aurell & Kirkpatrick 2004; Seitz, Alava & Orponen 2005).



Normalised (flips/n) solution times for finding satisfying assignments using WalkSAT, $\alpha = 3.8 \ldots 4.3$.
Left: complete data; right: medians and quartiles.

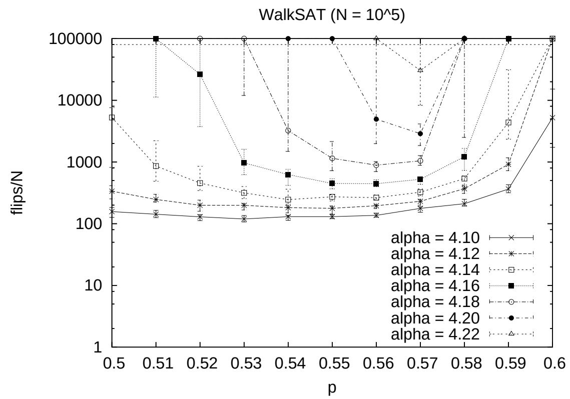
Data suggest linear solution times for $\alpha \gg \alpha_{\mathrm{dyn}} \approx 2.7$.

WalkSAT linear scaling



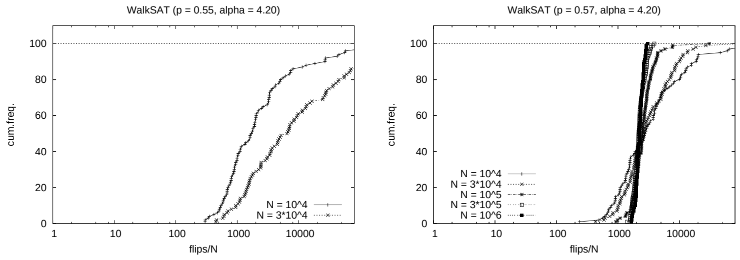
Cumulative solution time distributions for WalkSAT with $p = 0.55$.

WalkSAT optimal noise level?



Normalised solution times for WalkSAT with $p = 0.50 \ldots 0.60$, $\alpha = 4.10 \ldots 4.22$.

WalkSAT sensitivity to noise

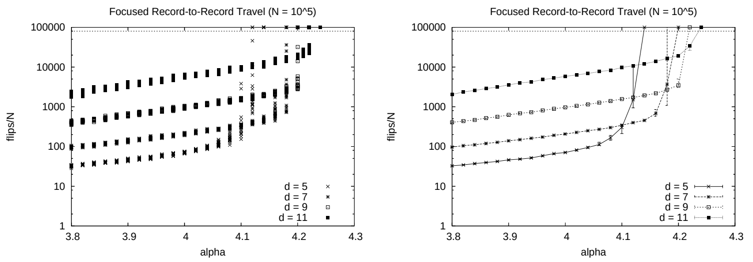


Cumulative solution time distributions for WalkSAT at $\alpha = 4.20$ with $p = 0.55$ and $p = 0.57$.

RRT applied to random 3-SAT

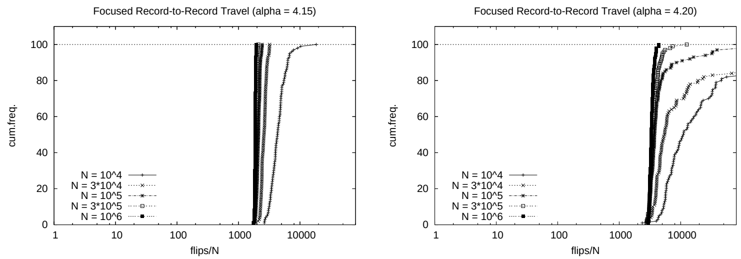
- Similar results as for WalkSAT are obtained with the Record-to-Record Travel algorithm.
- In applying RRT to SAT, $E(s)$ = number of clauses unsatisfied by truth assignment s. Single-variable flip neighbourhoods.
- *Focusing:* flipped variables chosen from unsatisfied clauses. (Precisely: one unsatisfied clause is chosen at random, and from there a variable at random.) $\Rightarrow$ FRRT = focused RRT.

FRRT experiments (3-SAT)



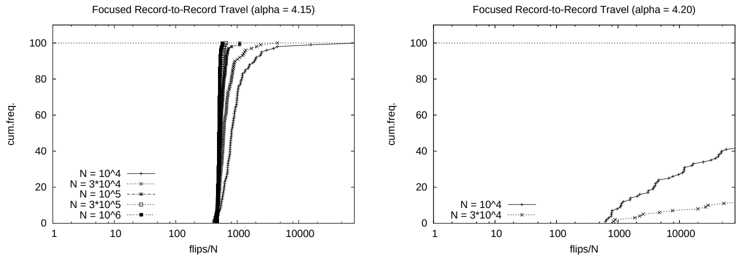
Normalised solution times for FRRT, $\alpha = 3.8 \ldots 4.3$.
Left: complete data; right: medians and quartiles.

FRRT linear scaling (1/2)



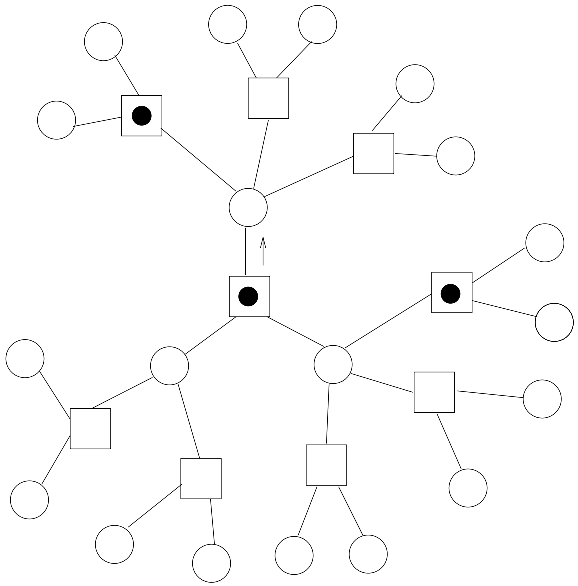
Cumulative solution time distributions for FRRT with $d = 9$.

FRRT linear scaling (2/2)

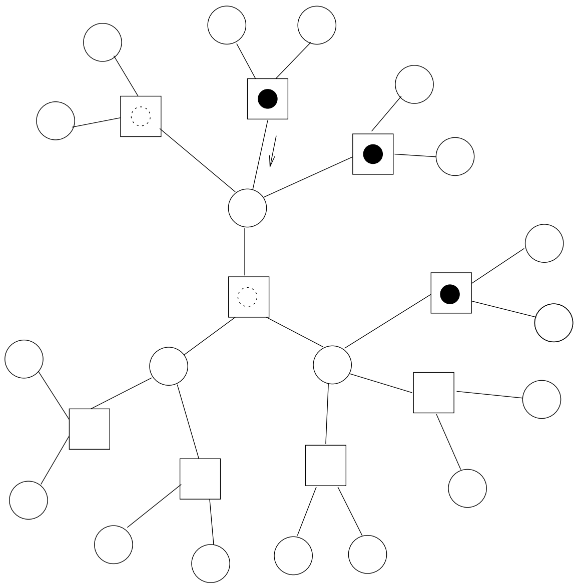


Cumulative solution time distributions for FRRT with $d = 7$.

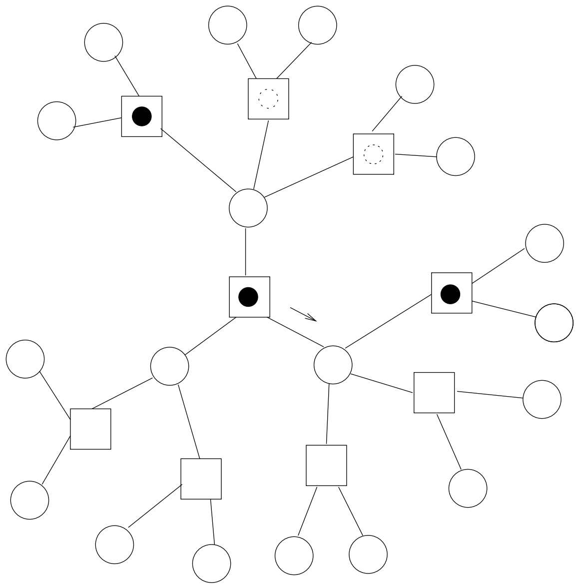
Focused search as a contact process



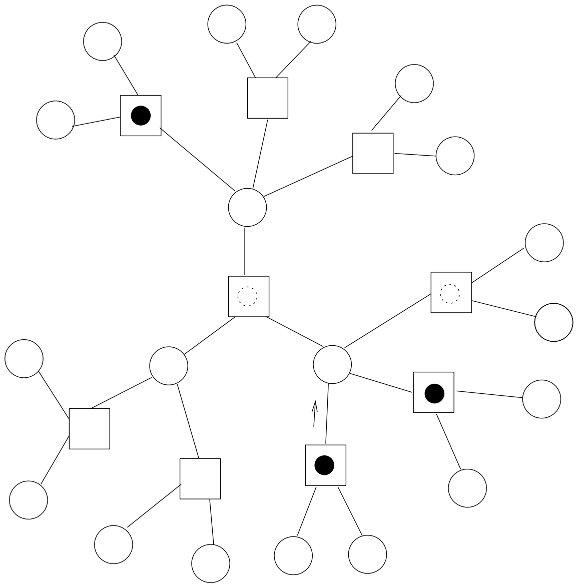
Focused search as a contact process



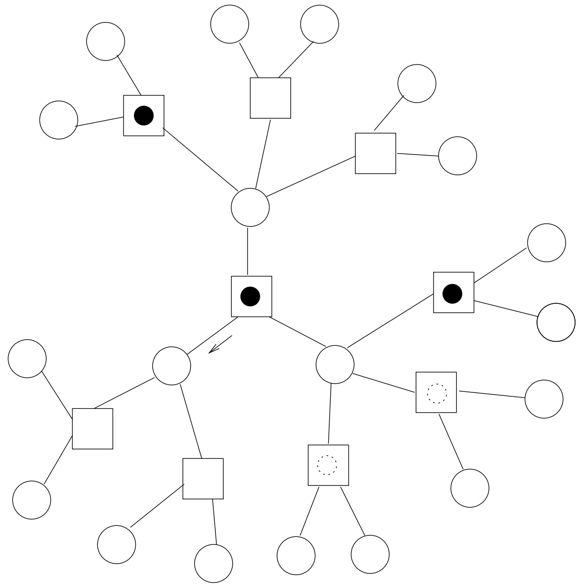
Focused search as a contact process



Focused search as a contact process



Focused search as a contact process



Focused search as a contact process