Statistical physics of search algorithms

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Lectures shortly available on http://www.lpt.ens.fr/~monasson

Trieste, september 2002

Content of the lectures

- *Today :*
  - Dynamical processes in physics …
    Algorithms for solving optimization problems
    Reminder on random 3-SAT
  - Analysis of random 3-SAT solving with a backtracking procedure

- *Tomorrow :*
  - Local search algorithms for random SAT
    - Gradient descent
    - Clause flip

Purpose: give technical ability to carry out calculations!

Dynamical processes in Physics

Configuration of variables $X=\{x_1,x_2,\ldots,x_N\}$ e.g. spins
Energy function H[X]
Equilibrium Probability Distribution $P_{gibbs}[X] = \exp(-H[X]/T) / Z$

Dynamics: *X at time T* ⇢ *Y at time T+1*

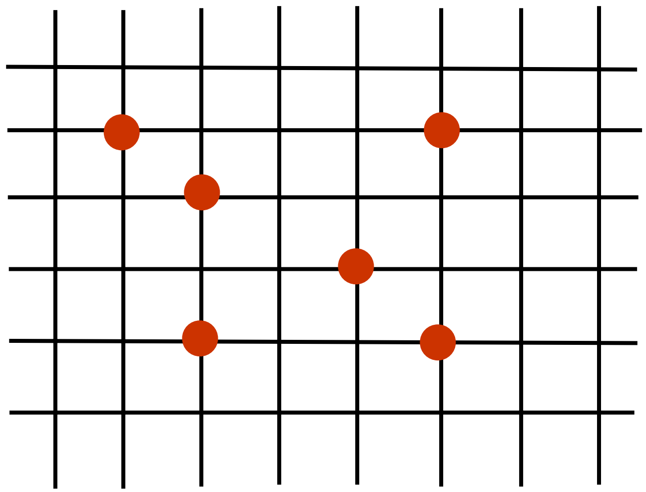
- $P[X,T=0] =$ d$_X$ or $1/2^N$
- $P[Y,T+1] =$ Ê$_X$ $M[Y,X]\ P[X,T]$ $\xrightarrow[\text{T ö ¶}]{}$ $P_{gibbs}[Y]$

e.g. Metropolis (one spin flip) $M[Y,X] = \begin{cases} 1 & \text{if } H[Y] \text{ § } H[X] \\ e^{-(H[Y]-H[X])/T} & \text{if } H[Y] \text{ ¥ } H[X] \end{cases}$

Convergence if T ö ¶, then N ö ¶

But what happens if N ö ¶, then T ö ¶ ?

Dynamical processes without Hamiltonian



Contact process:

- graph with vertices occupied or empty
- ocuppied becomes empty with prob. P
- empty becomes occupied with prob. Q×occup. neighbors

Evolution rules

- Large time limit: all empty!
- Non trivial if N infinite first
- Life time as a function of N (relaxation).

Combinatorial optimization algorithms

= set of evolution rules for an instance and/or a configuration of variables leading to a solution.

- Complete algorithms:

  tells you whether an instance of SAT has a solution or not (solves exactly a decision problem).

- Local search algorithms:

  looks for solutions through a sequence of small improvements of some initial configuration (cannot prove unsatisfiability).

- Probabilistic algorithms:

  Local search + upper bound on the probability of failure
  (one sided probabilistic algorithm)

Want to study various properties of algorithms, essentially average (or distribution) of running times.

A reminder on the Satisfiability of (random) Boolean constraints

(w or NOT x or y)
and
(NOT w or x or z)
and
(x or y or NOT z)

?

3-SAT NP-complete
(and >3)

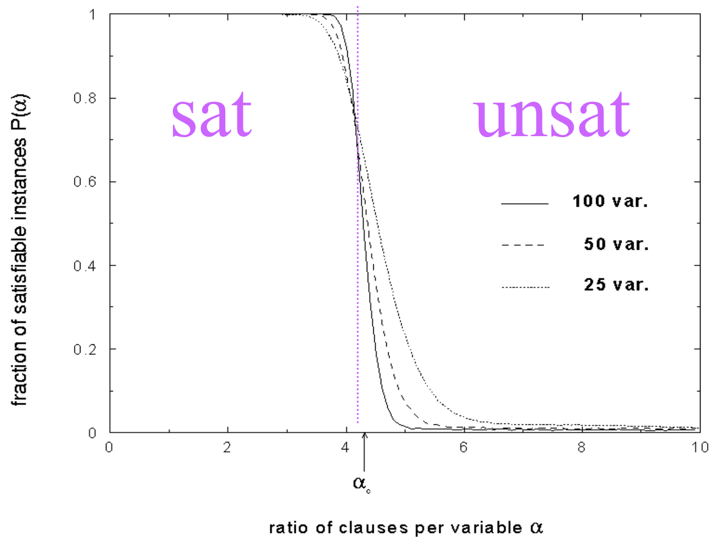
2-SAT P

$$\alpha = \frac{\text{nb. of clauses}}{\text{nb. of variables}}$$

Mitchell, Selman, Levesque ‘92
Crawford, Auton ‘93
Gent, Walsh ‘94

Chao, Franco ‘86, ‘90
Chvatal, Szmeredi ‘88

Phase transition and typical complexity

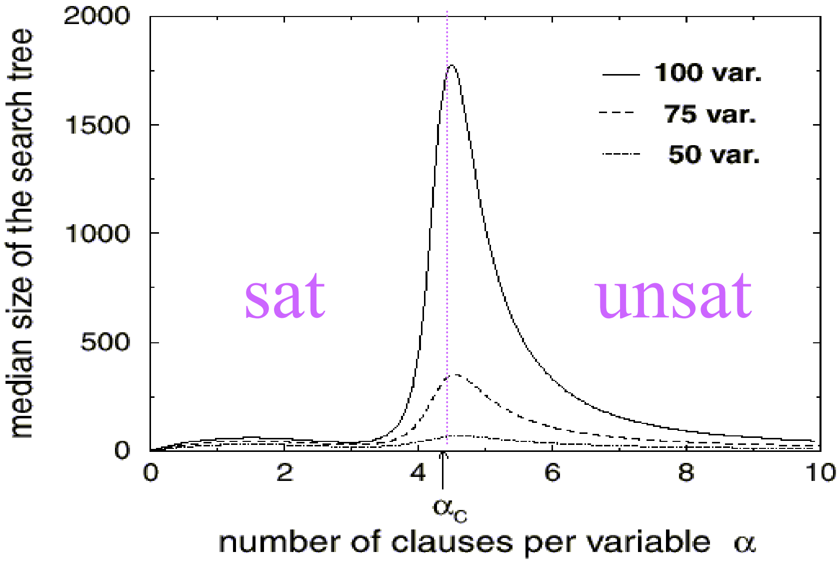


$\alpha_C \approx 4.3$

phase transition!

Rigorous results:

- $\alpha_C > 3.42$
- $\alpha_C < 4.51$
- transition region width $\rightarrow 0$



easy-hard-less hard pattern

Rigorous results:

- linear if $\alpha << \alpha_C$
- exponential if $\alpha > \alpha_C$
- "time" $< 1.5^N$

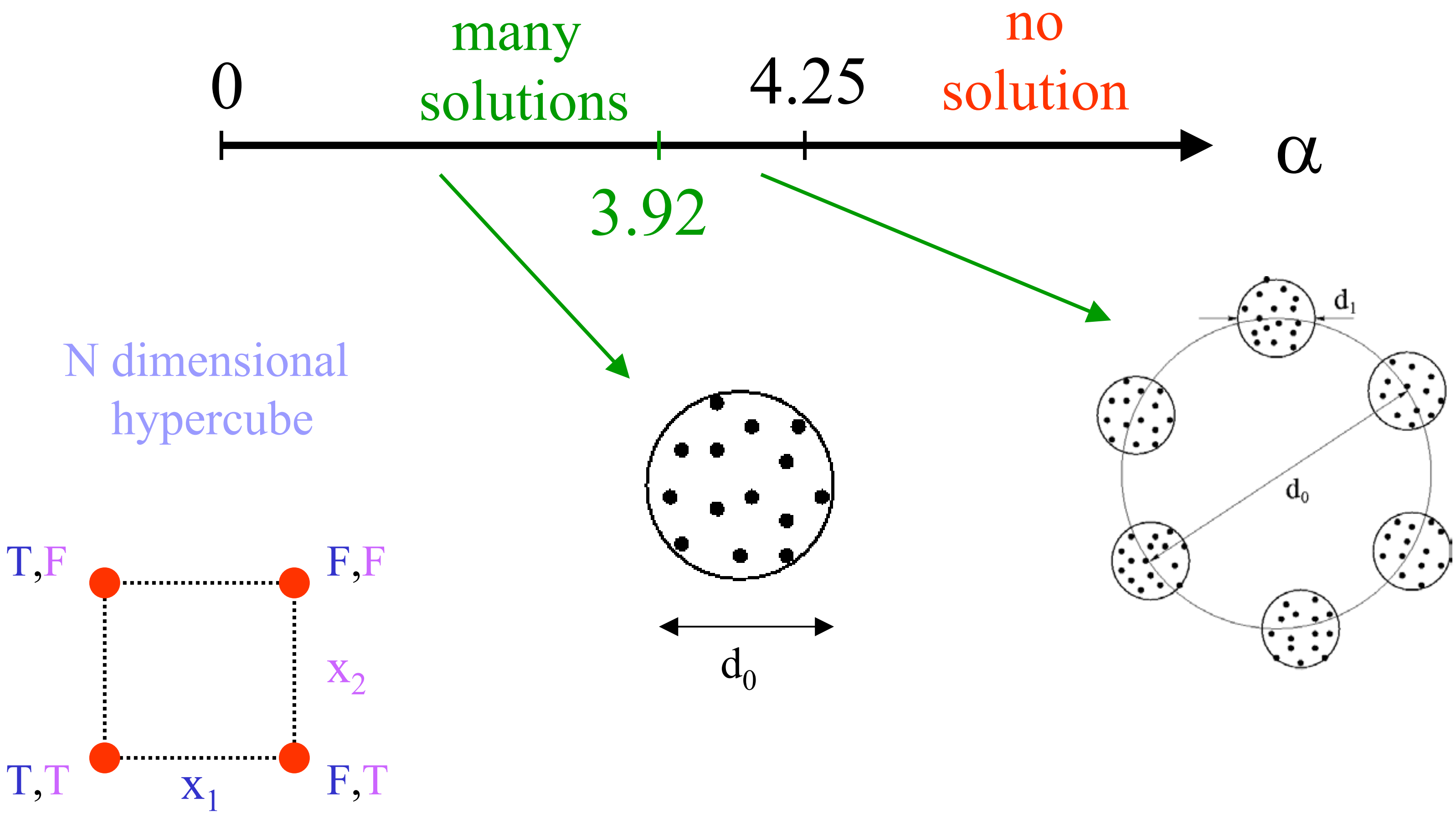
SAT,
a disordered
spin system
(at zero
temperature)

Dictionary

K-SAT	*statistical physics*
Boolean variable x = True , False	*Ising spin* $s_x = +1, -1$
Clauses	*Couplings and fields acting on spins*
Number of clauses violated by a logical configuration	*Energy E of the spins configuration*
some examples:	
2 SAT x or $\bar{y}$	$E = \frac{1}{4}(1-s_x)(1+s_y)$
(x or $\bar{y}$) and ($\bar{x}$ or z)	$E = \frac{1}{4}(1-s_x)(1+s_y) + \frac{1}{4}(1+s_x)(1-s_y)$
3 SAT x or $\bar{y}$ or z	$E = \frac{1}{8}(1-s_x)(1+s_y)(1-s_z)$
Minimal number of violated clauses	*Ground state energy*
The problem is satisfiable	*Ground state energy* = 0
The problem is not satisfiable	*Ground state energy* > 0

Cf. Lecture on Stat. Mech. by C. Borgs and J. Chayes.

Phase diagram of random 3-SAT



Cf. Lecture on Stat. Mech. Of Disordered Systems by M. Mezard.

Dynamics of the Davis-Putnam-Loveland-Logemann algorithm

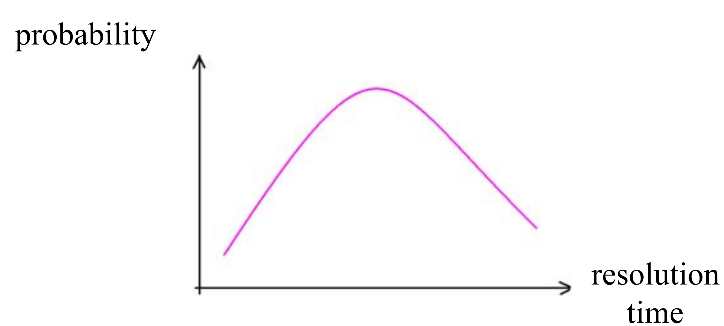
Rigorous analysis of search heuristics

Quantitative study of search trees (with backtracking)

$2^{N w}$

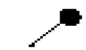
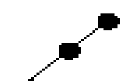
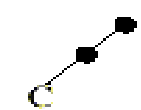
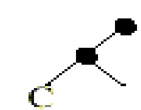
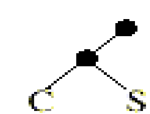
?

Distribution of resolution times (left tail)



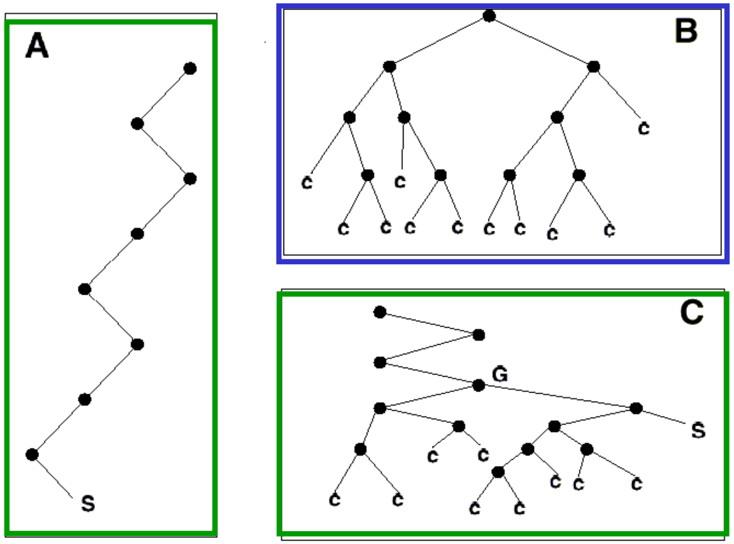
How to solve 3-SAT?

DPLL "Branch & bound" search algorithm

step	clauses	search tree
0	$w \vee \bar{x} \vee y$ $\bar{w} \vee x \vee z$ $\bar{w} \vee \bar{x} \vee \bar{y}$ $\bar{w} \vee \bar{x} \vee y$ $x \vee y \vee \bar{z}$	
1	split : $w = T$	
2	$x \vee z$ $\bar{x} \vee \bar{y}$ $\bar{x} \vee y$ $x \vee y \vee \bar{z}$	
3	split : $x = T$	
4	$\bar{y}$ y	
5	propagation : $y = F$, $y = T$ contradiction	
6	backtracking to stage 1 : $x = F$	
7	z $y \vee \bar{z}$	
8	propagation : $z = T$, $y = T$ solution : $w = T$, $x = F$, $y = T$, $z = T$	

Backtrack algorithm, search tree and heuristic

Davis-Putnam algorithm = heuristic + backtracking
↓
search tree



A satisfiable instance (easy)

B unsatisfiable instance (hard)

C satisfiable instance (hard)

Complexity = size of search tree (= number of nodes –or leaves-)

- Unit-Clause (UC): pick variable in 1-clause if any, or any unset variable
- Generalized unit-clause (GUC): pick variable in shortest clause
- Shortest Clause With Majority (SC): pick most frequent variable in 3-clauses

Trajectories and the 2+p-SAT problem

clauses with 3 var.

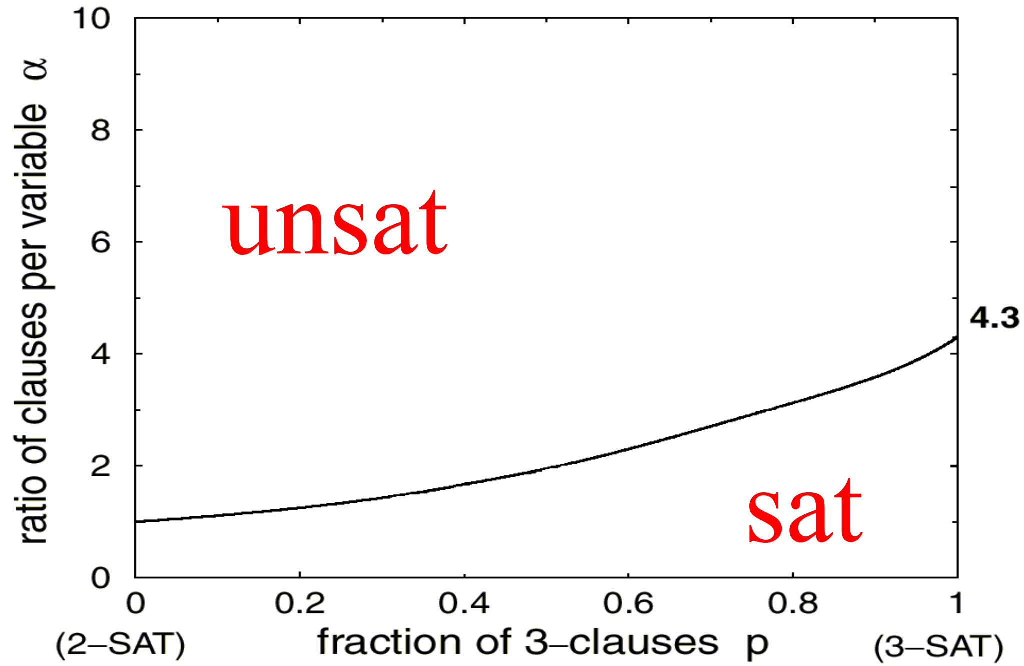
α

"dynamics" of the algorithm

clauses with 2 or 3 var.

α , p

phase diagram of the 2+p-SAT model



Analysis of the GUC heuristic (I)

NO BACKTRACKING !

Evolution rules:

1. If no clause left, output « Satisfiable »;
2. Otherwise, select randomly a shortest clause e.g. *(not y)*, and set one of its literals to True e.g. *y=F.*
3. Simplify remaining clauses;
   e.g. *(not y or z) is removed, (y or w or q)* ö *(w or q)*
3. If a unit clause with false literal appears e.g. *(y)*, output « Contradiction »;
   Else go to 2.

NB: Contradiction does not mean Unsatisfiable!

Analysis of the GUC heuristic (II)

Call $P^{(K)}[M;N]$ the measure over random K-SAT instances with M clauses and N variables.

Call P_T[instance] the measure over instances after T steps of the heuristic.

3-SAT instances $\xrightarrow[\text{heuristic}]{\text{GUC}}$ Mixed 1-,2-,3-SAT instances

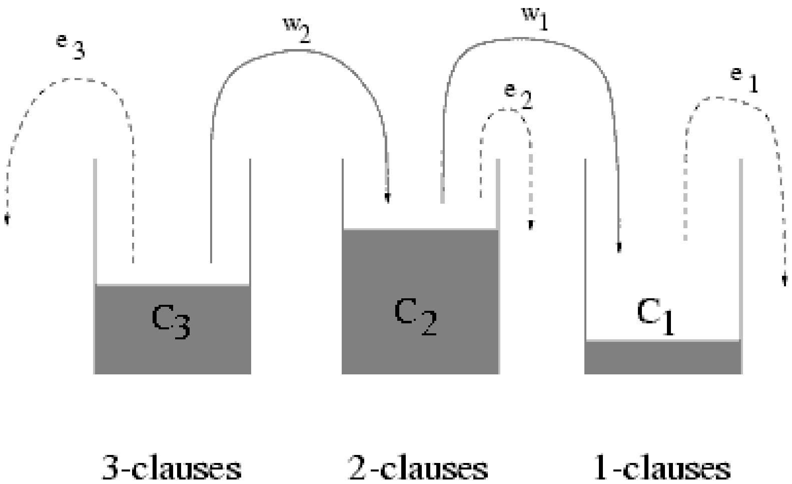
Initial measure
$P_{T=0}[instance] = P^{(3)}[M;N]$

Measure $P_T[instance]$?

Define the numbers $C_1(T)$, $C_2(T)$, $C_3(T)$ of 1-, 2-, 3-clauses after T steps;
Then:

$$\boxed{P_T[\text{instance} \mid C_1(T), C_2(T), C_3(T)] = P^{(1)}[C_1(T);N-T] \approx P^{(2)}[C_2(T);N-T] \approx P^{(3)}[C_3(T);N-T]}$$

Analysis of the GUC heuristic (III)



Flows of
clause populations

$$C_3(T+1) = C_3(T) - e_3(T) - w_2(T)$$
$$C_2(T+1) = C_2(T) - e_2(T) + w_2(T) - w_1(T)$$
$$C_1(T+1) = C_1(T) - e_1(T) + w_1(T) - 1$$

- Average values of e and w: $< e_3(T) > = < w_2(T) > = \dfrac{3}{2\,(N-T)} <C_3(T)> = O(1)$
- Concentration of clause densities:

$$C_j(T) = N\, c_j\left(\frac{T}{N}\right) + o(N) \qquad (j = 2, 3)$$

Reduced time
t=T/N

fl $< e_3(t) > = < w_2(t) > = \dfrac{3\ c_3(t)}{2\ (1-t)}$

Analysis of the GUC heuristic (IV)

Set of coupled Ordinary Differential Equations:

$$
\begin{aligned}
\frac{\mathrm{d}c_3(t)}{\mathrm{d}t} &= -\frac{3}{1-t}c_3(t) - \rho_3(t) \\
\frac{\mathrm{d}c_2(t)}{\mathrm{d}t} &= \frac{3}{2(1-t)}c_3(t) - \frac{2}{1-t}c_2(t) - \rho_2(t)
\end{aligned}
$$

where $r_j(t)$ is the probability that a literal is chosen from a j-clause at time t,

$$r_1(t) + r_2(t) + r_3(t) = 1$$

What are the values of these probabilities?

Analysis of the GUC heuristic (V)

Estimate the initial creation rate of 2-clauses: $< w_2(0) > = \dfrac{3\,a}{2}$

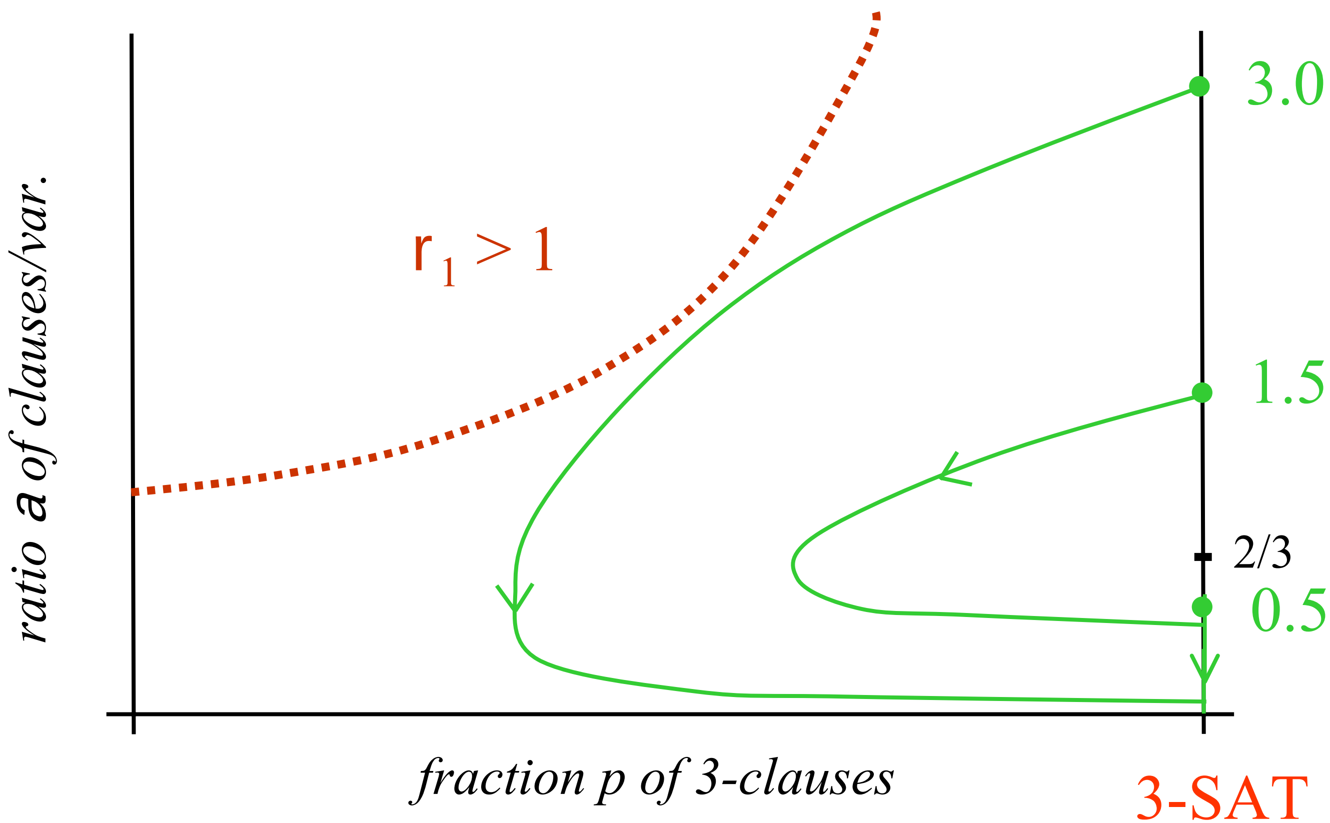
Case $a < 2/3$ $$\rho_1(t) = 0; \quad \rho_2(t) = \frac{3c_3(t)}{2(1-t)}; \quad \rho_3(t) = 1 - \rho_2(t)$$

Case $a > 2/3$ $$\rho_1(t) = \frac{c_2(t)}{1-t}\ ; \quad \rho_2(t) = 1 - \rho_1(t); \quad \rho_3(t) = 0$$

should always be smaller than unity!!!

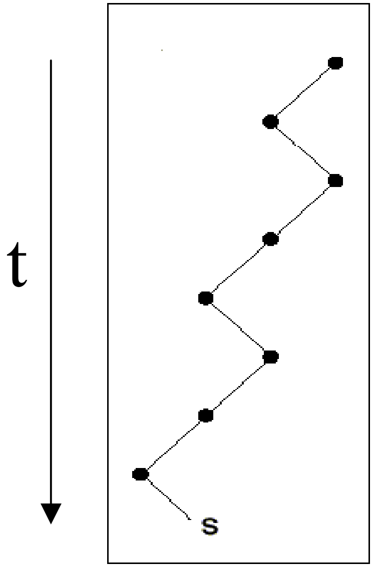
Analysis of the GUC heuristic (VI)

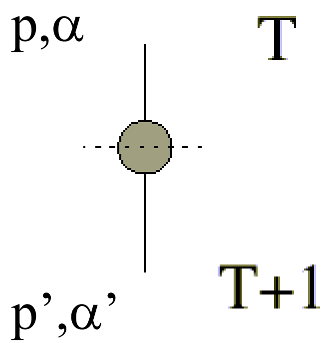
$$p(t) = \frac{c_3(t)}{c_2(t) + c_3(t)}, \qquad \alpha(t) = \frac{c_2(t) + c_3(t)}{1 - t}$$



OK if a < 3.003… (also sufficient condition)

Analysis of the GUC heuristic (VII)



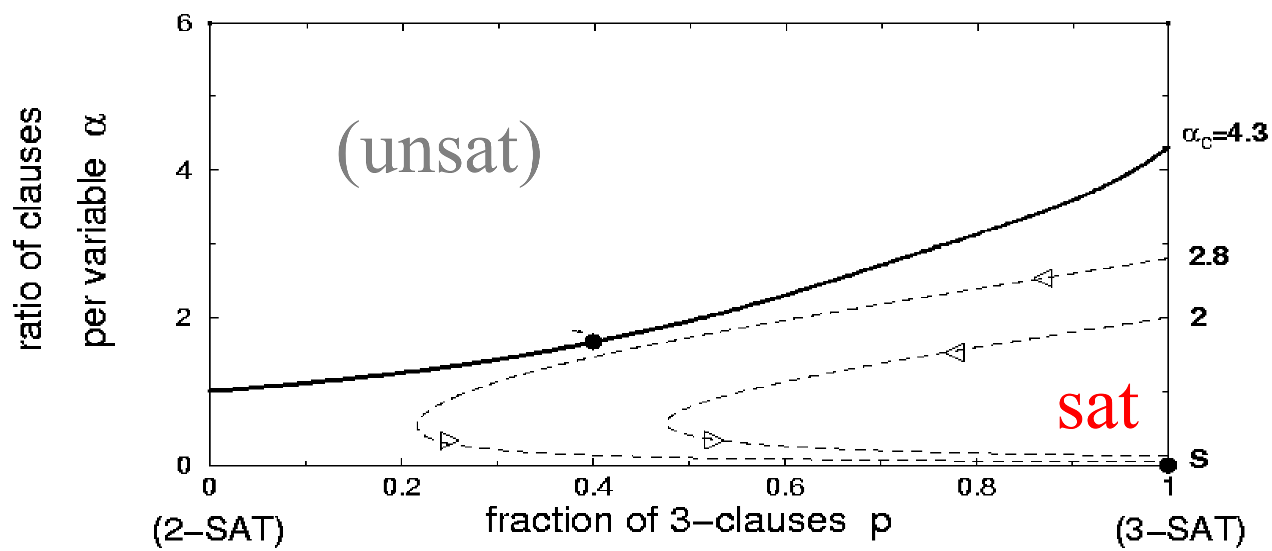


$$p(0)=1\ ,\ \alpha(0)=\alpha_0$$

$$\frac{dp}{dt}=F_p(p,\alpha,t)$$

$$\frac{d\alpha}{dt}=F_\alpha(p,\alpha,t)$$

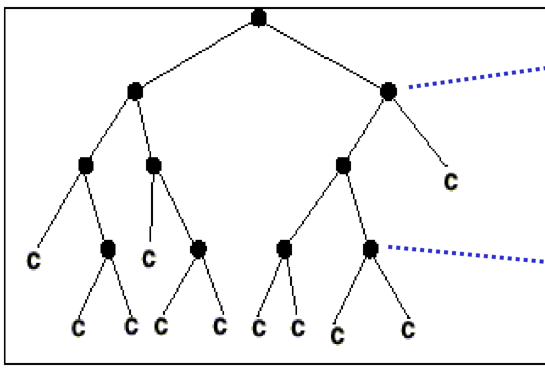
(ODE)



Complete search trees (I)

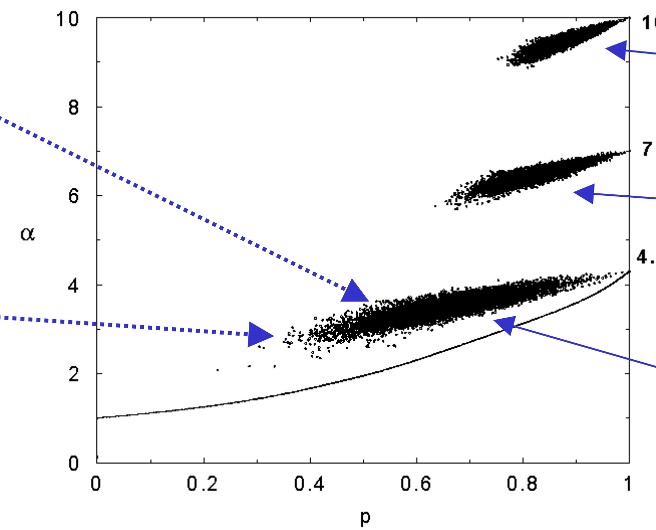
$a > a_C$

2+p-SAT phase diagram



p_1, a_1

p_2, a_2



N=300
6600 nodes

N=200
6300 nodes

N=120
7600 nodes

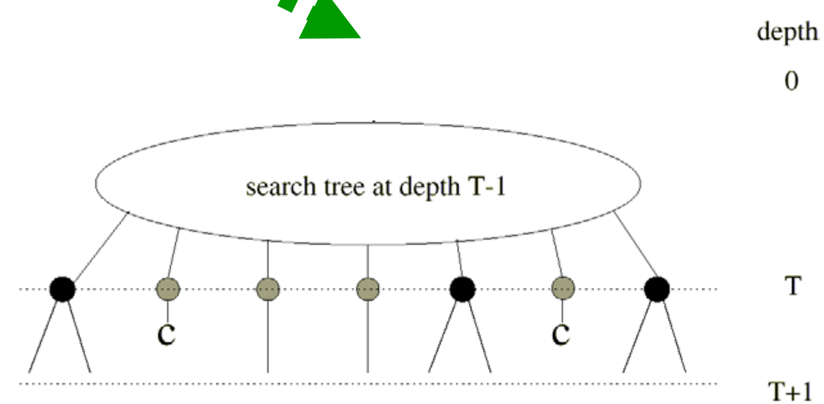
Proof of unsatisfiability

one branch: *$p(t)$, $\alpha(t)$* *ODE* → many branches: *$\omega\,(p,\alpha,t)$* *PDE*

Complete search trees (II)

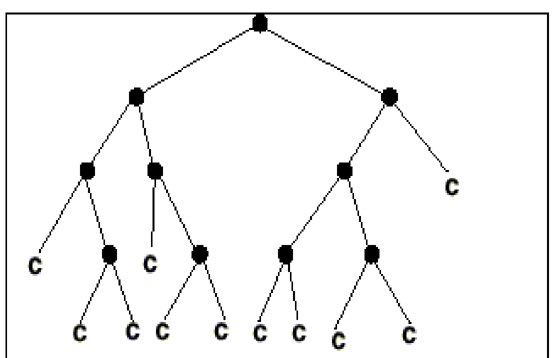
Instance to be solved

DPLL induces a non Markovian evolution of the search tree



Imaginary, parallel building up of the search tree

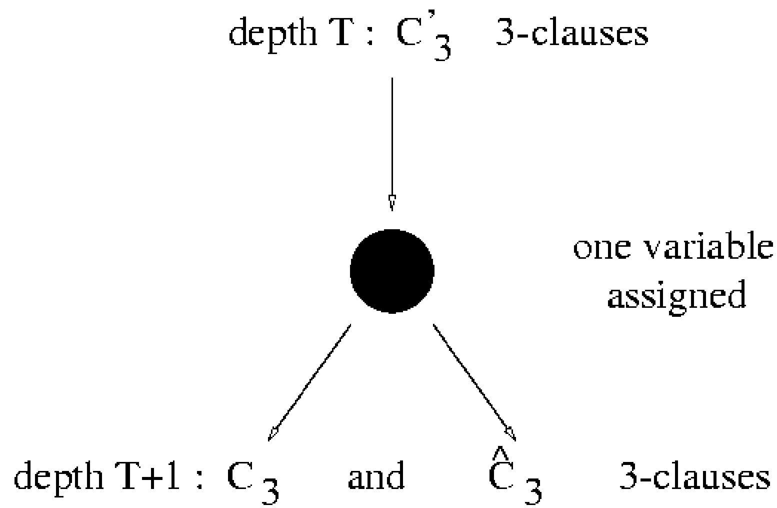
Final Search tree



Toy model of search tree (I)

Consider only
clauses with 3 variables

(Dont'care about empty clauses!)



• Obviously the total number of branches at depth T equals $B(T)=2^T$.

• Consider the number of branches B with C_3 3-clauses:

$$B(C_3; T+1) = \sum_{C_3'=0}^{\infty} K_{\mathrm{toy}}\,(C_3, C_3'; T)\, B(C_3'; T).$$

branching matrix

Toy model of search tree (II)

Branching matrix is simply (twice) a Binomial law:

$$K_{\text{toy}}\,(C_3, C_3'; T) = 2\binom{C_3'}{C_3' - C_3}\left(\frac{3}{N-T}\right)^{C_3'-C_3}\left(1-\frac{3}{N-T}\right)^{C_3}$$

Consider the action of the algorithm during the interval,

$$T_0 = t\,N \leq T \leq T_1 = (t+\epsilon)\,N$$

Then, clause densities are expected to change by O(ϵ), and

$$K_{\text{toy}}(C_3', C_3, t) = 2\,\chi\,(C_3' - C_3)\,e^{-m_3(t)}\,\frac{m_3(t)^{C_3'-C_3}}{(C_3'-C_3)!} + O(\epsilon)$$

where $\quad m_3(\text{t}) = \dfrac{3\,c_3(\text{t})}{2\,(1\text{-t})}$

Toy model of search tree (III)

During time interval $\mathcal{T} = T_1 - T_0 = \epsilon\, N$, branches numbers change according to

$$\boxed{B(C_3; t\, N + \mathcal{T}) = \sum_{C_3'=0}^{\infty} \left[K_{\mathrm{toy}}\right]^{\mathcal{T}} \, (C_3', C_3; t)\, B(C_3'; t\, N)}$$

- Diagonalization of the (Toeplitz) matrix K_{toy}:

Eigenvectors: $v(q_3, C_3) = \mathrm{e}^{\mathrm{i}\, q_3\, C_3} / \sqrt{2\pi}$ with $0 \le q_3 < 2\,\pi$
(wave number)

Eigenvalues: $\lambda_{q_3}(t) = 2\ \exp\left[m_3(t)\ \left(\mathrm{e}^{\mathrm{i}\, q_3} - 1\right) \right]$

- Exponential scaling Ansatz for the numbers of branches:

$$\lim_{N\to\infty} \frac{1}{N} \ln B(c_3\, N; t\, N) = \omega(c_3, t).$$

Toy model of search tree (IV)

Finally, changing the sum over clauses number into an integral through,

$$C_3' - C_3 = r_3\,\mathcal{T}$$

allows to obtain

$$\boxed{\begin{aligned}\exp\Big(N\,\omega(c_3, t+\epsilon)\Big) = \mathcal{T}\int_0^{c_3/\epsilon} \mathrm{d}r_3 \int_0^{2\pi} \frac{\mathrm{d}q_3}{2\pi} \\ \times \exp\Big[N\,\big(\epsilon\ln\lambda_{q_3}(t) - \mathrm{i}\,\epsilon\,r_3\,q_3 + \omega(c_3+\epsilon\,r_3, t)\big)\Big]\end{aligned}}$$

Now:

1. Estimate integrals through saddle-points;
2. Expand up to first order in e assuming w is once differentiable with respect to t and c_3.

Toy model of search tree (V)

We obtain:

$$\frac{\partial \omega}{\partial t}(c_3, t) = \max_{r_3, q_3} \left(\ln \lambda_{q_3}(t) - \mathrm{i}\, r_3\, q_3 + r_3 \frac{\partial \omega}{\partial c_3}(c_3, t) \right)$$

Saddle point over r_3: $q_3 = -\mathrm{i}\frac{\partial \omega}{\partial c_3}$

$$\boxed{\frac{\partial \omega}{\partial t}(c_3, t) = \ln 2 - \frac{3\, c_3}{1-t} + \frac{3\, c_3}{1-t}\; \exp\left[\frac{\partial \omega}{\partial c_3}(c_3, t)\right]}$$

Initial condition:

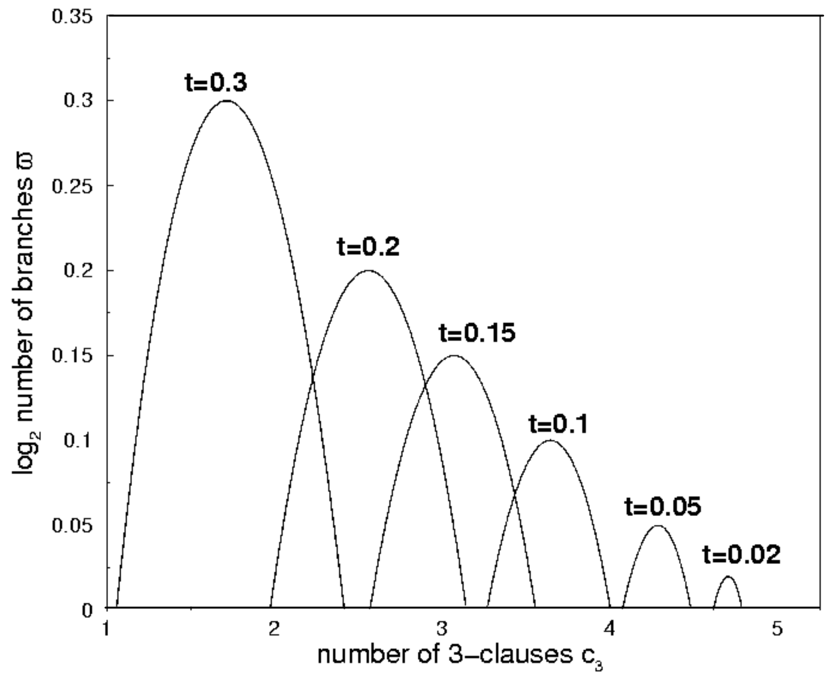
$$\boxed{\mathrm{w}(c_3\,, t{=}0) = \begin{cases} 0 \;\; \text{if } c_3 = \mathrm{a} \\ \text{-¶} \;\; \text{otherwise} \end{cases}}$$

Toy model of search tree (VI)

Solution:

$$\omega(c_3,t) = t\ \ln 2 + 3c_3\ \ln(1-t) + \alpha\ \ \ln\alpha \\ - c_3 \ln c_3 - (\alpha\ \ - c_3)\ln\left[\frac{\alpha\ \ - c_3}{1-(1-t)^3}\right]$$

Graphical representation



NB: max of $w(c_3\ , t)$ gives back most probable $c_3(t)$ for GUC heuristic trajectory.

Analysis of DPLL search tree (I)

Average number of branches with clause populations C_1, C_2, C_3

$$B(C_1, C_2, C_3; T+1) = \sum_{C'_1, C'_2, C'_3 = 0}^{\infty} K\left(C_1, C_2, C_3, C'_1, C'_2, C'_3; T\right) B(C'_1, C'_2, C'_3; T)$$

Branching matrix

$$\begin{aligned} K(C_1,C_2,C_3;C'_1,C'_2,C'_3;T) = & \binom{C'_3}{C'_3 - C_3} \left(\frac{3}{N-T}\right)^{C'_3 - C_3} \left(1 - \frac{3}{N-T}\right)^{C_3} \sum_{w_2=0}^{C'_3 - C_3} \left(\frac{1}{2}\right)^{C'_3 - C_3} \binom{C'_3 - C_3}{w_2} \\ & \times \Bigg\{ (1 - \delta_{C'_1}) \sum_{z_2=0}^{C'_2} \binom{C'_2}{z_2} \left(\frac{2}{N-T}\right)^{z_2} \left(1 - \frac{2}{N-T}\right)^{C'_2 - z_2} \sum_{w_1=0}^{z_2} \left(\frac{1}{2}\right)^{z_2} \binom{z_2}{w_1} \delta_{C_2 - C'_2 - w_2 + z_2}\, \delta_{C_1 - C'_1 - w_1 + 1} + \delta_{C'_1} \\ & \times \sum_{z_2=0}^{C'_2 - 1} \binom{C'_2 - 1}{z_2} \left(\frac{2}{N-T}\right)^{z_2} \left(1 - \frac{2}{N-T}\right)^{C'_2 - 1 - z_2} \sum_{w_1=0}^{z_2} \left(\frac{1}{2}\right)^{z_2} \binom{z_2}{w_1} \delta_{C_2 - C'_2 - w_2 + z_2 + 1} \left[\delta_{C_1 - w_1} + \delta_{C_1 - 1 - w_1}\right] \Bigg\}, \end{aligned}$$

- $B(C_1, C_2, C_3;T) \sim \exp[\, N\ w(c_2, c_3;t)\ ]$ where $c_i = C_i/N$, $t = T/N$
- Distribution of C_1 becomes stationary over $O(1)$ time scale

Analysis of DPLL search tree (II)

Eigenvectors of K: $$v_{q,q_2,q_3}(C_1',C_2',C_3') = \mathrm{e}^{\mathrm{i}(q_2 C_2' + q_3 C_3')}\,\tilde{v}_q(C_1)$$

$$\tilde{K}_{q_2}(C_1,C_1') = \sum_{z_2=0}^{\infty} \mathrm{e}^{-m_2}\,\frac{(m_2\,\mathrm{e}^{\mathrm{i}q_2})^{z_2}}{z_2!} \sum_{w_1=0}^{z_2} \binom{z_2}{w_1} \frac{1}{2^{z_2}}$$
$$\times \left\{ \delta_{C_1-C_1'-w_1+1}\,(1-\delta_{C_1'}) + \mathrm{e}^{\mathrm{i}\,q_2}(\delta_{C_1-w_1}+\delta_{C_1-1-w_1})\,\delta_{C_1'} \right\}$$

Effective matrix in (C_1,C_1’) sector

Analysis of DPLL search tree (III)

Generating function of Eigenvector components

$$V_q(x) = \sum_{C_1=0}^{\infty} \tilde{v}_q(C_1)\, x^{C_1} = V_q(0) \frac{L(x)\; N(x)}{\Lambda_q - L(x)}$$

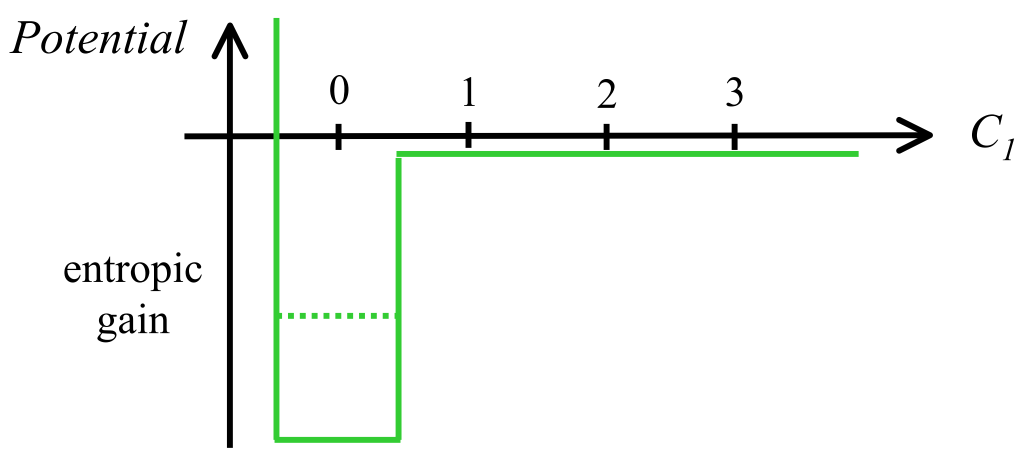
$$N(x) = \mathrm{e}^{-y_2}\,(x+x^2) - 1, \quad L(x) = \frac{1}{x}\,\exp\left(\frac{m_2}{2}\,\mathrm{e}^{-y_2}\,x\right)$$

Asymptotic behavior:

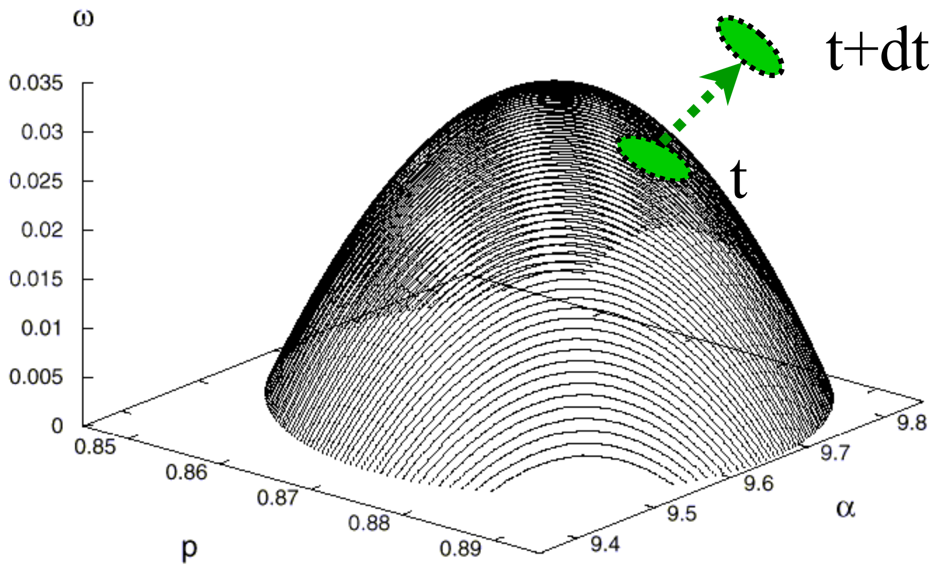
$$\tilde{v}_0(C_1) \sim \left(\frac{1}{R}\right)^{C_1} \longrightarrow V_0(x) \sim (R-x)^{-1}$$

Pole of V_0 located in R>1 (localized eigenvector), or R=1 (extended eigenvector)

Analogy with
1D-Quantum Mechanics
(discrete, non hermitean)



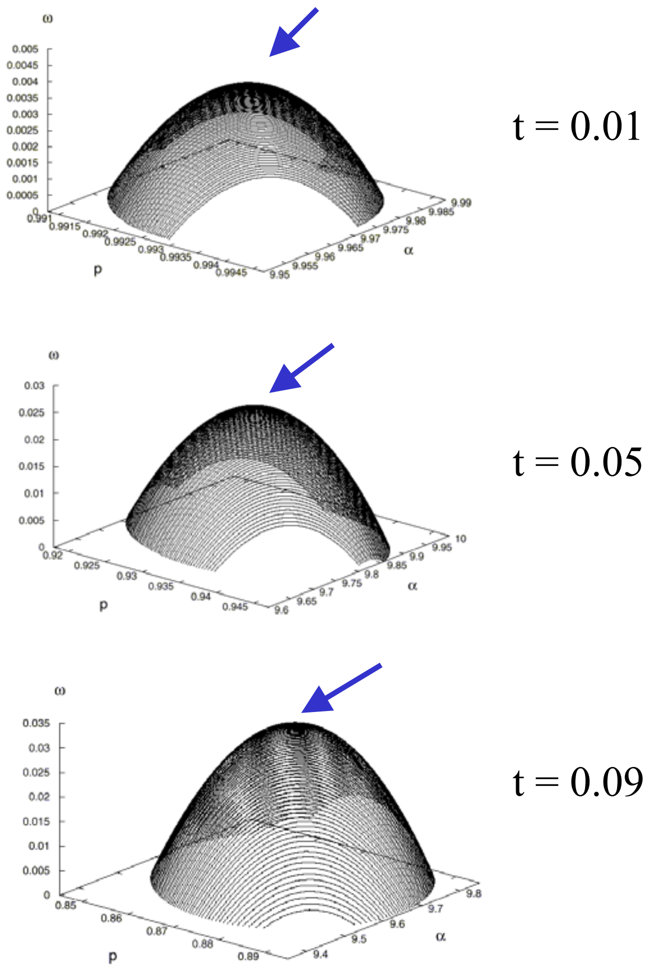
Analysis of DPLL search tree (IV)

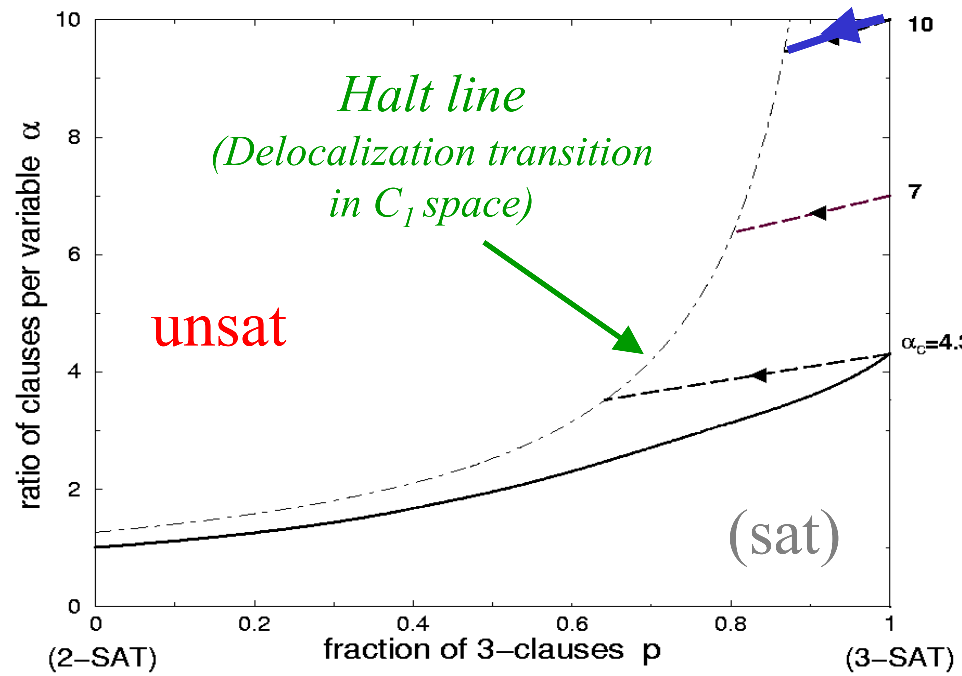


$$\frac{\partial \omega}{\partial t} = \mathcal{H}\left[p, \alpha, \frac{\partial \omega}{\partial p}, \frac{\partial \omega}{\partial \alpha}, t \right] \qquad \text{(PDE)}$$

+ moving frontier between alive (finite C_1) and dead branches (C_1=O(N))

Analysis of DPLL search tree (V)





$\alpha_0 = 10$

Comparison to numerical experiments

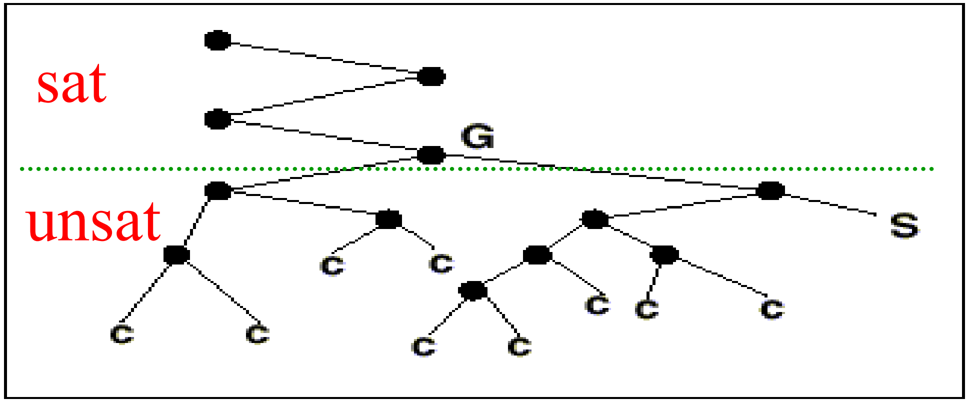
$$Q = 2^{N\omega}$$

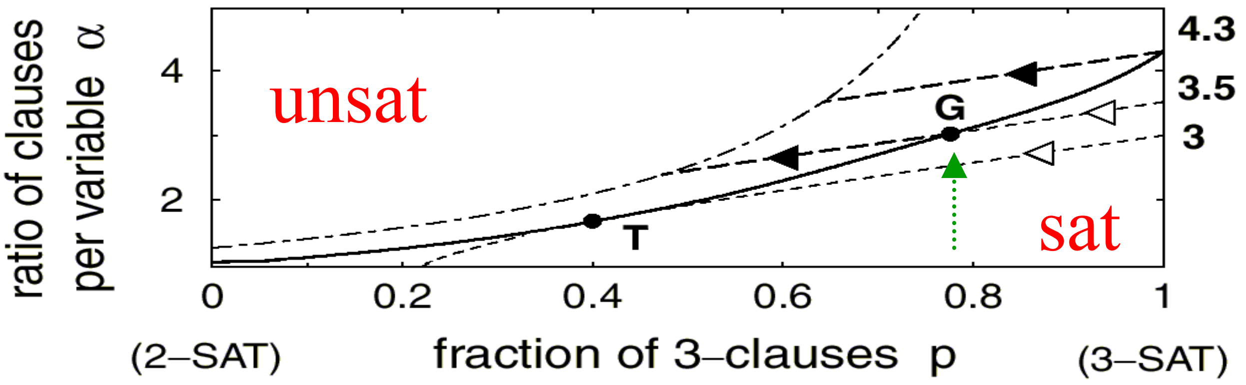
	Initial Ratio α_0	Experiments $\log_2 Q$	$\log_2 B$	Theory $\hat{\omega}$
unsat	20	0.0153 ± 0.0002	0.0151 ± 0.0001	0.0152
	15	0.0207 ± 0.0002	0.0206 ± 0.0001	0.0206
	10	0.0320 ± 0.0005	0.0317 ± 0.0002	0.0319
	7	0.0482 ± 0.0005	0.0477 ± 0.0005	0.0477
	4.3	0.089 ± 0.001	0.0895 ± 0.001	0.0875
sat	3.5	0.034 ± 0.003		0.035
	G	0.040 ± 0.002	0.041 ± 0.003	0.044
		(nodes)	(leaves)	

$$\omega = \frac{3+\sqrt{5}}{6\ln 2}\left[\ln\left(\frac{1+\sqrt{5}}{2}\right)\right]^2 \frac{1}{\alpha} \approx \frac{0.292}{\alpha}$$

Satisfiable, hard instances 3.003< α < 4.3

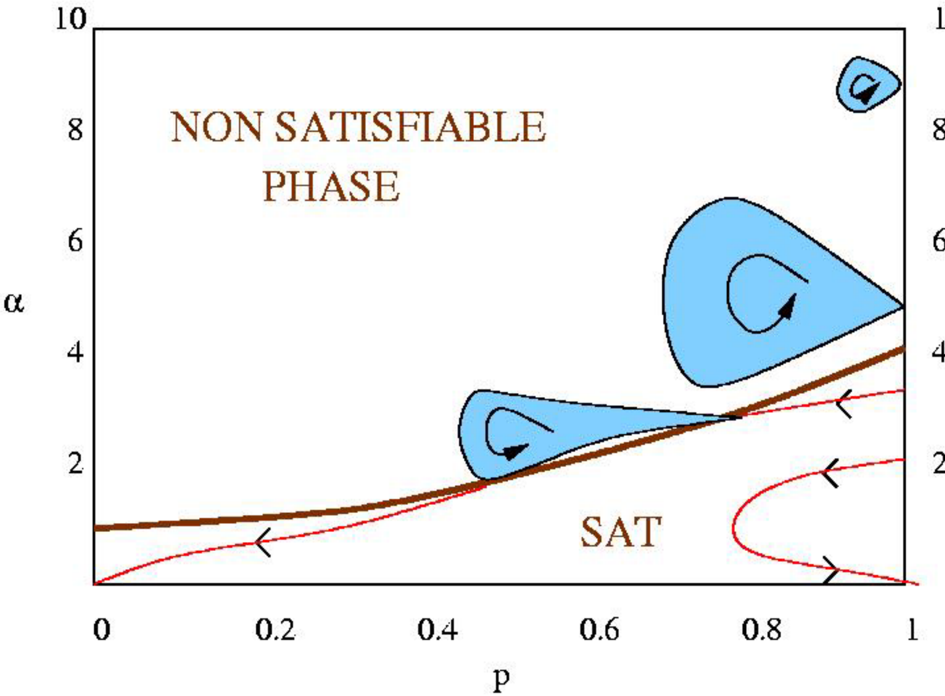
(which could made be easier?)

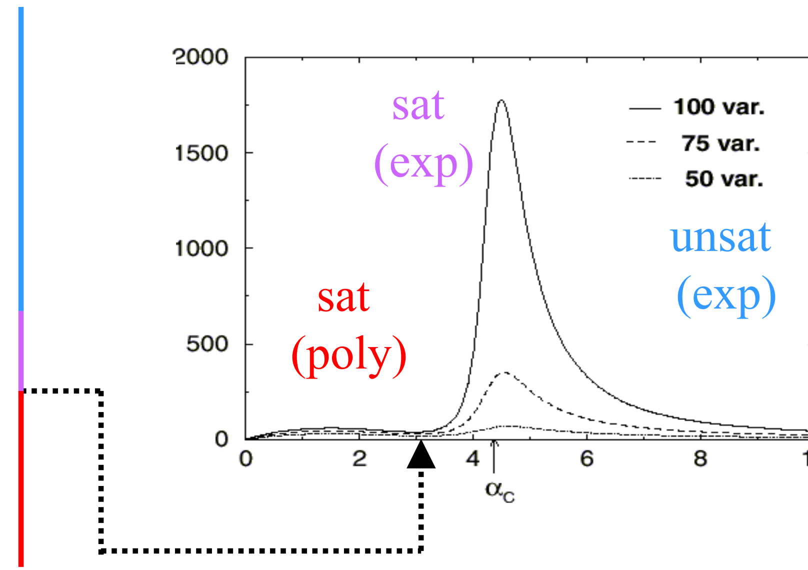




The complexity of 3-SAT solving is strongly affected by the phase transitions of 2+p-SAT .

The polynomial/exponentiel crossover





"dynamical" transition
(depends on the heuristic)

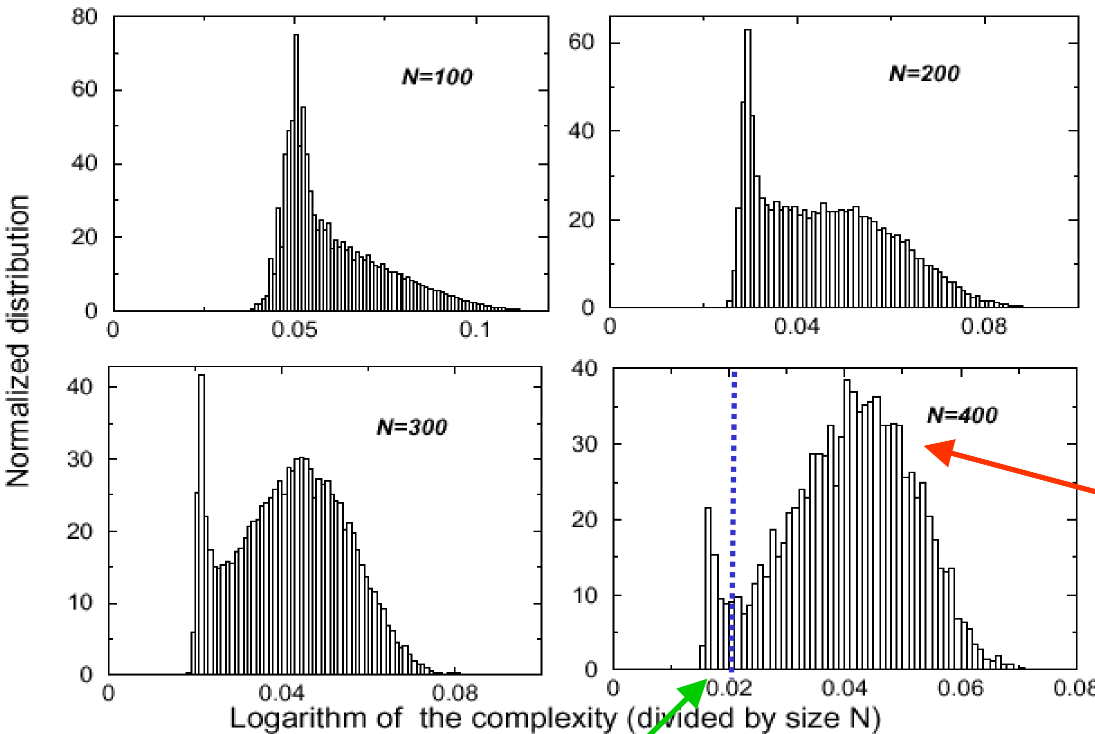
$$\begin{aligned} UC &: \quad 2.667 \\ GUC &: \quad 3.003 \\ SC &: \quad \approx 3 \end{aligned}$$

but

$$p_T = \frac{2}{5}, \alpha_T = \frac{5}{3}$$

T is largely heuristic independent (universality)

Fluctuations of complexity for finite instance size



Histograms of solving times

α=3.5

Exponential regime Complexity $= 2^{0.035\, N}$ + fluctuations !

Linear regime
Very rare! frequence $= 2^{-0.011\, N}$

Talks later this week by S. Cocco and A. Montanari

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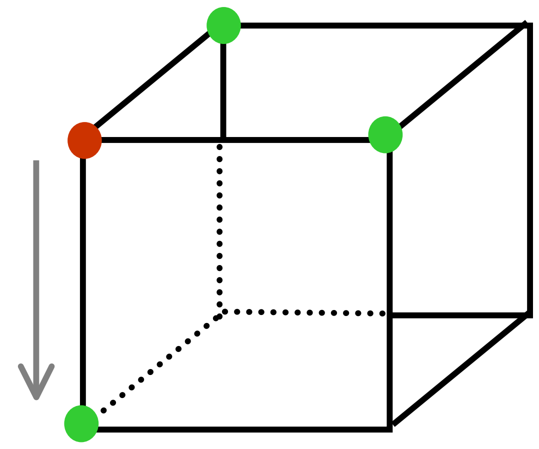
Local search algorithm

Configuration: set of N Boolean variables or spins $x_i = 0,1$
Goal: minimize some cost function over the x's.

Configuration space
for N=3



Local search algorithm:
1. Start from some (more or less) random configuration C (●);
2. Look at neighbors of C in Configuration Space (●), and their attached costs;
3. Move to one of these neighbors (⟶) with some transition rate, or remain in C.
4. Go to 2.

Gradient descent procedure

= Monte Carlo Algorithm at zero temperature

- The procedure:

  a. *Start from a random configuration, call E the number of unsatisfiable clause (energy).*
  b. *If E=0, STOP.*
  c. *If E>0, pick up a variable randomly; flip it if the corresponding energy E' is smaller or equal to E. Goto b.*

- Possible relationship between Replica results and MC method

- Example of 3-XORSAT

Random 3-XORSAT (I)

Logical XOR instead of OR = system of linear equations modulo 2

- N Boolean variables $x_1, x_2, x_3, \ldots, x_N$;
- M clauses (pick up randomly three variables and a second member equal to 0 or 1), e.g.

$$x_1 + x_3 + x_{12} = 0 \mod 2$$

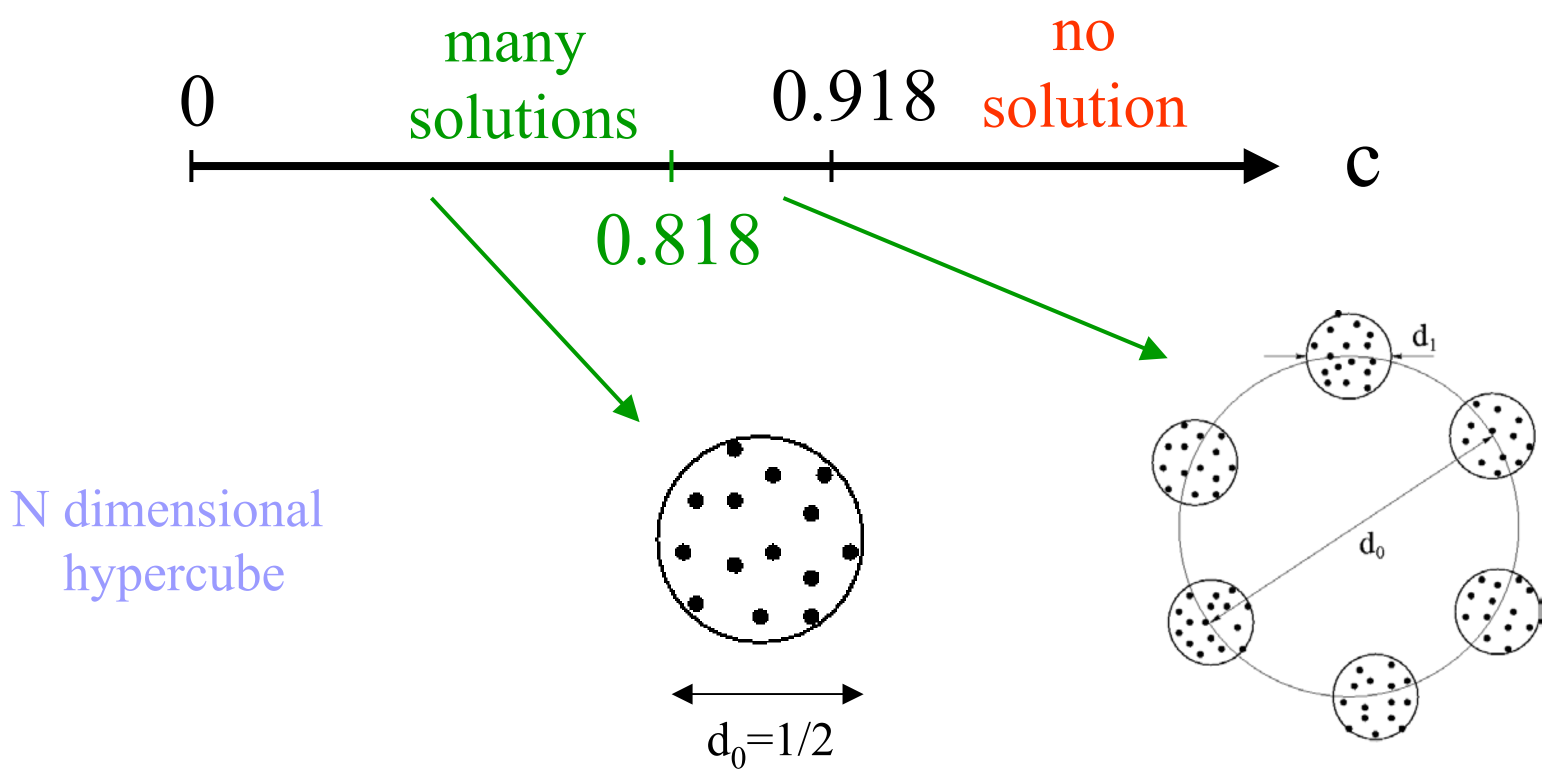
- repeat M times.

Are all clauses (equations) satisfiable together?

…. depends on ratio $c=M/N$!

Random 3-XORSAT (II)

Phase diagram derived from Replica method, then Rigorous analysis:

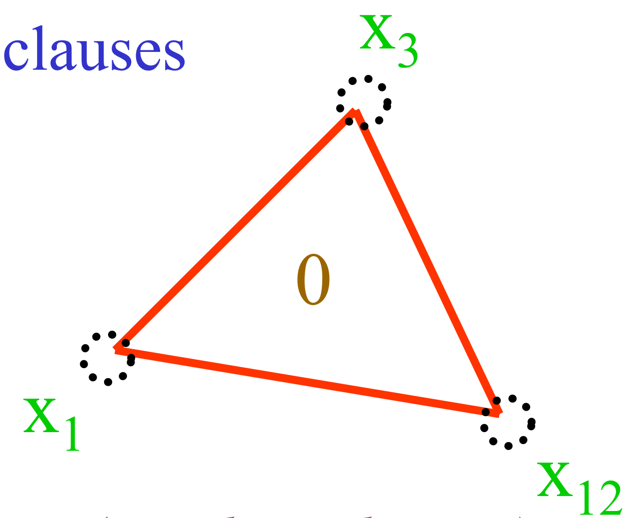


Hamming distance (fraction of
variables that differ) between solutions

Random 3-XORSAT (III)

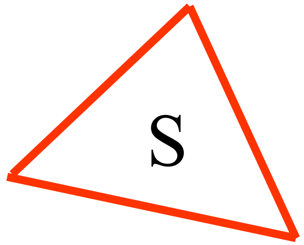
Graphical representation of clauses

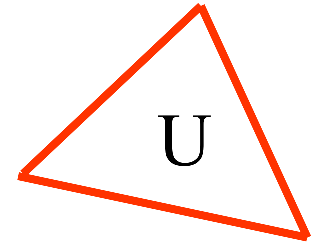
$$x_1 + x_3 + x_{12} = 0 \quad \longrightarrow$$



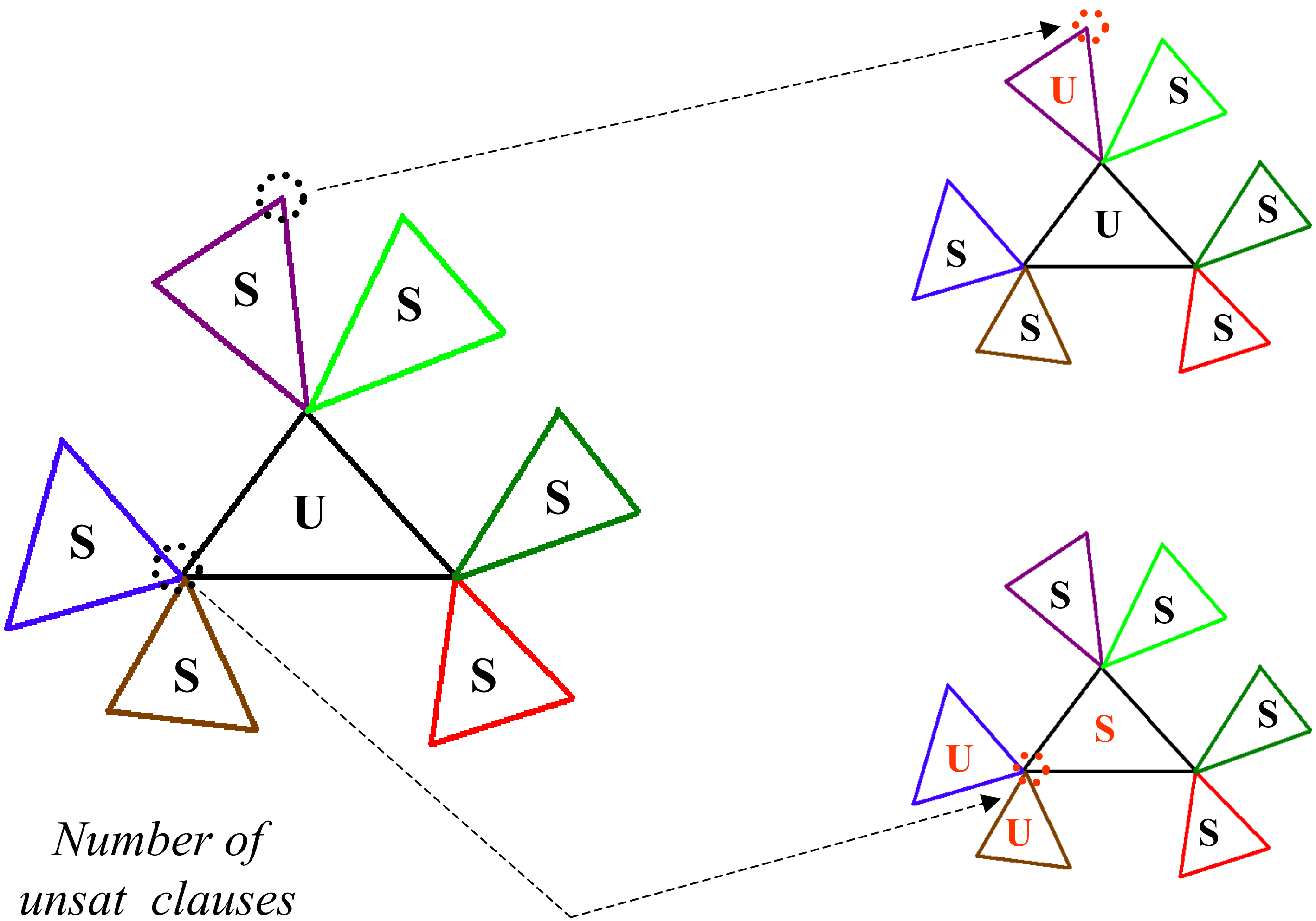
(triangle, or plaquette)

Depending on values of variables, the clause is Satisfied or Unsatisfied,





Blocked Islands (I)



Number of unsat clauses = 1

Unsat = 2

Unsat = 2

Blocked Islands (II)

Statement:

Blocked islands prevent the algorithm from reaching the ground state

Proof:

• *show that, with high probability, there is an extensive number*

$$\text{Islands} = \frac{729}{8} c^7 e^{-45c} N + o(N)$$

of islands, a finite fraction of which are blocked.

• *deduce a lower bound to the final energy reached by Gradient descent*

Energy ¥ q(c) . N

Blocked Islands (III)

NB: Fixed probability (not fixed number) statistical ensemble

Any triplet p of vertices carries a clause with prob. $\boxed{\mu = \frac{cN}{\binom{N}{3}} = \frac{6c}{N^2} + O\left(\frac{1}{N^3}\right)}$

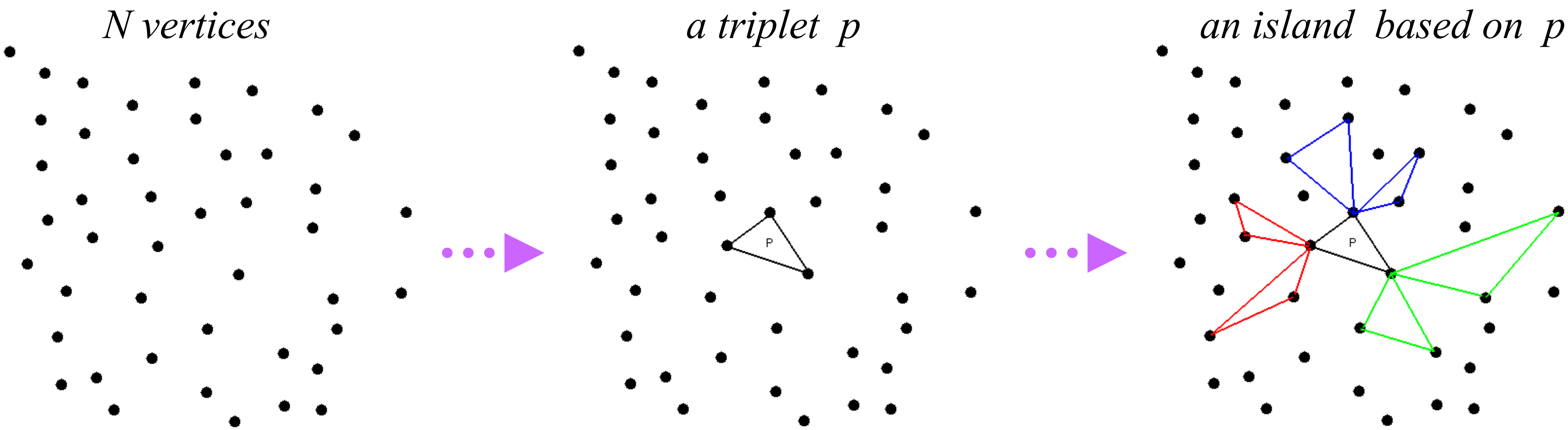
Draw randomly a set of clauses, i.e. a set of triangles joining vertices

Define $\boxed{\mathcal{I}_p = \begin{cases} 1 & \text{if triplet } p \text{ is the center of an island} \\ 0 & \text{if not} \end{cases}}$

Show that $$\mathcal{I} = \sum_p \mathcal{I}_p = \text{Number of islands}$$

is highly concentrated and calculate its typical value.

Blocked Islands (IV)



$$E[I_p] = \frac{(N-3)(N-4)(N-5)(N-6)}{8} \times \frac{(N-7)(N-8)(N-9)(N-10)}{8}$$

$$\times \frac{(N-11)(N-12)(N-13)(N-14)}{8}$$

$$\times \mu^A (1-\mu)^B$$

with $A = 7$, $B = \underbrace{\binom{N}{3}}_{\text{total \# triplets}} - \underbrace{\binom{N-15}{3}}_{\text{\# triplets external to the island}} - 7$

Blocked Islands (V)

Average number of islands per vertex:

$$\lim_{N\to\infty} \frac{1}{N} E[\mathcal{I}] = \lim_{N\to\infty} \frac{1}{N} \binom{N}{3} E[\mathcal{I}_p] = \boxed{\frac{729}{8}\, c^7 \;\exp(-\,45\, c)}$$

Concentration:

E[x]

consider $x = \mathcal{I}/N$

Chebyshev's inequality: for all e > 0, $\mathrm{Prob}\left(\left|x - E[x]\right| \geq \epsilon\right) \leq \frac{\mathrm{Var}[x]}{\epsilon^2}$

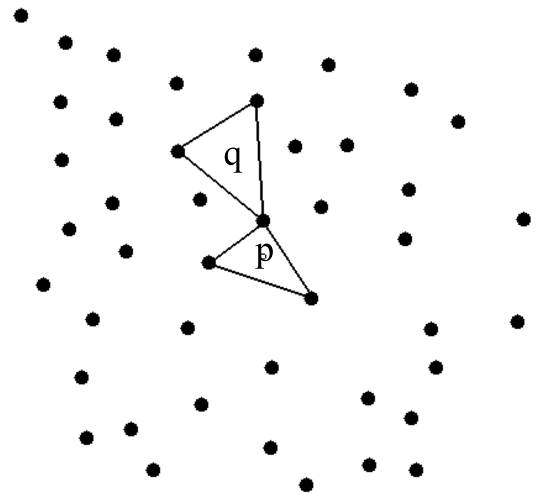
show that Var[x] tends to 0 as N tends to infinity …

Blocked Islands (VI)

Need to calculate second moment:

$$E[\mathcal{I}^2] = \sum_{p,q} E[\mathcal{I}_p \mathcal{I}_q]$$

Depends only upon the number *l* of common vertices between *p* and *q* = 0, 1, 2 or 3



$$\begin{aligned}
E_{\ell=3} &= E[\mathcal{I}_p^2] = E[\mathcal{I}_p] = \frac{3^7}{2^2}\, c^7\, e^{-45\,c}\, N^{-2} + O(N^{-3}) \\
E_{\ell=2} &= E_{\ell=1} = 0 \\
E_{\ell=0} &= \frac{(N-6)\ldots(N-17)}{2^9}\,\frac{(N-18)\ldots(N-29)}{2^9}\mu^{14}\,(1-\mu)^{\binom{N}{3}-\binom{N-30}{3}-14} \\
&= \frac{3^{14}}{2^4}\, c^{14}\, e^{-90\,c}\, N^{-4} + O(N^{-5})
\end{aligned}$$

Blocked Islands (VII)

$$
\begin{aligned}
E[\mathcal{I}^2] &= \binom{N}{3} E_{\ell=3} + \binom{N}{3}\binom{N-3}{3} E_{\ell=0} \\
&= E[\mathcal{I}]^2 + O(N)
\end{aligned}
$$

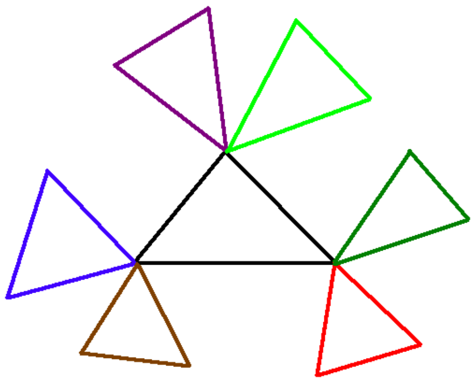
î $\lim_{N\to\infty} \mathrm{Var}[x] = 0$

Thus, with high probability, *x* does not deviate from the expectation value,

$$\mathrm{E}[x] = \frac{729}{8} c^7 \exp(-45\,c)$$

Blocked Islands (VIII)

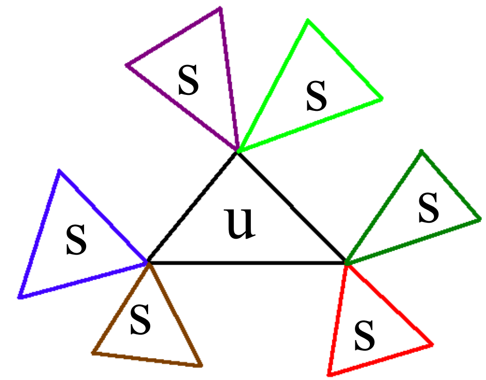
island



with prob.

$$\frac{1}{2^7}$$

blocked island



Thus with high probability, there is an number

$$BI = \frac{729}{1024}\, c^7\, e^{-45c}\, N + o(N)$$

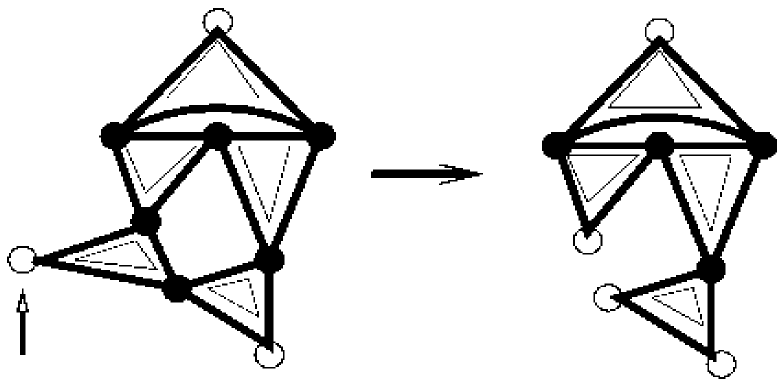
of blocked islands, each with an energy equal to unity.
This gives a lower bound to the final energy reached by Gradient descent

Energy ¥ BI

Comments on Gradient descent and XORSAT

- 3-XORSAT easy to solve (linear algebra problem)

- Easy to solve up to c_d=0.818 with a polynomial algorithm looking at vertex degrees (non local)



- Cannot be solved by gradient descent, even when looking Q steps ahead for any finite Q!

  BUT bound is very small: q(c,Q) N < q(c,1) N < 1.5 10^{-9} N

  cannot be seen for sizes < 1 billion spins

  Necessary condition for convergence: q(c,Q) N ö 0, i.e. Q ~ log N

- What happens for other energy functions e.g. ferromagnets, random 3-SAT?

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Unsatisfied clause flip procedure

- The clause flip procedure
- Exact results for 2-SAT and 3-SAT
  upper bounds on resolution times valid for worst case
- Mean Field approach
  approximate analysis of average performances for 3-SAT
- Conclusion

Clause flip procedure

1. Pick up an initial (random) configuration of variables;
2. If all clauses are satisfied, STOP.
3. Else, choose randomly one unsat clause and flip one of its attached variables; Goto 2.

Example:

set of clauses

$$
\begin{array}{lcl}
(\text{NOT } x_1 \text{ or } x_2 \text{ or } x_3) & \longrightarrow & F \\
(x_1 \text{ or } x_2 \text{ or NOT } x_4) & \longrightarrow & T \\
(\text{NOT } x_1 \text{ or } x_2 \text{ or } x_4) & \longrightarrow & T
\end{array}
$$

1. random configuration x_1=T, x_2=F, x_3=F, x_4=T
2. pick up first clause and flip one variable it contains

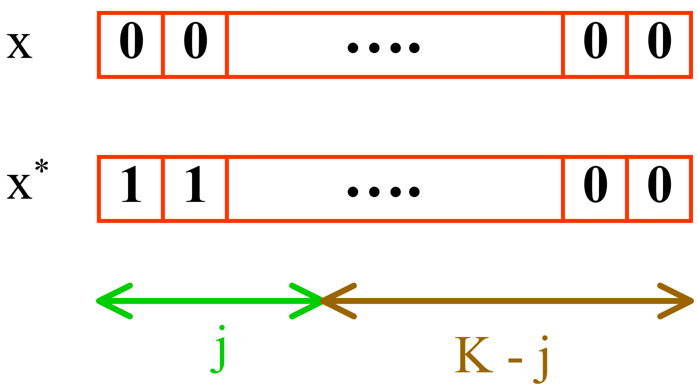
   e.g. x_2=F ö x_2=T then all clauses are satisfied

   e.g. x_1=T ö x_1=F then clause 1 is satisfied, but clause 2 is not any longer.

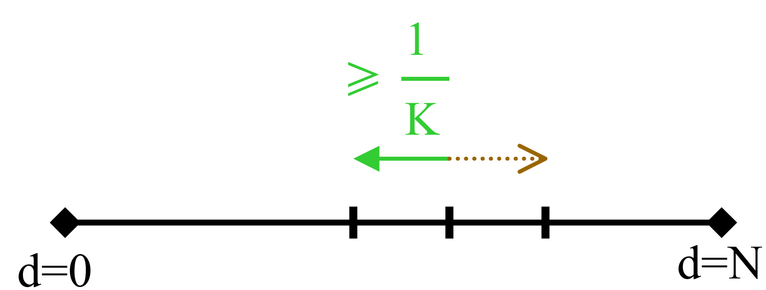
Energy is not guaranteed to decrease!

Exact results for 2-Sat and 3-Sat

Suppose the formula is satisfiable, and call $(x^*)_i$ a solution. Consider a clause not satisfied by x,



$$d=j \quad \text{ö} \quad d' = \begin{cases} j+1 & \text{with prob. } (K-j)/K \\ j-1 & \text{with prob. } j/K \end{cases}$$



2-SAT: free 1-D diffusion, resolution time growing as N^2 at most.

3-SAT: probability of success $> (1/2)^{d^*}/O(N^{1/2}) > (3/4)^N / O(N^{1/2})$
thus resolution time growing as $(4/3)^N$
recently: 1.329… instead of 1.333…

Mean field analysis (I)

Parameters:

N = number of variables
M = number of clauses = a N
K = number of variables in each clause (K-SAT)

- Define $M_j(T)$ the number of clauses satisfied by j literals after T clause flips with j = 0, 1,…, K.
  ($M_0(T)$ is the number of unsatisfied clauses)

- Normalization condition: $$\sum_{j=0}^{K} M_j(T) = M$$

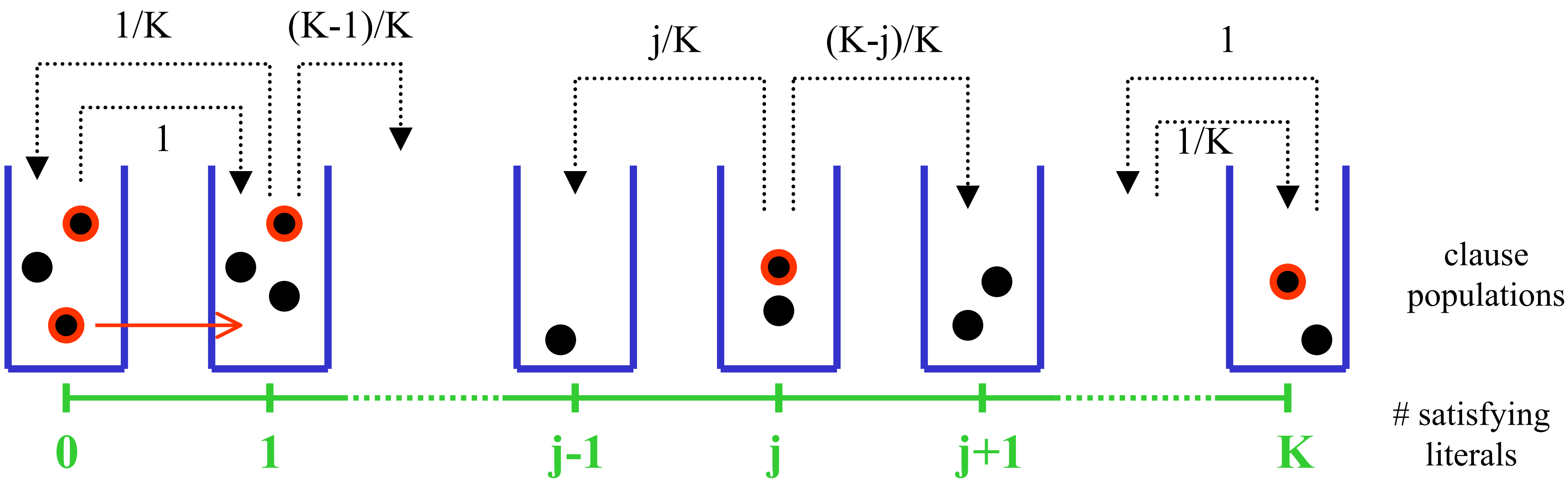
- Define fractions of j-clauses: $$\phi_j(t) = M_j(T)/M$$

Question: evolution equations for the fractions when T Ø T+1 ?

Mean field analysis (II)

Initial conditions for the fractions of j-clauses: $$\phi_j(0) = \frac{1}{2^K}\binom{K}{j}$$

After a new clause flip, i.e. from T Ø T+1:



$$M_j(T+1) - M_j(T) = \frac{K}{N}\Big((K-j+1)/K \;\; M_{j-1}(T) + (j+1)/K \;\; M_{j+1}(T) \Big) - d_j + d_{j-1}$$

Mean field analysis (III)

DT = 1 leads to DM_j = q(1). Thus, fractions F_j vary by q(1) on time scale DT = q(M). Define reduced time: t = T/M.

Evolution equation:

$$\frac{d\vec{\phi}}{dt} = \vec{v} + \alpha\, K\, W_r.\vec{\phi}$$

with

$$\vec{v} = \begin{pmatrix} -1 \\ 1 \\ 0 \\ .. \\ 0 \end{pmatrix} , \qquad W_r = \begin{pmatrix} -1 & \frac{1}{K} & 0 & 0 & 0 & .. & 0 \\ 1 & -1 & \frac{2}{K} & 0 & 0 & .. & 0 \\ 0 & \frac{K-1}{K} & -1 & \frac{3}{K} & 0 & .. & 0 \\ .. & .. & .. & .. & .. & .. & ... \\ 0 & 0 & 0 & 0 & .. & & -1 \end{pmatrix}$$

NB: normalization of fractions comes from nullity of matrix elements summed over columns.

Mean field analysis (IV)

Introduction of the generating function:

$$\varphi(x,t) = \sum_{j=0}^{K} \phi_j(t)\, x^j \qquad \text{with} \qquad \varphi(x,0) = \left(\frac{1+x}{2}\right)^K$$

$$\boxed{\frac{\partial \varphi}{\partial t}(x,t) = -1 + x + \alpha K(x-1)\varphi(x,t) + \alpha(1-x^2)\frac{\partial \varphi}{\partial x}(x,t)}$$

1. *Homogeneous equation:* $\varphi_0(x,t) = -\dfrac{1}{\alpha K}$

$$\psi(x,t) = \varphi(x,t) - \varphi_0(x,t)$$

$$\frac{\partial \psi}{\partial t}(x,t) = \alpha K(x-1)\psi(x,t) + \alpha(1-x^2)\frac{\partial \psi}{\partial x}(x,t)$$

First order linear Partial Differential Equation

Mean field analysis (V)

2. Wave propagation …

$$\chi(x,t) = (1+x)^K \;\psi(x,t)$$

$$\frac{\partial \chi}{\partial t}(x,t) = \alpha(1-x^2)\frac{\partial \chi}{\partial x}(x,t)$$

$$\chi(x,t) = \Omega\left(\frac{1}{\alpha}\,\tanh^{-1}(x) + t\right)$$

Initial conditions allow to determine the wave envelope

$$\Omega(u) = \frac{1}{2^K} + \frac{1}{\alpha K}\,[1+\tanh(\alpha u)]$$

Solution

$$\boxed{\varphi(x,t) = \left(\frac{1+x}{2}\right)^K + \frac{1}{\alpha K}\left\{\left[\frac{1+x\tanh(\alpha t)}{1+\tanh(\alpha t)}\right]^K - 1\right\}}$$

Mean field analysis (VI)

Existence of a critical value of the ratio clause/variable

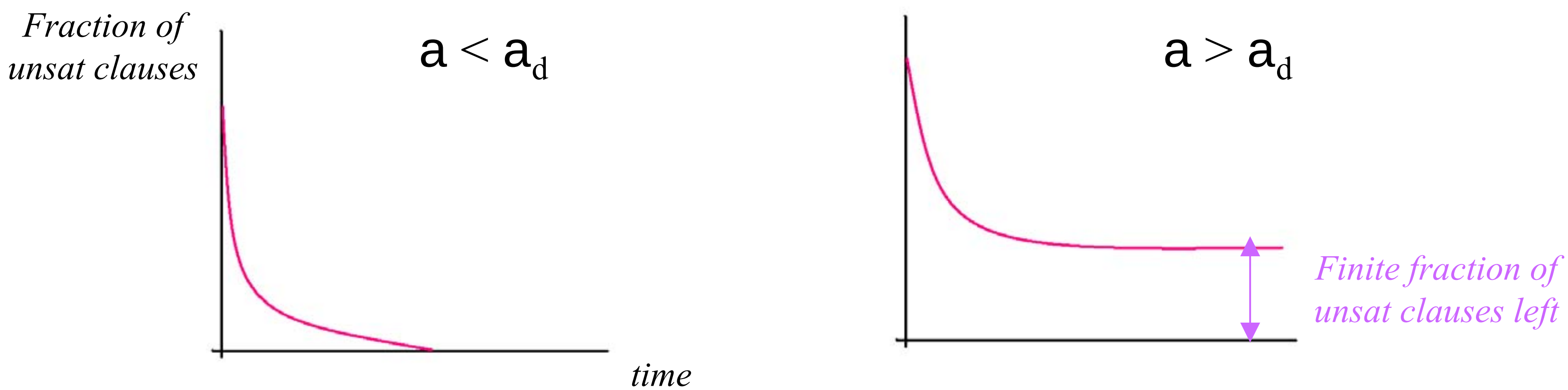
$$\boxed{\alpha_d(K) = \frac{2^K - 1}{K}}$$

- If $\alpha < \alpha_d$, then the procedure stops after a finite time with no unsat clause left.
- If $\alpha > \alpha_d$, then the procedure never stops, and a finite fraction of clauses remain unsatisfied.

$$\begin{aligned}
\phi_0^* &= \frac{1}{2^K} - \frac{1}{\alpha K}\left(1 - \frac{1}{2^K}\right) = \frac{1}{2^K}\left(1 - \frac{\alpha_d(K)}{\alpha}\right) \\
\phi_j^* &= \left(1 + \frac{1}{\alpha K}\right)\frac{1}{2^K}\binom{K}{j} \qquad .
\end{aligned}$$

Comments on the analysis

• Numerical simulations confirm scenario is qualitatively correct …

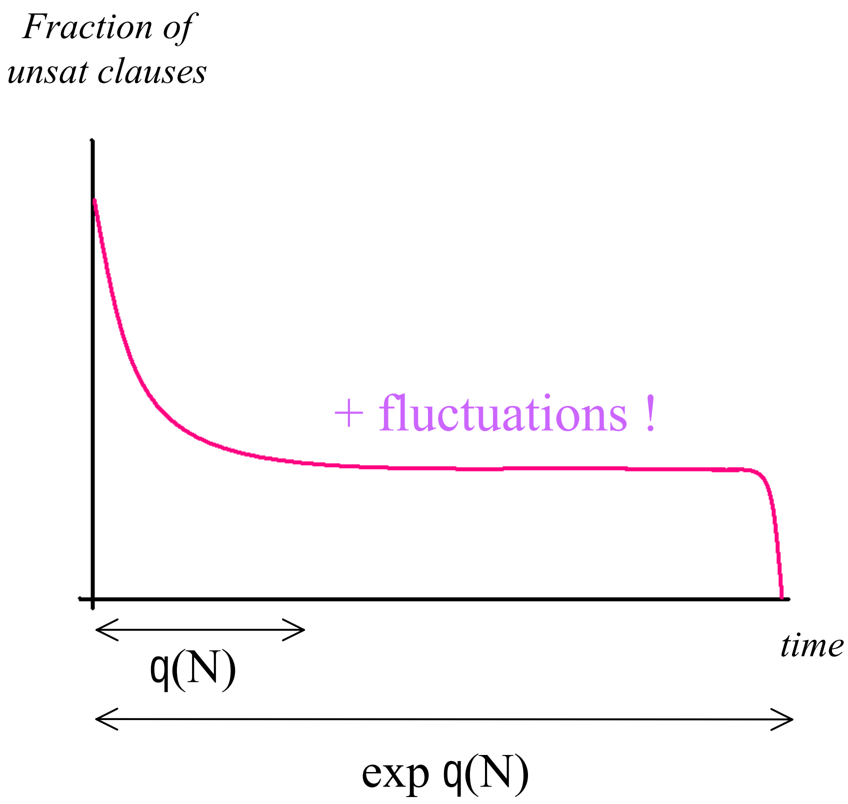


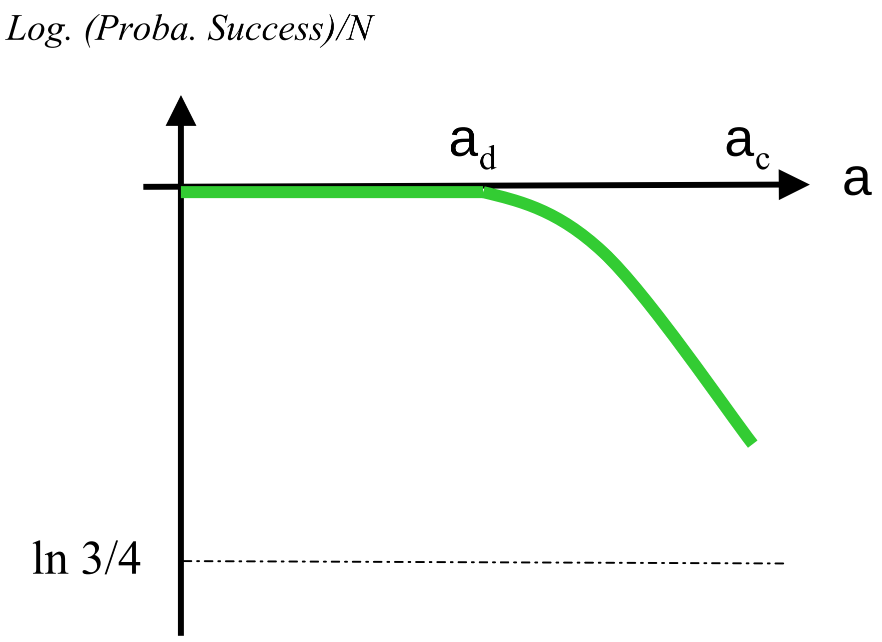
… but numerical estimates for a_d are larger than theoretical predictions.

• Quantitative agreement seems to improve for larger K or a in agreement with theoretical argument by G. Semerjian (2001).

• Behavior at very large times (exponential in N) for $a > a_d$ …

Rare deviations





Also work by
W. Barthel and M. Weigt

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Conclusion

Few examples of solving algorithms which can be studied using statistical mechanics tools
= *more or less legitimate extension of mathematical studies*

- Average properties of algorithms for random distribution of instances.

- Can we obtain results true for any instance?