## PHASE CHANGES IN RANDOM STRUCTURES AND ALGORITHMS

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(1) Binary search trees, Quicksorts, and phase changes
(2) Method of moments and its refinements
(3) Differential equations with polynomial coefficients
(9) Profiles of random log-trees

## BINARY SEARCH TREE CONSTRUCTED FROM \{6,2,4,8,7, 1,5,3,10,9\}



## WHO STUDIED BSTs FIRST? AND WHEN?

Knuth (1997, Art Comput. Programming), Vol. III, p. 453

- Windley (1960) Computer Journal
- Booth and Colin (1960) Information and Control
- Hibbard (1962) Journal ACM
- Hoare (1961) Communications ACM (Quicksort)

The first published descriptions of tree insertion were by P. F. Windley [Comp. J. 3 (1960), 84-88], A. D. Booth and A. J. T. Colin [Information and Control 3 (1960), 327-334], and Thomas N. Hibbard [JACM 9 (1962), 13-28]. Each of these authors seems to have developed the method independently of the others, and each paper derived the average number of comparisons (6) in

## Computer algorithms

- Simple, fundamental, prototypical data structure
- Many variants, generalizations: balanced BSTs, weighted BSTs, quadtrees, median BSTs, ...
- Closely connected to quicksort (one of the most widely used sorting algorithms)

Appeared in other fields
Statistical physics, probability, evolution, population genetics, chemistry, ...

Mathematically intriguing
Many fascinating phenomena and challenging problems

## RANDOM BSTs

## The probability model

Assume that all $n$ ! permutations of $n$ elements are equally likely.

Construct the BST from a random permutation. Call it a random BST.


$$
\begin{gathered}
\mathbb{P}\left(U_{n}=j\right)=\frac{1}{n} \\
j=0, \cdots, n-1
\end{gathered}
$$

$$
\mathbb{P}\left(U_{n}=j\right)=\frac{1}{n}
$$


(1) probabilistic: $X_{n} \stackrel{d}{=} X_{U_{n}}+X_{n-1-U_{n}}+T_{n}$
(2) recurrence: $a_{n}=\frac{2}{n} \sum_{0 \leq j<n} a_{j}+b_{n}$
(3) differential equation: $f^{\prime}(z)=\frac{2}{1-z} f(z)+g(z)$
(4) bivariate parameter: $a_{n, k}=\frac{2}{n} \sum_{0 \leq j<n} a_{j, k}+b_{n, k}$

## A short list

- Quicksort algorithms
- Discrete probability: random pairwise selections (or an unfriendly seating arrangement problem)
- Statistical physics: Eden model, diffusion-limited aggregates, ...
- Combinatorial structures: binary increasing trees
- Chemistry: random sequential adsorption (or random dimer filling, ...)
- Evolutionary trees: Yule (or Markov) model
- Population genetics: Kingman's coalescent
- Parking problems: discrete and continuous
- Random fragmentation process
- Branching Markov processes


## CLOSELY CONNECTED STRUCTURES

Quicksort (Hoare, 1961, Comm. ACM)
Selected to be among the top 10 algorithms in the 20th century with "the greatest influence on the development and practice of science and engineering in the 20th century" (appeared in the January/February issue of Computing in Science \& Engineering).


Widely used; many variants.

PART II: PHASE CHANGE PHENOMENA

## Random search trees and related models



## PHASE CHANGE

## $f(n ; m)$ change behaviors as $n \rightarrow \infty$ and $m \geq m_{0}$



## CLASSICAL CENTRAL LIMIT THEOREM

$X_{1}, \ldots, X_{n}$ iid, continuous, zero mean, finite variance $\sigma^{2}>0$

$$
\mathbb{P}\left(\frac{X_{1}+\cdots+X_{n}}{\sigma \sqrt{n}}<x\right) \rightarrow \Phi(x):=\frac{1}{\sqrt{2 \pi}} \int_{-\infty}^{x} e^{-t^{2} / 2} d t
$$

so $\Phi(x)$ is used to bridge the transition between "events unlikely to happen" and "events happening almost always".

Binomial from Normal to Poisson
If $X_{n} \sim \operatorname{Binomial}(n ; p)$, then

- $X_{n} \sim \mathscr{N}(p n, p(1-p) n)$ if $p n \rightarrow \infty$;
- $X_{n} \sim$ Poisson $(\lambda)$ if $p n \rightarrow \lambda<\infty$.
- Analytically, singularity changes nature (or regular $\rightarrow$ singular)
$\mathbb{P}\left(X_{1}+\cdots+X_{n}>x\right)=\frac{1}{2 \pi i} \int_{-\infty}^{\infty} t^{-1} e^{-i x t}\left(\mathbb{E}\left(e^{i i X_{1}}\right)\right)^{n} d t$.
coalescence of pole and the saddle-point.
- Asymptotically, the consequence of increasing errors: $\mathbb{E}\left(Y_{n}\right)=c n+O\left(n^{\alpha}\right)$,

$$
\mathbb{V}\left(Y_{n}\right) \asymp \begin{cases}n, & \text { if } \alpha<1 / 2 ; \\ n \log n, & \text { if } \alpha=1 / 2 ; \\ n^{2 \alpha}, & \text { if } \alpha>1 / 2 .\end{cases}
$$

- Algorithmically, hardest instances often (but not always) occur in or near the phase transition range.


# DESIGN AND ANALYSIS OF ALGORITHMS: A NEW TREND 

> Massive data or data streams everywhere
> Many algorithms need to be redesigned and asymptotic analysis is gaining its increasing importance.

The current mega-giga-era will soon be replaced by the tera-peta-era.

- Quantitatively, phase transitions more informative than static states
- Structurally, phase transitions useful in describing the structural stability
- Theoretically, many aspects of phase transitions like classification, universality $\Longrightarrow$ theory
- Computationally, identifying phase transitions helpful in improving algorithms
- Methodologically, more powerful tools always needed


## VARIANTS OF BSTs



## VARIANTS OF QUICKSORT


$\therefore \% 80$ $\therefore 0 \theta_{0}+\infty$

## m-ARY SEARCH TREES

## Introduced by Muntz and Uzgalis (1971)


$m$ branches

## An example: space requirements

Mahmhoud and Pittel (1989), Lew and Mahmoud (1994), Chern and H. (2001): The space requirement $X_{n}$ exhibits the phase change: if $3 \leq m \leq 26$, then

$$
\frac{X_{n}-\mu n}{\sigma \sqrt{n}} \longrightarrow N(0,1) ;
$$

if $m \geq 27$, then the sequence of random variables $\left(X_{n}-\mathbb{E}\left(X_{n}\right)\right) / \sqrt{\mathbb{V}}\left(X_{n}\right)$ does not converge (periodicity dominates).

For other results, see H. (2003), Janson (2005), Chauvin and Pouyanne (2005), Fill and Kapur (2005), Dean and Majumdar (2005).

## THE SECOND PHASE CHANGE

Convergence rate to normal limit law
H. (2003)

$$
\begin{aligned}
& \sup _{x \in \mathbb{R}}\left|\mathbb{P}\left(\frac{X_{n}-\mathbb{E}\left(X_{n}\right)}{\sqrt{\mathbb{V}\left(X_{n}\right)}}<x\right)-\Phi(x)\right| \\
&= \begin{cases}O\left(n^{-1 / 2}\right), & \text { if } 3 \leq m \leq 19 \\
O\left(n^{-3\left(\frac{3}{2}-\alpha\right)}\right), & \text { if } 20 \leq m \leq 26\end{cases}
\end{aligned}
$$

where $\alpha \in\left(\frac{4}{3}, \frac{3}{2}\right)$ denotes the real part of the second largest zero of the equation

$$
z(z+1) \cdots(z+m-2)=m!.
$$

Rate optimal, up to implied constants

## THE SECOND PHASE CHANGE

Approximate numerical values of $\alpha$ and $3\left(\frac{3}{2}-\alpha\right)$

| $m$ | $\alpha$ | $3\left(\frac{3}{2}-\alpha\right)$ |
| :---: | :---: | :---: |
| 20 | 1.34892881 | 0.45321354 |
| 21 | 1.38079786 | 0.35760639 |
| 22 | 1.40936978 | 0.27189065 |
| 23 | 1.43512896 | 0.19461309 |
| 24 | 1.45847025 | 0.12458925 |
| 25 | 1.47971848 | 0.06084455 |
| 26 | 1.49914326 | 0.00257020 |

Dean and Majumdar (2002)
a physical model for random m-ary search trees.


Stop if length $<1$
Number of nodes in the corresponding tree is an RV

## Dean and Majumdar (2002)

They argue heuristically (called scientifically modeling math by Aldous, in contrast to theorem-proof math) that

$$
\mathbb{V}\left(X_{n}\right) \asymp \begin{cases}n, & \text { if } 3 \leq m \leq 26 ; \\ n^{2 \alpha-2}, & \text { if } m>26 .\end{cases}
$$

## They conclude

... we have shown that a fragmentation process with an atomic threshold can undergo a nontrivial phase transition in the fluctuations of the number of splittings at a critical value of the branching number $m$. ... The mechanism of this transition is remarkably simple and therefore one expects it to be rather generic with broad applications ....

Dean and Majumdar (2002): a cuboid splitting tree

- A random point splits $[0, x]^{d}$ into $2^{d}$ hyper-rectangles.
- Continue as long as the volume is $>1$.

Call the tree corresponds to the resulting configuration a random fragmentation tree.

## The phase change at $d=8$

The number $X_{n}$ of nodes in the tree undergoes a phase change:

$$
\mathbb{V}\left(X_{n}\right) \asymp \begin{cases}n, & \text { if } 1 \leq d \leq 8 \\ n^{2 \cos (2 \pi / d)-1}, & \text { if } d>8\end{cases}
$$

$$
\left\{2 \cos \frac{2 \pi}{d}-1\right\}_{d \geq 5}=\{-.38,0,0.24,0.41,-.53,0.61, \ldots\}
$$

## A 2-DIMENSIONAL POINT QUADTREE



## $d$-DIMENSIONAL QUADTREE

Introduced by Finkel and Bentley (1974)

$$
x \in \mathbb{R}^{d}
$$



## The model

If the $n$ given points are iid from $[0,1]^{d}$, then the resulting tree is called a random quadtree.

## The phase change

Chern, Fuchs, H. (2005): If $1 \leq d \leq 8$, then the number $X_{n}$ of leaves is asymptotically normally distributed; if $d \geq 9$, then the random variables $\left(X_{n}-\mathbb{E}\left(X_{n}\right)\right) / \sqrt{\mathbb{V}\left(X_{n}\right)}$ do not converge.

Second phase change at $d=7$.

## RANDOM d-DIMENSIONAL GRID-TREES

A combination of $m$-ary search tree and quadtree
Devroye (1998):

- $m$ - 1 random points split $[0, x]^{d}$ into $m^{d}$ grids.
- Repeat if volume $>1$.

Call the corresponding tree a random grid-tree.
Chern, Fuchs, H. (2005): all pairs ( $m, d$ ) leading to asymptotic normality for the number of leaves

| $m$ | 2 | 3 | 4 | $5, \ldots, 8$ | $9, \ldots, 26$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $d$ | $1, \ldots, \underline{8}$ | $1, \ldots, 4$ | $1, \ldots, 3$ | 1,2 | 1 |

## MEDIAN-OF-( $2 t+1$ ) BSTs (FRINGE-BALANCED)



$\Rightarrow$



How to construct from a sequence of numbers?
Bell (1965) and Walker and Wood (1976):

- Find the median of $2 t+1$ random elements
- Place this median at the root with the smaller $t$ elements going to the left, larger to the right
- Keep inserting as usual (small $\rightarrow \mathbf{L}$, large $\rightarrow \mathbf{R}$ )
- Split recursively if size $=2 t+1$


## Phase change at $t=58$

Chern and H. (2001): The number of nodes with subtree sizes $\geq 2 t+1$ is asymptotically normally distributed for $1 \leq t \leq 58$, and does not converge for $t>58$.

## GENERALIZED m-ARY SEARCH TREES

Combine m-ary search trees and median BSTs All pairs $(m, t)$ for which asymptotic normality holds.

| $m$ | 2 | 3 | 4 | 5 | 6 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $t$ | $1, \ldots, 58$ | $0, \ldots, 19$ | $0, \ldots, 10$ | $0, \ldots, 6$ | $0, \ldots, 4$ |
| $m$ | 7 | 8,9 | $10, \ldots, 13$ | $14, \ldots, 26$ | $>27$ |
| $t$ | $0, \ldots, 3$ | $0,1,2$ | 0,1 | 0 | $\emptyset$ |

## A SIMPLE SCHEME FOR PHASE CHANGES

Chern, H. and Tsai (2002)
Phase changes are clarified for random variables defined recursively by

$$
X_{n} \stackrel{d}{=} X_{l_{n}}+X_{n-1-l_{n}}^{*}+1 \quad(n \geq r)
$$

where

$$
\mathbb{P}\left(I_{n}=k\right)=\sum_{0 \leq j<r} p_{j} \frac{\binom{k}{j}\binom{n-1-k}{r-1-j}}{\binom{n}{r}}, \quad \sum_{0 \leq j<r} p_{j}=1 .
$$

More than a dozen of examples addressed there.

## A DIFFERENT TYPE OF PHASE CHANGE

## H. and Neininger (2002)

General cost measures on BSTs satisfy
$X_{n} \stackrel{d}{=} X_{\text {uniform }_{[0, n-1]}}+X_{n-1-\text { uniform }_{[0, n-1]}^{*}}+Y_{n} \quad(n \geq 2)$, where $Y_{n}$ is known.

## The phase change

If $Y_{n}=O\left(n^{1 / 2}\right)$, then the limit law of $X_{n}$ is normal; if $Y_{n} \gg n^{1 / 2}$, then nonnormal.

A large number of applications.

## CONCLUSION

Analysis of algorithms: a rich source of phase changes

- Many intriguing phenomena and challenging math
- More research needed to unveil new phase changes
- More collaboration needed (with statistical physicists, biologists, ... )
- Simple models are often ubiquitous

