

# A Local Limit Theorem for QuickSort Key Comparisons

Jim Fill

Department of Applied Mathematics and Statistics  
The Johns Hopkins University

October 25, 2016

BIRS Workshop in Analytic and Probabilistic Combinatorics

This is joint work with Béla Bollobás and Oliver Riordan.

# QuickSort: The Algorithm

- Assume distinct keys (numbers—or perhaps symbol strings—to be sorted).
- Choose “pivot” key uniformly at random.
- Use pivot to partition into two subsets: smaller and larger.
- Apply **QuickSort** recursively to subsets. Measure runtime by

$$\begin{aligned} K_n &:= \text{number of comparisons, with } K_0 = 0 \\ &\stackrel{\mathcal{L}}{=} K_{U_n-1} + K_{n-U_n}^* + n - 1, \quad n \geq 1, \end{aligned}$$

where on the RHS:

$$U_n \sim \text{unif}\{1, \dots, n\}$$

and

$$U_n; K_0, \dots, K_{n-1}; K_0^*, \dots, K_{n-1}^*$$

are all *independent*.

- Applied focus: the law  $\mathcal{L}(K_n)$  and asymptotics as  $n \rightarrow \infty$

# The importance of QuickSort

- In a special issue of *Computing in Science & Engineering* (2000), guest editors Jack Dongarra and Francis Sullivan chose QuickSort as one of the ten algorithms “with the greatest influence on the development and practice of science and engineering in the 20th century.”
- QuickSort is the standard sorting procedure in Unix systems.
- QuickSort is among “some of the most basic algorithms—the ones that deserve deep investigation.” — Ph. Flajolet (1999)
- “probably most widely used sorting algorithm” — U. Rösler (1991)
- “one of the fastest, the best-known, the most generalized, the most completely analyzed, and the most widely used algorithms for sorting” — W. F. Eddy and M. J. Schervish (1995) (But *much* more analysis has followed!)

# 1: Basics of QuickSort analysis

Conditioning on the pivot index  $U_n$  and using the law of total expectation, the distributional recurrence

$$K_n \stackrel{\mathcal{L}}{=} K_{U_n-1} + K_{n-U_n}^* + n - 1, \quad n \geq 1$$

implies a simple **divide and conquer** recurrence relation for expected values with explicit solution

$$\kappa_n := \mathbf{E}K_n = 2(n+1)H_n - 4n, \quad n \geq 0.$$

We have

$$\kappa_n \sim 2n \ln n.$$

The law of total variance gives another recurrence relation, with solution

$$\begin{aligned} \mathbf{Var} K_n &= 7n^2 - 4(n+1)^2 H_n^{(2)} - 2(n+1)H_n + 13n \\ &\sim \left(7 - \frac{2}{3}\pi^2\right)n^2 =: \sigma^2 n^2 \end{aligned}$$

[e.g., Exercise 6.2.2-8 in **D. E. Knuth (1973, vol. 3)**].

- Higher-order cumulants: **Pascal Hennequin (1991 PhD diss.)**

## 2a: Convergence in distribution: heuristic derivation

Is there convergence in distribution?

$$Y_n := \frac{K_n - \kappa_n}{n} \xrightarrow{\mathcal{L}} ?$$

Note

$$K_n \stackrel{\mathcal{L}}{=} K_{U_n-1} + K_{n-U_n}^* + n - 1, \quad n \geq 1$$

implies

$$Y_n \stackrel{\mathcal{L}}{=} \frac{U_n - 1}{n} Y_{U_n-1} + \frac{n - U_n}{n} Y_{n-U_n}^* + C_n, \quad n \geq 1,$$

where  $Y_0 :=$  arbitrarily, with  $C_n := c_n(U_n)$  and

$$c_n(i) := \frac{n-1}{n} + \frac{1}{n}(\kappa_{i-1} + \kappa_{n-i} - \kappa_n).$$

Here  $\mathbf{E}Y_n = 0 = \mathbf{E}C_n$ .

## 2a: Convergence in distribution: heuristic derivation

Note: Can get  $U_n$  as  $\lceil nU \rceil$  with  $U \sim \text{unif}(0, 1)$ .

Can show by calculus:

$$c_n(\lceil nu \rceil) \rightarrow c(u) := 2u \ln u + 2(1 - u) \ln(1 - u) + 1;$$

this suggests

$$Y_n \xrightarrow{\mathcal{L}} Y \stackrel{\mathcal{L}}{=} UY + (1 - U)Y^* + c(U)$$

where on the RHS:  $Y$  has mean 0 and variance  $\sigma^2$ ,

$$U \sim \text{unif}(0, 1),$$

and

$U, Y, Y^*$  are *independent*.

## 2b: Convergence in distribution: three methods of proof

Heuristics have suggested

$$Y_n \xrightarrow{\mathcal{L}} Y \stackrel{\mathcal{L}}{=} UY + (1-U)Y^* + c(U)$$

with

$$\mathbf{E}Y = 0 \quad \text{and} \quad \mathbf{Var} Y = \sigma^2 = 7 - \frac{2}{3}\pi^2 < \infty.$$

This is **TRUE!**, and at least three methods of proof are possible:

**Method 1:**  $Y_n \xrightarrow{\mathcal{L}} Y$  by *method of moments* [P. Hennequin (1991)]

**Method 2:**  $Y_n \rightarrow Y$  a.s. and in  $L^p \forall 0 < p < \infty$  by *martingale* arguments [M. Régnier (1989)]

**Method 3:**  $Y_n \rightarrow Y$  in *Mallows*  $d_p \quad \forall p = 1, 2, \dots$  by *contraction method* [U. Rösler (1991)]

**OPEN PROBLEM** 6.2 in F and Janson (2002):

Is there a *local* limit theorem for distns.?

**YES!:** this talk, based on B. Bollobás, F, and O. Riordan (2016+)

### 3: Selected contributions to analysis of QS (2002-)

The following contributions are highlighted because they are relevant to establishment of a LLT!

- K. H. Tan and P. Hadjicostas (1995) — limit distribution is absolutely continuous; density is positive a.e.
- F and S. Janson (*Mathematics and Computer Science: Algorithms, Trees, Combinatorics, and Probabilities*, 2000) — smoothness and decay properties of the limiting density and its derivatives; in particular (Theorems 3.1 and 3.3 and Corollary 4.2 there), there is an infinitely smooth (analytic?) everywhere positive limiting density  $f$  satisfying

$$\max_x f(x) < 16 \quad \text{and} \quad \max_x f'(x) < 2466$$

(with the true bounds probably closer to 1 and 2, resp.).

Aside: These bounds were one ingredient used by L. Devroye, F, and R. Neininger (2000) to devise an algorithm for perfect simulation from the limiting distribution  $F$  for QuickSort.



# Plot of the (smooth) density function $f$ for $F$

*Kok Hooi Tan, P. Hadjicostas / Statistics & Probability Letters 25 (1995) 87–94*

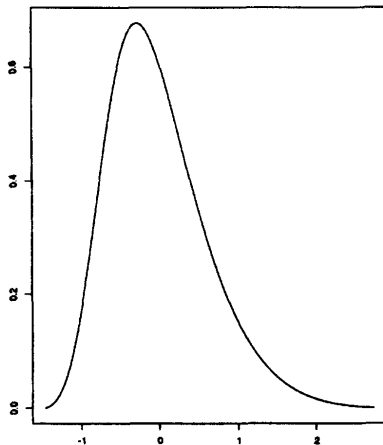


Fig. 4. Density function  $f_X(x)$  of limiting distribution.

# Thinness of the tails of $F$ (rigorous)

- Invariably, someone asks: How thin are the tails of  $F$ ?
- A **rigorously** established answer, sharp to lead order in log-probability, was provided by **S. Janson (Electron. J. Probab., 2015)**, improving significantly on results of **F and S. Janson (RSA, 2000)**.
- Let  $Y \sim F$ . The left tail is doubly-exponentially thin, and the right tail is Poisson(1)-thin:

## Theorem (**Janson, 2015**)

(a) Let  $\gamma := \left(2 - \frac{1}{\ln 2}\right)^{-1}$ . As  $x \rightarrow \infty$  we have

$$\exp\left[-e^{\gamma x + \ln \ln x + O(1)}\right] \leq \mathbf{P}(Y \leq -x) \leq \exp\left[-e^{\gamma x + O(1)}\right].$$

(b) As  $x \rightarrow \infty$  we have

$$\exp\left[-x \ln x - x \ln \ln x + O(x)\right] \leq \mathbf{P}(Y \geq x) \leq \exp\left[-x \ln x + O(x)\right].$$

# Thinness of the tails of $F$ (non-rigorous)

- Using the non-rigorous WKB method, C. Knessl and W. Szpankowski (*Discrete Math. Theor. Comput. Sci.*, 1999) found very sharp log-asymptotics for both tails:

(a) As  $x \rightarrow \infty$ , for some constant  $c$  we have

$$\mathbf{P}(Y \leq -x) = \exp \left[ -e^{\gamma x + c + o(1)} \right].$$

(b) As  $x \rightarrow \infty$  we have

$$\mathbf{P}(Y \geq x) = \exp \left[ -x \ln x - x \ln \ln x + (1 + \ln 2)x + o(x) \right].$$

**OPEN PROBLEMS:** Prove that  $f$  is unimodal. Is  $f$  in fact *strongly* unimodal? What can one say about changes of signs of the derivatives of  $f$ ? Is  $F$  infinitely divisible?

### 3: Selected contributions to analysis of QS (2002-)

Let  $F_n$  denote the distribution function of  $Y_n = (K_n - \kappa_n)/n$ . The following two results about convergence of  $F_n$  to its limit  $F$  are from **F and S. Janson** (*J. of Algorithms*, 2002), and the upper bounds are proved by first treating  $d_p$ -distances inductively using the *contraction method* á la **Rösler's** (1991) proof of convergence and then relating *Kolmogorov–Smirnov distance* to  $d_p$ -distances:

- We have  $F_n \rightarrow F$  at rate  $O\left(n^{-(\frac{1}{2}-\epsilon)}\right)$  in the K-S distance (for every  $\epsilon > 0$ ); but our lower bound is only  $\Omega(n^{-1})$  (and **improving either bound** in this global theorem remains an **open problem**).
- There is a constant  $C$  such that, for any  $x$  and any  $n \geq 1$ ,

$$\left| \frac{F_n(x + \frac{\delta_n}{2}) - F_n(x - \frac{\delta_n}{2})}{\delta_n} - f(x) \right| \leq Cn^{-1/6},$$

where  $\delta_n = 2Cn^{-1/6}$  (w/ no claim of sharpness in the bound).

## 4: From a semi-local LT to a local LT

Recall that  $F_n$  denotes the distribution function of

$$Y_n = (K_n - \kappa_n)/n$$

and that we have the following **semi-local limit theorem**:

- There is a constant  $C$  such that for any  $x$  and any  $n \geq 1$  we have

$$\left| \frac{F_n(x + \frac{\delta_n}{2}) - F_n(x - \frac{\delta_n}{2})}{\delta_n} - f(x) \right| \leq Cn^{-1/6},$$

where  $\delta_n = 2Cn^{-1/6}$ .

Our **new result** is that  $\delta_n$  can be decreased to  $n^{-1}$ , with the error bound increasing from  $O(n^{-1/6})$  to a little more than  $O(n^{-1/18})$ .

Expressed in terms of the distribution of the unnormalized comparisons-count  $K_n$ , the result is as follows (**again with no claim of sharpness in the bound**).

# Main theorem: A LLT for QuickSort

The following **local limit theorem** is our main result and gives a positive answer to **Open Problem 6.2** in **F and S. Janson** (*J. of Algorithms*, 2002):

## Theorem (Local Limit Theorem for QuickSort)

Let  $K_n$  denote the (random) number of key comparisons required by **QuickSort** to sort a file of  $n$  distinct keys, let  $\kappa_n = \mathbf{E}K_n$ , and let  $f$  denote the continuous density of the limiting distribution for the normalized random variable  $Y_n = (K_n - \kappa_n)/n$ . Then there is a constant  $C$  such that for any integer  $k$  and any  $n \geq 1$  we have

$$|\mathbf{P}(K_n = k) - n^{-1}f((k - \kappa_n)/n)| \leq n^{-1} \times Cn^{-1/18} \log n.$$

We obtain the LLT from the semi-LLT by multiple rounds of a **smoothing argument**. The proof is a bit too complex even for a 60-minute talk, but I will give some ideas.

## 5: Obtaining the LLT from the semi-LLT: main ideas

We obtain the LLT from the semi-LLT by multiple rounds of a **smoothing argument**. The basic idea of strengthening a distributional (often normal) limit theorem to a local one by smoothing is by now quite old, but we find it necessary (and sufficient) to do this smoothing in multiple rounds. [Multi-round smoothing has recently been used independently by **Diaconis and Hough (2015)** in a different context.]

- We know that there is global (and, indeed, semi-local) convergence to a well-behaved distribution. (GLT)
- To deduce a LLT from the GLT it would suffice to show that “nearby” values for  $K_n$  have probabilities that are close, namely: If  $k_n, k'_n = \kappa_n + O(n)$  and  $|k_n - k'_n| = o(n)$ , then

$$\mathbf{P}(K_n = k_n) = \mathbf{P}(K_n = k'_n) + o(n^{-1}). \quad (1)$$

- For this, in turn, we might (as in **D. R. McDonald (1979)**) try to find a “smooth part” within the distribution of  $K_n$ . More precisely, ...

# Obtaining the LLT from the semi-LLT: main ideas

- We might try to find a “smooth part” within the distribution of  $K_n$ . More precisely, we might try to write

$$K_n = A_n + B_n$$

where, for some  $\sigma$ -field  $\mathcal{F}_n$ , we have that  $A_n$  is  $\mathcal{F}_n$ -measurable and the conditional distribution of  $B_n$  given  $\mathcal{F}_n$  (wvhp) obeys a “closeness” relation corresponding to (1).

- Then it follows easily (by first considering conditional probabilities given  $\mathcal{F}_n$ ) that (1) holds.
- One idea is to choose  $\mathcal{F}_n$  so that  $B_n$  has a very well understood conditional distribution, such as binomial.
- In some contexts, this approach works directly. Here it does not. We can get such a decomp. with (conditionally)  $B_n \sim \text{Bin}(\Theta(n), 2/3)$ . But then the variance of  $B_n$  grows linearly, while the variance of  $K_n$  grows quadratically. Roughly speaking, this allows us to prove (1) when  $|k_n - k'_n| = o(\sqrt{n})$ , but we need (1) for  $|k_n - k'_n| = o(n)$  [or, in light of the semi-LLT, at least for  $|k_n - k'_n| = O(n^{5/6})$ ].



## 6: The tree-exploration lemma

The key idea, then, is not to try to jump straight from the GLT (or from the semi-LLT) to the LLT, but to proceed in stages (rounds). Rather than outline the entire argument (which makes use of the CLT for sums of independent random variables after suitable exponential tilting, among many other things), I will discuss a **tree-exploration** lemma (along with its proof using **martingale arguments**) that lies at the heart of the argument. Let  $c := 1/100$ .

### Lemma (tree-exploration lemma)

Let  $r \geq 2$  be even, and assume that  $r \leq n/75$ . Then setting  $s = \lceil cn/r \rceil$ , we may write  $K_n = A + B$  where, for some  $\sigma$ -field  $\mathcal{F}$ :

- $A$  is  $\mathcal{F}$ -measurable, and
- with probability at least  $1 - e^{-s}$ , the conditional distribution of  $B$  given  $\mathcal{F}$  is the sum of  $s$  independent random variables  $B_1, \dots, B_s$  with each  $B_i$  having the distribution  $K_{r_i}$  for some  $r_i$  with  $r/2 \leq r_i \leq r$ .

## 7: Proof of the tree-exploration lemma

The remainder of the talk is devoted to the proof of the **tree-exploration lemma**. Before any **claims**, much preliminary discussion:

- $T_n$  = random binary search tree for  $n$  nodes labeled  $1, \dots, n$ .
- $T(v)$  denotes the subtree of  $T_n$  consisting of a given node  $v$  and its descendants (the **"fringe" subtree** of  $T_n$  rooted at  $v$ ). We consider two counts,  $X_n$  (primary) and  $Y_n$  (auxiliary):
- $X_n :=$  number of nodes  $v$  such that (i)  $r/2 \leq |T(v)| \leq r$  and (ii) either  $v$  is the root or  $|T(\text{parent of } v)| > r$ . Call such a node **special**.
- Observe: If  $v$  and  $w$  are distinct special nodes, then  $T(v)$  and  $T(w)$  are disjoint.
- We will show that, with probability at least  $1 - e^{-s}$ , there are at least  $s$  special nodes in  $T_n$ , i.e.:  $\mathbf{P}(X_n \geq s) \geq 1 - e^{-s}$ .
- $Y_n :=$  number of fringe trees with at least  $r + 1$  nodes.

# Proof of the tree-exploration lemma (cont.): exploration

For convenience in presenting the arguments that follow, attach (unlabeled) external nodes as necessary to each node of  $T_n$  so that as a result each of the original nodes of  $T_n$  has two children; these external nodes do not have labels and do not contribute to the sizes of subtrees.

Consider the following discrete-time procedure for **exploring** the original nodes of  $T_n$  in order to learn their search-tree labels.

- At time 0 nothing is known.
- At time 1, the label of the root is revealed, thus also revealing the sizes of the left and right subtrees.

Now let  $2 \leq t \leq n$ . ...

# Proof of the tree-exploration lemma: exploration (cont.)

Now let  $2 \leq t \leq n$ . At time  $t - 1$ , it will be true inductively that nodes with revealed labels will have fringe subtree size at least  $r + 1$  and the subtree sizes of their two children will be known.

- At time  $t$ , choose an unrevealed child  $v$  of a revealed node such that  $|T(v)| \geq r + 1$  and reveal its label, if such a  $v$  exists.
  - For definiteness, among such nodes  $v$  with smallest level, choose the leftmost one.
  - If there are no such nodes  $v$ , then nothing is revealed at time  $t$  (nor at later times).
  - At any time  $t \in [1, n]$ , call the unrevealed children (including all external nodes) of revealed nodes “leaves”.
- Note that each time the label of a node is revealed, two new leaves (namely, the children of that node) are created; for later technical reasons, we consider the left child to be created as a leaf before the right child.

# Proof of the tree-exploration lemma (cont.): martingales

- $\tau := Y_n$  is the random time at which the procedure ends, i.e., the first time at which all of the leaves have subtree sizes  $\leq r$ .
- $\mathcal{F}_t :=$  the  $\sigma$ -field corresponding to the labels that have been revealed through time  $t$ .
- **Observe!:** For any random variable  $W$  with finite expectation, the stochastic process  $(\mathbf{E}[W|\mathcal{F}_t])_{0 \leq t \leq n}$  is a (Doob's) **martingale** with values  $\mathbf{E}W, W$  at times  $t = 0, n$ , resp.
- We will apply this observation taking  $W$  to be  $X_n$  [with martingale  $(M_t)$ ] and  $Y_n$  [with martingale  $(N_t)$ ]. Clearly  $N_\tau = Y_n = \tau$ .
- The respective means  $\xi_n := \mathbf{E}X_n$  and  $\eta_n := \mathbf{E}Y_n$  of the martingales  $(M_t)$  and  $(N_t)$  can be computed by solving standard **divide-and-conquer recurrence relations**.
- From those computations it is simple to deduce that

$$-2 < N_t - N_{t-1} \leq 1, \quad -\frac{1}{2} < M_t - M_{t-1} < 1$$

for every  $t$ .

# Proof of the tree-exploration lemma (cont.): bound on $\tau$

**First claim:**  $\mathbf{P}(\tau < \frac{3n}{r+1}) \geq 1 - \exp\left[-\frac{2}{27} \left(\frac{n}{r+1}\right)\right]$ .

**Proof:** Recalling that  $\tau = N_\tau$ , we have

$$\mathbf{P}\left(\tau \geq \frac{3n}{r+1}\right) \leq \mathbf{P}\left(N_t = t \text{ for some } t \geq \frac{3n}{r+1}\right).$$

By the **generalized Azuma inequality** we have

$$\begin{aligned} & \mathbf{P}\left(\tau \geq \frac{3n}{r+1}\right) \\ & \leq \mathbf{P}\left(N_t - \eta_n = t - \left\lfloor \frac{2(n+1)}{r+2} - 1 \right\rfloor \text{ for some } t \geq \frac{3n}{r+1}\right) \\ & \leq \mathbf{P}\left(N_t - \eta_n \geq \frac{1}{3}t \text{ for some } t \geq \frac{3n}{r+1}\right) \\ & \leq \exp\left[-\frac{2}{81} \left\lfloor \frac{3n}{r+1} \right\rfloor\right] \\ & \leq \exp\left[-\frac{2}{27} \left(\frac{n}{r+1}\right)\right] =: \varepsilon. \quad \square \end{aligned}$$

**First claim:**  $\mathbf{P}(\tau < \frac{3n}{r+1}) \geq 1 - \exp\left[-\frac{2}{27} \left(\frac{n}{r+1}\right)\right]$ . □

**Second claim:**  $\mathbf{P}\left(X_n \geq \frac{(1/100)n}{r}\right) \geq 1 - \exp\left[-\left\lceil\frac{1}{100}\left(\frac{n}{r}\right)\right\rceil\right]$ .

**Proof:** By the **first claim**, because  $t \geq \tau$  implies  $M_t = X_n$ , we have

$$\mathbf{P}\left(X_n < \frac{(1/2)(n+1)}{r+1}\right) \leq \mathbf{P}\left(\tau \geq \frac{3n}{r+1}\right) + \mathbf{P}\left(M_{\lceil 3n/(r+1) \rceil} < \frac{(1/2)(n+1)}{r+1}\right).$$

Further, by **Azuma's inequality** we have

$$\begin{aligned} & \mathbf{P}\left(X_n < \frac{(1/100)n}{r}\right) \\ & \leq \mathbf{P}\left(X_n < \frac{(1/2)(n+1)}{r+1}\right) \leq \varepsilon + \mathbf{P}\left(M_{\lceil 3n/(r+1) \rceil} < \frac{(1/2)(n+1)}{r+1}\right) \\ & = \varepsilon + \mathbf{P}\left(M_{\lceil 3n/(r+1) \rceil} - \xi_n < -\frac{(1/2)(n+1)}{r+1}\right) \\ & \leq \varepsilon + \exp\left[-\frac{8}{9} \left[\frac{(1/2)(n+1)}{r+1}\right]^2 / \lceil 3n/(r+1) \rceil\right] \leq \varepsilon + \exp\left[-\frac{1}{18} \left(\frac{n}{r+1}\right)\right] \\ & \leq \exp\left[-\frac{4}{81} \left(\frac{n}{r}\right)\right] + \exp\left[-\frac{1}{27} \left(\frac{n}{r}\right)\right] \leq \exp\left[-\left\lceil\frac{1}{100}\left(\frac{n}{r}\right)\right\rceil\right], \quad \text{where} \end{aligned}$$

- the orange ineq. holds because  $\lceil 3n/(r+1) \rceil \leq 4n/(r+1)$ ,
- the blue inequality holds because  $r+1 \leq (3/2)r$ , and
- the green inequality holds because

$$e^{-4x/81} + e^{-x/27} \leq e^{-(x/100)+1} \leq e^{-\lceil x/100 \rceil} \text{ for } x \geq 75.$$

We have proven the second claim that the number  $X_n$  of special nodes is at least  $s = \lceil (1/100)n/r \rceil$  wp at least  $1 - e^{-s}$ .

The proof of the tree-exploration lemma, and hence of the LLT, concludes on the next slide.



# Proof of the tree-exploration lemma (conclusion)

- Let  $\sigma \leq \tau$  denote
  - the stopping time at which the exploration process has discovered either  $s$  or (by means of having simultaneously discovered two special-leaf children with a single reveal)  $s + 1$  special leaves, in the event  $E$  that such a time exists;
  - otherwise set  $\sigma = n$ .
- If the event  $E$  occurs, fully explore the subtrees rooted at all leaves except the first  $s$  special leaves that have been discovered by time  $\sigma$ .
- Take the desired  $\sigma$ -field  $\mathcal{F}$  to be (informally stated) the  $\sigma$ -field corresponding to all the information uncovered as we have just described.
- Taking  $B_i$ ,  $i = 1, \dots, s$ , to be (when  $E$  occurs) the total (internal) path length (i.e., number of key comparisons for **QuickSort**) of the  $i$ th special leaf discovered by time  $\sigma$ , the **tree-exploration lemma** follows. □

# Thanks for attending this talk!



**Method 1:**  $Y_n \xrightarrow{\mathcal{L}} Y$  by *method of moments* [Hennequin (1991)]

- **Hennequin** (who more generally studied  $s$ -ary QuickSort with pivots chosen as medians of samples of size  $2t + 1$ ) “pumped moments” and developed asymptotics for them.
- He proved that for  $r = 1, 2, \dots$  we have

$$\mathbf{E} Y_n^r \rightarrow m_r \in (-\infty, \infty),$$

where no general expression for  $m_r$  seems possible, but a recurrence relation can be established.

- From the recurrence relation he proved that the radius of convergence  $[\limsup_r (|m_r|/r!)^{1/r}]^{-1}$  of  $\sum_r (m_r/r!)t^r$  is positive. (**Rosler:**  $\text{Mgf}_Y$  is finite everywhere!) So  $Y_n \xrightarrow{\mathcal{L}} Y$ , where  $\mathcal{L}(Y)$  is the unique distribution with moments  $m_r$ .
- **Hennequin's** recurrence relation for  $(m_r)$  states *precisely* that (i)  $\mathbf{E} Y = 0$  and (ii)  $Y$  and  $UY + (1 - U)Y^* + c(U)$  have the same moments, so the distributional identity follows, too.

# An interesting sidelight from Hennequin

A mathematically interesting sidelight from **Hennequin (1991)** is that the cumulants  $k_r$  of  $Y$  (that is, the sequence defined by  $\sum_{r=1}^{\infty} (k_r/r!)t^r = \ln \mathbf{E} e^{tY}$ ) are for every  $r \geq 2$  of the form

$$k_r = (-1)^r 2^r [a_r - (r-1)! \zeta(r)],$$

where the constants  $a_r$  are all rational and  $\zeta(\cdot)$  is **Riemann's zeta function**.

# Martingale approach: discovering the martingale

**Method 2:**  $Y_n \rightarrow Y$  a.s. and in  $L^p \forall 0 < p < \infty$  by *martingale* arguments [Régnier (1989)]

- There are  $n + 1$  external nodes in the binary search tree built from  $X_1, \dots, X_n$ .
- $K_n = \text{IPL}_n = \text{internal path length}$  in the binary search tree built from  $X_1, \dots, X_n$ .
- By induction,  $\text{XPL}_n = \text{external path length} = \text{IPL}_n + 2n$ .  
[When  $n = 0$  this says  $0 = 0$ . When an external node at distance  $d$  from the root is converted to an internal node, IPL increases by  $d$  and XPL increases by  $2(d + 1) - d = d + 2$ ; so  $\text{XPL} - \text{IPL}$  increases by  $(d + 2) - d = 2$ .]
- So, conditionally given the evolution of the random binary search tree through time  $n$ , the expected increase in  $K = \text{IPL}$  at time  $n + 1$  is  $\text{XPL}_n / (n + 1) = (K_n + 2n) / (n + 1)$ .

# Martingale approach: application of $L^p$ Martingale Convergence Theorem

**Method 2:**  $Y_n \rightarrow Y$  a.s. and in  $L^p \forall 0 < p < \infty$  by *martingale* arguments [Régnier (1989)]

- Summarizing from preceding slide,

$$\mathbf{E}(K_{n+1} | \mathcal{F}_n) = K_n + \frac{K_n + 2n}{n+1}.$$

This is easily rearranged to reveal that the process

$(\hat{Y}_n := \frac{n}{n+1} Y_n = \frac{K_n - \kappa_n}{n+1})$  is a *martingale* with respect to  $(\mathcal{F}_n)$ .

- $L^p$  Martingale Convergence Theorem:** Fix  $p \in [1, \infty)$ . A martingale  $(Z_n)$  such that  $(|Z_n|^p)_{n=1,2,\dots}$  is uniformly integrable converges both almost surely and in  $L^p$  to a (common) limit  $Z$ .
- We get the desired conclusions by checking that, for each fixed  $r$ , the sequence of absolute moments of order  $r$  is bounded. This check does not require the delicacy of *Hennequin!*

# Convergence in distribution: contraction method

**Method 3:**  $Y_n \rightarrow Y$  in *Mallows*  $d_p$   $\forall p = 1, 2, \dots$  by *contraction method* [Rösler (1991)]

Rösler's method also shows that  $F := \mathcal{L}(Y)$  is the *unique* fixed point of the distributional transformation

$$G = \mathcal{L}(V) \mapsto SG := \mathcal{L}(UV + (1 - U)V^* + c(U))$$

subject (*only!*) to

$$\mathbf{E}V = 0, \quad \mathbf{Var} V < \infty.$$

Recall that the method of moments used by *Hennequin* only gave uniqueness subject to  $\mathbf{E}V = 0$  and finiteness of *all* moments of  $V$ .

**NOTE.** (F & S. Janson, *Electron. Commun. Probab.*, 2000a)

$F := \mathcal{L}(Y)$  is the *unique* fixed point of

$$G = \mathcal{L}(V) \mapsto SG := \mathcal{L}(UV + (1 - U)V^* + c(U))$$

subject to

$$EV = 0 \quad (\text{only!!}).$$

It's easy to check that the convolution of  $F$  with *any* Cauchy (any location, any scale) is also a fixed point.

F & Janson (2000a): Those are *all* the fixed points!



# Rösler: Existence and uniqueness of fixed point

- Due to time constraints, let's limit attention to  $d_2$  here.

**Rösler's proof** of the existence and uniqueness of a  $d_2$ -fixed point for  $S$ : Let  $d \equiv d_2$ . Then

$$\begin{aligned}d(G, H) &:= \inf_{\text{couplings with } V \sim G, W \sim H} \|V - W\|_2 \\ &= \|G^{-1}(U) - H^{-1}(U)\|_2.\end{aligned}$$

This is a metric on

$$D := \{\text{distns. with mean 0 and finite variance}\}.$$

Note

$(D, d)$  is a Polish space (i.e., a complete separable metric space);  
 $\rightarrow$  in  $d$  iff  $\xrightarrow{\mathcal{L}}$  and conv. of 2nd moments.

# Contraction

Existence & uniqueness of a fixed point for  $S$  follows directly from

## Proposition

$S$  is a strict contraction on  $(D, d)$ .

**Proof.** Given  $G$  and  $H$  in  $D$ , let

$$\begin{aligned}U &\sim \text{unif}(0, 1) \\(V, W) &\sim \text{coupling achieving } d(G, H) \\(V^*, W^*) &\sim \text{coupling achieving } d(G, H),\end{aligned}$$

with these three **independent**. Then  $S : D \rightarrow D$  and  $d^2(S(G), S(H))$

$$\begin{aligned}&\leq \| [UV + (1 - U)V^* + c(U)] - [UW + (1 - U)W^* + c(U)] \|_2^2 \\&= \| U(V - W) + (1 - U)(V^* - W^*) \|_2^2 \\&= \|U\|_2^2 \|V - W\|_2^2 + \|1 - U\|_2^2 \|V^* - W^*\|_2^2 = \frac{2}{3}d^2(G, H). \quad \blacksquare\end{aligned}$$

# Approximating the fixed point $F$

Rösler also showed that

$$\mathcal{L}(Y_n) \rightarrow \text{the fixed point } F \text{ of } S.$$

Trusting this for now, we can thus get approximations that converge **geometrically rapidly** in  $d_2$  to the limiting **QuickSort distribution** by choosing any  $G$  with mean zero and finite variance (e.g.,  $G = \delta_0$ ) and using  $S^n G$  with  $n$  large. Indeed, for any such  $G$ , Rösler showed that

$$d_2(S^n G, F) \leq \left(\frac{2}{3}\right)^{n/2} (\sigma^2 + \mathbf{Var} G)^{1/2}.$$

(Other metrics have been treated, but we don't have time today!)

*However*, note that computation of  $S^n G$  requires numerical integration (e.g., of densities).

### 3: Bound on $d_2$ -rate of convergence for QuickSort

Rösler proved  $Y_n \rightarrow Y$  (i.e.,  $F_n \rightarrow F$ ) in  $d$ ;

**rate of convergence?** From F & Janson (2002, J. Algo.):

#### Theorem

$$d(F_n, F) < \frac{2}{\sqrt{n}} \text{ for } n \geq 1.$$

**Remark:** By considering  $n = 2$ , the numerator 2 here is optimal within a factor of about 2.

Outline of **Proof:** Follow Rösler's outline for  $d(F_n, F) \rightarrow 0$ , but be more quantitative. Recall

$$Y_n \stackrel{\mathcal{L}}{=} \frac{\lceil nU \rceil - 1}{n} Y_{\lceil nU \rceil - 1} + \frac{n - \lceil nU \rceil}{n} Y_{n - \lceil nU \rceil}^* + c_n(\lceil nU \rceil),$$

$$Y \stackrel{\mathcal{L}}{=} UY + (1 - U)Y^* + c(U).$$

Proceed as in proof that  $S$  is contraction to get

$$\begin{aligned}d^2(F_n, F) &\leq \mathbf{E} \left[ \frac{\lceil nU \rceil - 1}{n} Y_{\lceil nU \rceil - 1} - UY \right]^2 \\ &\quad + \mathbf{E} \left[ \frac{n - \lceil nU \rceil}{n} Y_{n - \lceil nU \rceil} - (1 - U)Y \right]^2 \\ &\quad + \mathbf{E} [c_n(\lceil nU \rceil) - c(U)]^2 \\ &=: \text{(I)} + \text{(II)} + \text{(III)}\end{aligned}$$

using law of total variance. (Condition on  $U$ .)  
Can show (using calculus)

$$|c_n(\lceil nu \rceil) - c(u)| \leq c_1 \frac{\ln n}{n},$$

so

$$\text{(III)} \leq c_1^2 \left( \frac{\ln n}{n} \right)^2.$$

Next,

$$\begin{aligned} \text{(I)} &= \mathbf{E} \left[ \frac{\lceil nU \rceil - 1}{n} Y_{\lceil nU \rceil - 1} - UY \right]^2 \\ &= \mathbf{E} \left[ \frac{\lceil nU \rceil - 1}{n} (Y_{\lceil nU \rceil - 1} - Y) + \left( \frac{\lceil nU \rceil - 1}{n} - U \right) Y \right]^2 \\ &\leq \frac{1}{n} \sum_{i=1}^n \left( \frac{i-1}{n} d(F_{i-1}, F) + \frac{\sigma}{n} \right)^2. \end{aligned}$$

[Get this by Minkowski's inequality for  $\| \cdot \|_2$ ;  
factor of **2** in  $(a + b)^2 \leq 2(a^2 + b^2)$  would be disastrous.]

Handle **(II)** similarly.

Find

$$d^2(F_n, F) =: a_n^2 \leq \frac{2}{n^3} \sum_{j=1}^{n-1} j^2 a_j^2 + \frac{4\sigma}{n^3} \sum_{j=1}^{n-1} j a_j + c_1^2 \left( \frac{\ln n}{n} \right)^2 + \frac{2\sigma^2}{n^2}.$$

Show

$$a_n \leq c_2 n^{-1/4} \text{ using induction;}$$

then

$$\sum_{j=1}^{n-1} j a_j \leq c_3 n^{7/4}$$

and so

$$\begin{aligned} a_n^2 &\leq \frac{2}{n^3} \sum_{j=1}^{n-1} j^2 a_j^2 + c_4 n^{-5/4} + c_1^2 \left( \frac{\ln n}{n} \right)^2 + \frac{2\sigma^2}{n^2} \\ &\leq \frac{2}{n^3} \sum_{j=1}^{n-1} j^2 a_j^2 + c_5 n^{-5/4} \\ &=: \frac{2}{n^3} \sum_{j=1}^{n-1} j^2 a_j^2 + b_n. \end{aligned}$$

By standard **divide and conquer** recurrence (for  $n^2 a_n^2$ ),

$$a_n^2 \leq b_n + 2 \frac{n+1}{n^2} \sum_{k=1}^{n-1} \frac{k^2 b_k}{(k+1)(k+2)} \leq \frac{c_6}{n},$$

which gives the result up to a constant multiple. By both tuning up the argument and keeping track of constants, the result follows. ■



### 3: What *is* the $d_2$ -rate of convergence for QuickSort?

Is  $n^{-1/2}$  the right rate for  $d(F_n, F)$ ?

We don't know.

A trivial lower bound:

$$\begin{aligned}d(F_n, F) &= \inf_{\text{couplings}} \|Y_n - Y\|_2 \\ &\geq | \|Y_n\|_2 - \|Y\|_2 | \geq c_7 \frac{\ln n}{n}.\end{aligned}$$

# Exact rate of convergence in the Zolotarev metric $\zeta_3$

- R. Neininger and L. Rüschemdorf (2002) — **exact** rate  $\Theta(\frac{\log n}{n})$  in the *Zolotarev metric*  $\zeta_3$

The *Zolotarev metric*  $\zeta_3$  is defined as follows: If  $V \sim G$  and  $W \sim H$ , then

$$\zeta_3(G, H) := \sup_{f \in \mathcal{F}_3} |\mathbf{E} f(V) - \mathbf{E} f(W)| \quad \text{where}$$

$$\mathcal{F}_3 := \{f : |f''(x) - f''(y)| \leq |x - y| \text{ for all } x, y\}$$

is the class of functions having a Lipschitz-continuous second derivative with Lipschitz constant equal to 1.

The **precise statement** of their theorem matters!

# Perfect simulation from limiting QuickSort distribution

- Devroye, F, and R. Neininger (2000) — an algorithm for perfect simulation from the limiting distribution  $F$  for QuickSort. **Brief summary:** Combining
  - explicit integer bounds on density  $f$  and  $|f'|$  from F and S. Janson (2000),
  - an explicit integer bound on  $EY^4$ , and
  - standard arguments from the book of Devroye (1986) on simulation from distributions,

we can find a function  $g$  such that

- $g$  is of the form  $g(y) = \min(c_1, c_2 y^{-2})$  (and hence integrable),
- perfect simulation from density  $\text{normalized-}g$  is elementary, and
- $f \leq g$ .

Then we can use the rejection method to sample from  $f$ , if we can also find a sequence of explicitly computable approximations to  $f$  with explicitly computable error bounds. But F and S. Janson (2001) also supplies such a sequence.

# Knowledge about the fixed point $F = \mathcal{L}(Y)$

1.  $\mathbf{E}Y = 0$ ,  $\mathbf{Var}Y = \sigma^2 = 7 - \frac{2}{3}\pi^2$ .
2. Mgf  $M$  is finite everywhere (Rösler, 1991) and satisfies

$$M(\lambda) = \int_{u=0}^1 M(u\lambda)M((1-u)\lambda)e^{\lambda c(u)} du, \quad \lambda \in \mathbf{R}.$$

3. Moments of all orders can be “pumped.” (Hennequin, Rösler)
4. Characteristic function (ch.f.)  $\phi$  satisfies

$$\phi(t) = \int_{u=0}^1 \phi(ut)\phi((1-u)t)e^{itc(u)} du, \quad t \in \mathbf{R}.$$

5. Method of successive substitutions “works” both for  $M$  and for  $\phi$ .

# Knowledge about $F = \mathcal{L}(Y)$ : absolute continuity

6.  $F$  has a density  $f$ , which is  $> 0$  a.e. (Tan & Hadjicostas, 1995)

**Proof** of existence of density: For fixed  $y$  and  $z$ ,

$$h_{y,z}(U) := Uy + (1 - U)z + c(U)$$

is absolutely continuous, say with density  $g_{y,z}$ . Now mix densities:

$$f(t) := \int_{(y,z) \in \mathbb{R}^2} g_{y,z}(t) dF(y) dF(z), \quad t \in \mathbb{R}$$

gives density for  $F$ , satisfies integral equation

$$f(t) := \int_{(y,z) \in \mathbb{R}^2} g_{y,z}(t) f(y) f(z) dy dz, \quad t \in \mathbb{R}. \quad \blacksquare$$

But singularity of  $g_{y,z}(\cdot)$  at the left endpoint

$$\beta_{y,z} := 1 - 2 \ln \left( e^{-y/2} + e^{-z/2} \right)$$

of its support makes proving more about  $f$  *challenging*.

# Knowledge about $F = \mathcal{L}(Y)$ : behavior of density $f$

Knowledge about  $F$  from F and S. Janson (2000b):

- There is a density  $f$  that looks like the density plot (Fig. 4) in K. H. Tan and P. Hadjicostas (1995):
  - $f$  is positive everywhere (not just a.e.)
  - $f$  is infinitely differentiable [Is it analytic?]
  - $f$  and its derivatives are bounded (We proved  $f < 16$  and  $|f'| < 2466$  — far from sharp!)
  - $f^{(k)}(t) \rightarrow 0$  as  $t \rightarrow \pm\infty$ , superpolynomially quickly, for each  $k$
- $f$  satisfies this integral equation for  $x \in \mathbf{R}$  :

$$f(x) = \int_{u=0}^1 \int_{y \in \mathbf{R}} f(y) f\left(\frac{x - c(u) - (1-u)y}{u}\right) \frac{1}{u} dy du$$

**OPEN PROBLEMS:** Prove that  $f$  is unimodal. Is  $f$  in fact strongly unimodal? What can one say about changes of signs of the derivatives of  $f$ ? Is  $F$  infinitely divisible?

More knowledge about  $F$  from **F and S. Janson (2000b)**:

- Ch.f.  $\phi$  decays superpolynomially quickly. (NOTE: We proved this first!, with explicit bounds.) Thus, in particular,  $\phi \in L^1(\text{Lebesgue measure})$ , so  $f$  is continuous and given by the Fourier inversion formula

$$f(y) \equiv \frac{1}{2\pi} \int_{t \in \mathbf{R}} e^{-iyt} \phi(t) dt.$$

[*Note.* Several authors had used this without proof or comment.]

An example of knowledge about  $F$  contained in **F and S. Janson (2001)**:

- Applying the method of successive substitutions to the integral equation for  $f$  gives a sequence  $(f_n)$  that converges uniformly to  $f$  (method for Figure 4—authors have **disclaimer**), with a geometric rate of convergence, provided we start with a density having zero mean and finite variance (such as standard normal).
- We also have geometrically fast convergence of  $f_n$  to  $f$  in Kolmogorov–Smirnov and total variation distances.