Boltzmann sampling of irreducible context-free structures in linear time

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Abstract: We continue our program of improving the complexity of so-called ‘Boltzmann sampling’ algorithms, for the exact sampling of combinatorial structures, and reach average linear-time complexity, i.e. optimality up to a multiplicative constant. Here we solve this problem for ‘irreducible context-free structures’, a broad family of structures to which the celebrated Drmota–Laalley–Woods Theorem applies. Our algorithm is a ‘rejection algorithm’. The main idea is to single out some degrees of freedom, i.e. write $p(x) = p_1(y)p_2(x|y)$, which allows to introduce a rejection factor at the level of the $y$ object, that is almost surely of order 1.

Keywords: Boltzmann sampling, Exact sampling, Galton–Watson trees, Analysis of algorithms.

1 The quest for linear-time Boltzmann sampling

We continue our study of the so-called “Boltzmann” Exact Sampling Algorithm [1], a wide class of algorithms which allow to sample random combinatorial structures of size $n$ from a given measure, in an average time that scales algebraically with $n$. This algorithm has received many praises since its appearance in 2004, and it is fair to state that nowadays constitutes a small branch by its own with the Theory of Algorithms. It exists in various incarnations, such as labeled [1] and unlabeled [2] combinatorial structures, structures defined through differential specifications [3] and multi-parametric extensions [4]. In this paper we will mostly concentrate on the ‘original’ case, discussed in [1], of labelled structures.

The structures to which this family of algorithms mainly apply are described in detail in the Flajolet and Sedgewick monograph on Analytic Combinatorics [5], where a large stress is given to generating-function techniques and saddle-point methods for the asymptotic enumeration of the configurations. In short, the Boltzmann Algorithm explores the possibility of translating the informations implicit in this analysis into an efficient exact-sampling algorithm. Say that we have combinatorial objects $x \in \mathcal{X} = \bigcup_n \mathcal{X}_n$, and objects of size $n$ have measure $\mu_n(x)$, with support $\mathcal{X}_n$. In most cases, a one-parameter family of measures exist, $\mu(x; \beta)$, which takes the form $\mu(x; \beta) = \sum_n p_\beta(n)\mu_n(x)$, and is ‘natural’ in the sense that it is the one implicit in the construction of the generating function $X(z)$ for the objects (where $z$ and $\beta$ are easily related). In other words, the measures $\mu_n(x)$ and $\mu(x; \beta)$ are the canonical and grand-canonical Boltzmann–Gibbs measures, at energy $n$ and inverse-temperature $\beta$, for the statistical ensemble consisting of the combinatorial objects, and the name ‘Boltzmann Method’ is a tribute to the role of Ludwig Boltzmann in the foundations of Statistical Mechanics, whose ideas are of inspiration for the method. The recursive description of $X(n)$ implicit in the combinatorial specification translates into a linear-time algorithm for sampling from $\mu(x; \beta)$, which thus induces an algorithm for sampling from $\mu_n(x)$, with complexity $\sim n/p_\beta(n)$.

Essentially in all the cases of interest for us, the Shannon entropy of the measure $\mu_n(x)$, defined as $S[\mu_n] := -\sum_{x \in \mathcal{X}_n} \mu_n(x) \ln \mu_n(x)$, scales linearly with $n$, and, as well known, this provides a lower bound to the complexity for exact sampling, because any algorithm needs to sample on average at least $S[\mu_n]$ random bits, and the cost of a random bit is of order 1. (Note that, if the measure is the uniform measure, as in most of the concrete applications, then $S[\mu_n] = \ln \mathcal{A}_n$, and if $\mathcal{A}_n \sim \rho^{-n}n^\gamma$, then $S[\mu_n] = -n \ln \rho + o(n)$.) We say that an algorithm is optimal up to a multiplicative constant if

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1 This is a different, weaker notion w.r.t. optimality tout court, which, in the framework of exact-sampling algo-
it has average complexity bounded from above by $C \cdot S[p_n]$, for some constant $C \geq 1$. Unfortunately, the Boltzmann algorithm as is is not optimal, as normally $\max_j p_j(n)$ scales as $1/n$, or, at best, as $1/\sqrt{n}$. Thus, the average complexity scales as $\sim n/p_j(n) = n^{1+\gamma}$ for some $\gamma > 0$. For this reason we have started to explore under which circumstances we can improve the ideas of Boltzmann sampling, up to (possibly) reach optimality.

In a first paper [14], we devise a general method that applies to all the cases in which an object $x$ of size $n$ can be decomposed canonically as the union of two parts, $x = x_1 \cup x_2$, both of size $\sim n$. When this is the case, an improvement of the naive Boltzmann method for sampling from the Hadamard product of two distributions allows to decrease the complexity from $n^{1+\gamma}$ to $n^{1+\gamma}$. In our opinion, this is already an interesting result, as it is rather general, however it does not cover all the applications of Boltzmann sampling (as the forementioned canonical decomposition does not always exist), and, most importantly, still does not reach optimality.

In a second set of works [15,16], we describe how to exactly sample, in linear time, combinatorial structures which (up to bijections) are described by random bridges (i.e., random lattice walks from $(0,0)$ to $(n,0)$, with steps $(+1,h_j)$), even when the distributions $p_{n,j}(h_j)$ of the steps are not all equal, in particular (as described in [16]) provided that they satisfy a property that we call positive decomposition. We show that this technical constraint is not very restrictive, as the realm of applications includes, among other things, important combinatorial classes such as random set-partitions, that is partitions of a set of $n$ elements into $k$ non-empty subsets, counted by Stirling numbers of the second kind and related to the exact sampling of minimal automata [17], and its ‘dual’ problem, of random permutations of size $n$ with $k$ cycles, counted by Stirling numbers of the first kind, for which, to our knowledge, no linear-time sampling algorithms were previously available. However, admittedly, the problems solved by this algorithm are just a relatively small subclass of all those that are addressed by the Boltzmann method, so a quest for a new idea that could tackle very large classes of combinatorial objects still stands.

Let us put the Boltzmann Method and its variants more in context. Of course, this method is not the only available exact-sampling algorithm for combinatorial structures. One relatively ancient algorithm is due to Nijenhuis and Wilf [18] (with later modifications by Flajolet, Zimmermann and Van Cutsem [19], see also [20]). If the exact enumeration of certain combinatorial objects is described by a system of equations, of the form

$$A_n^{(i)} = \cdots + \sum_{n_1, n_2, \ldots, n_k \geq 0 \atop n_1 + n_2 + \cdots + n_k \leq n} c(n_1, n_2, \ldots, n_k, n) A_{n_1}^{(j_1)} A_{n_2}^{(j_2)} \cdots A_{n_k}^{(j_k)} + \cdots$$

where the coefficients $c$ are positive-valued functions (for their range of arguments), that can be evaluated as floats with $O(\ln n)$ digits in time $O(\ln n)$, then, for $(i_1, \ldots, i_k)$ being sets of indices appearing as left factors of the monomials above, the quantities $A_{n_1}^{(j_1)} \cdots A_{n_k}^{(j_k)} := \sum_{n_1, \ldots, n_k} \sum_{j_1, \ldots, j_k} A_{n_1}^{(j_1)} \cdots A_{n_k}^{(j_k)}$, can be evaluated recursively up to the size of interest, once and for all in a ‘preprocessing phase’, in a time of order $n^2 \ln n$, and the final data structure occupies a space of order $\ln \ln n$. At this point, a simple divide-and-conquer algorithm (with complexity improved by the so-called “boustrophedon method”) allows to perform exact sampling in average time of order $\ln \ln n$. So, if one is interested in exact sampling with the aim of performing a statistical average, when the number of samples is much larger than the size of the objects (as is often the case), and allows for extra logarithmic factors, even this “brute-force counting” strategy, once improved by the expedients outlined above, may be quasi-optimal.

In fact, when the system of equations is linear (as in the broad family of regular languages), the setting of this algorithm simplifies drastically, and a careful implementation of these ideas allows to achieve linear complexity even for the single-run sampling, that is, with an algorithm in which also

For various families of trees and walks, [10,12] for random permutations, [13] for “linear extensions in series-parallel posets” among others.
the preprocessing is quasi-linear \[O\left(n^{2/3}\right)\]. So, we should focus on combinatorial structures whose generating functions are determined by non-linear systems, which, indeed, are in general more complicated classes (just like in Algebra, non-linear systems are more complicated than linear systems).

Within these classes, there is an important family, in which the coefficients \(c(n_1, n_2, \ldots, n_k, n)\) above are in fact constants, depending only on \(n - (n_1 + n_2 + \cdots + n_k)\), and only finitely many are non-zero. In this case one says that the corresponding structures are context-free. As explained in [5, Sec. VII.1–6], under suitable hypotheses, the crucial Drmota–Lalley–Woods Theorem (DLW) [23–25] applies, and these structures fall under the so-called smooth inverse-function schema (SIFS), that is the generating function has a peculiar square-root singularity at the critical point, and the enumeration has asymptotics of the form \(A_n \sim \rho^{n^2} (\log n)^{-1/2} \exp(\Omega(1))\), where the exponent \(-\frac{3}{2}\) is ‘universal’, that is, it is shared by all classes within the SIFS.

This family contains examples ranging from simple cases, such as e.g. binary and unary-binary rooted planar trees, to rather complicated ones, such as two-terminal planar graphs with no \(W_5\) minor (a class of graphs included in the set of planar graphs, and including series-parallel graphs). Indeed, quoting [5, pg. 443]:

*There is a progression in the complexity of the schemas leading to square-root singularity. From the analytic standpoint, this can be roughly rendered by a chain [ inverse functions \(\rightarrow\) implicit functions \(\rightarrow\) systems ]. It is, however, often meaningful to treat each combinatorial problem at its minimal level of generality.*

This hierarchy of difficulty seems to stand also at the level of the Boltzmann Method. In fact, the simplest case of the SIFS corresponds to simple varieties of trees and inverse functions in [5], and is analysed in Section VII.3 there. In this situation, there exists an algorithm, due to Devroye [26], that achieves (quasi-)optimality \[2\] by considering a classical bijection with Lukasiewicz paths, using the cyclic lemma, and exploiting the exchangeability of the steps for the corresponding bridges. This algorithm has the small flaw of involving floating-point arithmetics, but it has the important merit of showing, for the first time, that linear-time average complexity can be achieved for ‘hard’ (i.e., non-linear) combinatorial structures. Also, when the step weights allow for a positive non-local correlations between the various steps. As a result, exchangeability is broken at the level of the single steps, and the whole Devroye strategy cannot be applied, without being complemented by some new idea. This fact is also evidentiated in the original Devroye paper [26], which explains clearly to which situations his algorithm applies (and, implicitly, to which situations his algorithm does not apply).

The goal of this paper is to provide an average linear-time algorithm, variant of the Boltzmann sampling method, that works in the broader setting of irreducible context-free structures, thus performing “two leaps forward in one stroke”, on the complexity scale of the SIFS, in the program of making the Boltzmann Method linear. Note however that more complicated, non-context-free structures...
non-linear classes, such as what is called ordinary differential equations and systems in \cite{5}, and treated in Section VII.9 there, are still not covered by the treatment of this paper, despite the fact that, as mentioned above, some linear non–context-free problems are solved by our \cite{16} (we hope to address this level of generality in future work).

Our main idea is to decompose the combinatorial object \( x \), in order to extract one family of degrees of freedom which are specially simple, and postpone the sampling of these degrees of freedom after the evaluation of the acceptance rate. By some magics that we try to elucidate in Section 2 on a simple example (and discuss in full length in Section 8), this allows to gain the factor \( 1/p_\beta(n) \approx n^\gamma \), and reach optimality. Ideas of this sort are not completely new (for example, a version of this appears in our \cite{16} and another version appears in \cite{27}), but are used here in a different twist, that requires a number of subtle tweaks that we try to introduce here in a pedagogical way.

The paper is organised as follows: besides the simple motivational example of Section 2 in Section 3 we discuss some (more or less) well-known facts in Analytic Combinatorics, concerning irreducible context-free structures. This section is complemented by Section 4 that is mainly devoted to examples. Sections 5 and 6 discuss some preliminary aspects of our algorithm (more of combinatorial flavour in the first section, and of analytical flavour in the second one). Finally, Section 7 describes the structure of the algorithm, and the functional form of the involved quantities, while Section 8 describes how to optimise the parameters, in such a way to reach a certification of optimal complexity.

Section 8 is complemented by an appendix that discusses some facts in Perron–Frobenius Theory (which, as well known, has a crucia role in the DLW Theorem). A second appendix provides a reminder of the BalancedShuffle algorithm of Bacher, Bodini, Hollender and Lumbroso \cite{11}, which is used as a black box within our algorithm. A third appendix collects some technicalities required for the certification of optimality discussed in Section 8.

2 A simple example

As a warm-up before introducing our full-fledged algorithm, let us consider the exact sampling of lattice walks from \((0, 0)\) to \((n, 0)\), with steps \(+1, \nu\), with \(\nu \in \{-1, 0, +1\}\). Steps with \(\nu = 0\) come with a factor 2, that is, calling \( x \) a walk, and \(n_+, n_0\) and \(n_-\) the number of steps \(\nu = +1, 0, -1\) in \( x \), respectively, we have

\[
\mu_\nu(x) \propto 2^{n_\nu(x)}.
\]

The weight 2 has been chosen in order to have a trivial normalisation: walks of this sort are just ‘walks of length 2n in disguise’: if \( x' \) is a walk from \((0, 0)\) to \((2n, 0)\) with steps \(\pm 1\), we obtain a map from walks \( x' \) to \( x \) by just taking steps in pairs, and the factor \(2^{n_0}\) is nothing but the number of preimages under this map. As a result, we have the more explicit

\[
\mu_\nu(x) = \left(\frac{2n}{n}\right)^{-1} 2^{n_\nu(x)},
\]

and more generally

\[
A_{n,h} := \sum_{x:(0,0) \to (n,h)} 2^{n_\nu(x)} = \left(\frac{2n}{n+h}\right).
\]

As a result, a simple divide-and-conquer algorithm allows to sample these walks in linear time. We grow the walk step by step. Say that the concatenation of the first \( j \) steps has reached the position \((j, h)\). Then we must continue with a step \(\nu = +1, 0\) or \(-1\) with probabilities \( A_{n-j-1, h+\nu}/A_{n-j, h} \), that is, given by the triple of rational functions

\[
\left(\frac{2(n-j-h)(n-j-h+1)}{(2n-2j)(2n-2j+1)}\right), \quad \left(\frac{2(n-j-h+1)(n-j+h)}{(2n-2j)(2n-2j+1)}\right), \quad \left(\frac{(n-j+h)(n-j+h+1)}{(2n-2j)(2n-2j+1)}\right).
\]

Keeping probabilities \(\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)\) as first approximation, and refining the evaluation only if the sampling procedure requires it, allows to avoid spurious logarithmic factors in bit complexity.
So, in this case we have no need of inventing a new algorithm. However, it is instructive to see other algorithms at work here, where all the calculations can be performed explicitly, and a number of subtleties are not required, before trying to generalising their ideas to more complicated situations.

Before doing this, we shall remind that, for every $k$ of order 1, and every $(n_1, \ldots, n_k)$ with $n = n_1 + n_2 + \cdots + n_k$, it is possible to sample uniformly random shuffles $\sigma \in S_{n_1, \ldots, n_k}$ of the string

$$(1, 1, \ldots , 1, 2, 2, \ldots , 2, k, \ldots , k)$$

(that is, permutations in $\mathfrak{S}_n/(\mathfrak{S}_{n_1} \times \cdots \times \mathfrak{S}_{n_k})$) in a time linear in $n$. If we allow for an extra $\ln n$ factor in the complexity, this can be done just by sampling a random permutation, e.g. with the classical Fisher–Yates algorithm [28,29]. Random-bit optimality (that is, using $\sum_{j=1}^k n_j \ln(n_j/n) + o(n)$ random bits) is reached by the BALANCEDSHUFFLE algorithm of Bacher, Bodini, Hollender and Lumbroso [11]. We will need uniform random shuffles repeatedly in the following, where it will be understood that ‘BBHL shuffling’ refers to this algorithm, and BBHL($n_1, \ldots, n_k$) is the corresponding sampler.

Boltzmann Method. Let us see how the ordinary Boltzmann sampling would work in this case. Call $\mu_\infty(\nu)$ the measure $\mu_\infty(0) = 1/2$, $\mu_\infty(\pm 1) = 1/4$. We just have:

**Algorithm 1:** Boltzmann Method for $(1/4, 1/2, 1/4)$-bridges.

begin
repeat
$\quad x = (x_1, \ldots, x_n) \leftarrow \mu_\infty^n$;
$\quad \text{until } \sum_j x_j = 0$;
return $x$
end

Each run costs $\Theta(n)$ (and exactly $3n$ random bits on average), and the probability that a run is accepted is $4^{-n \binom{n}{2}} \approx 1/\sqrt{n}$. So the overall complexity is of order $n^{3/2}$, as anticipated.

Devroye Method. The method described in [26], specialised to this case, works as follows. First, we sample admissible triples $(n_+, n_0, n_-)$, with the appropriate probability distribution. As we must have $\sum_j x_j = 0$, admissible triples have the form $(n_+, n_0, n_-) = (m, n-2m, m)$ for $m \in \{0, 1, \ldots, [n/2]\}$, and the probability distribution is

$$p_n(m) = \binom{2n}{n}^{-1} \left( \frac{n}{m} \left( \frac{n}{n} - \frac{m}{n} \right)^2 \right)^{2n-2m}$$

Then, we perform a random shuffle of the string consisting of $m$ symbols $-1$, followed by $n-2m$ zeroes, and by $m+1$’s:

**Algorithm 2:** Devroye Method for $(1/4, 1/2, 1/4)$-bridges.

begin
$\quad m \leftarrow p_n(m)$;
$\quad x = (\ldots, -, 0, \ldots, 0, +, \ldots, +)$;
$\quad \sigma \leftarrow \text{BBHL}(m, n-2m, m)$;
$\quad x = \sigma \circ x$;
return $x$
end

Sampling from $p_n(m)$ is complicated but feasible in sublinear time (it is easily done in average time $\sim \sqrt{n}$, by sampling $y$ uniformly in $[0, 1]$, one digit at the time as long as they are needed, calculating once and for all $p_n(\lceil n/4 \rceil)$ as a high-precision float, and summing up the $p_n(m)$’s, in order of distance from $m = \lceil n/4 \rceil$, up to reach the threshold $y$, which is done quickly as the ratio $p_n(m+1)/p_n(m)$ is a simple rational function and w.h.p. we need $O(\sqrt{n})$ summands). The rest of the algorithm requires no other subtlety, and takes linear time. So this algorithm is optimal.
Accelerated Boltzmann Method. Let us now see how our acceleration method improves the complexity of Boltzmann sampling. Call \( \mu'_\infty(\nu) \) the measure \( \mu'_\infty(0) = \frac{2}{3}, \mu'_\infty(1) = \frac{1}{3} \). The structure of our algorithm is as follows:

**Algorithm 3:** Accelerated Boltzmann Method for \((\frac{1}{4}, \frac{1}{2}, \frac{1}{4})\)-bridges.

```plaintext
begin
repeat
    \( t = 1; \)
    \( u = 0; \)
    \( x = (-1, -1, \ldots, -1); \)
    while \( u < n \) do
        \( x_t \leftarrow \mu'_\infty; \)
        \( t \rightarrow t + 1; \)
        \( u \rightarrow u + 1 + x_t; \)
    until \( u = n \) and \( \text{rand}_{[0,1]} < r_n(n-t); \)
    \( \sigma \leftarrow \text{BBHL}(t,n-t); \)
    \( x = \sigma \circ x; \)
return \( x \)
```

In words, we sample a random walk, with steps 0 and +1, and probabilities \( \frac{2}{3} \) and \( \frac{1}{3} \) (thus with average slope \( \frac{1}{3} \)), up to reach or jump over the line passing through \((n,0)\) with slope \(-1\). The probability of jumping over is roughly \( \frac{1}{4} \) (with exponentially small corrections). The most important fact is that, assuming that we reached the line at position \((t,n-t)\), we keep what we have constructed so far with a suitable acceptance rate \( r_n(n-t) \), and restart otherwise. Once this acceptance step has been verified, we just sample a random shuffle, for shuffling the set of steps +1 and 0 altogether with the set of steps -1, and we are done.

So, our algorithm is optimal up to a multiplicative constant if we can determine a function \( r_n(m) \) such that:

1. the algorithm samples according to the desired measure;
2. \( r_n(m) \in [0,1] \) for all \( n \geq 1 \) and \( 0 \leq m \leq \lfloor n/2 \rfloor \);
3. the function \( r_n(m) \) can be calculated efficiently, i.e., in time at most \( O(n) \);
4. \( \mathbb{E}(r_n(m)) = \Theta(1) \).

Let us first address the most obvious constraint: that we are sampling the desired measure. We do this by analysing the probability of getting any given output string \( x \), with \((n_+, n_0, n_-) = (m, n-2m, m)\). We have a factor \( 2^{n-2m}/3^{n-m} \) for sampling the 0/+1 walk up to the line, then a factor \((\binom{n}{m})^{-1}\) for sampling the unique shuffle that produces the string under investigation, and finally we have the acceptance rate \( r_n(m) \). The resulting product must be proportional to \( 2^{n-2m} \). This gives the equation

\[
r_n(m) \frac{2^{n-2m}}{3^{n-m} \binom{n}{m}} = K_n 2^{n-2m}
\]

for some \( K_n \). That is,

\[
r_n(m) = K_n 3^{n-m} \binom{n}{m}.
\]

Then, we have to choose \( K_n \) as large as possible (in order to have good hopes on the fourth condition), while satisfying the second and third condition, that is, we have to choose \( K_n \) as large as possible, while keeping it easy to evaluate, and certified to be smaller than \( 1/\max_n(3^{n-m} \binom{n}{m}) \). For all \( n \), the sequence \( c_{n,m} = 3^{n-m} \binom{n}{m} \) is log-concave, so it has a unique maximum, at the value \( m^*\)

\[4\text{Because we jump over the } n \text{-th diagonal if we are in } n - 1, \text{ and we take a } +1 \text{ step, so the probability } p \text{ of not occupying a diagonal satisfies the steady-state equation } p = (1-p)\frac{1}{2}, \text{ that gives } p = \frac{1}{3}.\]
where \( c_{n,m}/c_{n,m-1} \geq 1 \) and \( c_{n,m+1}/c_{n,m} \leq 1 \). As we have \( c_{n,m+1}/c_{n,m} = \frac{n-m}{3(m+1)} \), this gives \( m^* = \lfloor \frac{n-3}{4} \rfloor \). So we can choose
\[
 r_n(m) = \frac{3^{m^*} (n - m^*)! m^!}{3^m (n - m)! m!}.
\]

Typical values of \(|m - m^*|\) are of order \( \sqrt{n} \), thus calculating the quantity above, as a \( d \)-digit float, by calculating the corresponding Pochhammer functions, takes on average \( \Theta(\sqrt{n}(d + \ln n)) \). Of course, we can do much better. Recalling the Robbins bound on factorials \( \left[ 30 \right] \)
\[
e \frac{n!}{\sqrt{2\pi}n^{n+\frac{1}{2}}e^{-n}} \leq e^{\frac{1}{12n+1}}
\]
we can determine if a random uniform number in \([0, 1]\) is larger or smaller than the acceptance rate above, in time \( \Theta(1) \), with probability \( 1 - \Theta(1/n) \), and then for the remaining probability we can perform the product in the way outlined above, this giving overall complexity \( \Theta(1) \times (1 - \Theta(1/n)) + \Theta(\sqrt{n}\ln n) \times \Theta(1/n) = \Theta(1) \).

So, we are ready to address the one and only subtle point, which shall illustrate the reason of the acceleration. That is, we shall understand why \( E(r_n(m)) = \Theta(1) \), while for ordinary Boltzmann \( \mathbb{P}(\sum_j x_j = 0) = \Theta(n^{-\frac{3}{2}}) \), just as a result of the fact that we have sampled a 0/+1 random walk up to the line with slope \(-1\) passing through \((n, 0)\), instead of sampling a \(-1/0/+1\) random walk up to the vertical line passing through \((n, 0)\).

In fact, we would have had the very same complexity of ordinary Boltzmann if we did perform the ’wrong’ na"ıve choice \( r_n(m) = \frac{\binom{m}{n}}{\binom{m}{n^*}} \) (which, by the way, is manifestly bounded by 1 because \( \sum_m r_n(m) = 1 \)). However, we could push up the acceptance rate, by a factor that is the inverse of the maximum over \( m \) of the naïve function, and this quantity indeed is of order \( \sqrt{n} \).

For what concerns the evaluation of \( E(r_n(m)) \), we could just use the CLT for showing that \( (m - m^*)/\sqrt{n} \) is asymptotically normal distributed, and then check that \( r_n(m) \) is also asymptotically Gaussian, scaled \textit{not} as to be normalised, but rather as to have maximum value 1. That is, roughly,
\[
E(r_n(m)) \sim \int \frac{dx}{\sqrt{2\pi}n\sigma^2} \exp(-x^2/(2\sigma^2)) \exp(-x^2/(2n\tau^2)) = \tau/\sqrt{\sigma^2 + \tau^2},
\]
where \( x = m - m^* \), the first Gaussian is the approximation of the probability of reaching \( m \), and the second Gaussian is the acceptance rate. This CLT principle applies in general. Furthermore, in our simple example we can perform the calculations explicitly, as we have
\[
E(r_n(m)) = \frac{\sum_m \binom{n-m}{m} \frac{3^{m^*+m}}{3^{m^*}m^!}}{\sum_m \binom{n-m}{m} \frac{3^{m^*}m^!}{3^{m^*}m!}}
\]
The denominator is nothing but \( (3 + (-3)^{-n})/4 \approx 3/4 \), which, incidentally, is also the probability of reaching the \( n \)-th diagonal. The numerator is the slightly more complicated expression \( 3^{m^*+n}(2n)!m^!(n - m^*)!/n! \). Note that there are three factorials in the numerator, and three in the denominator, so, as \( m^*/n = \Theta(1) \), there are no \( \sqrt{2\pi}n \) factors coming from Stirling approximation, and indeed, for large \( n \) the numerator converges to \( \sqrt{3/8} \), with corrections of order \( 1/n \). That is, combining numerator and denominator, \( E(r_n(m)) \approx \sqrt{2/3} \), which in turns, multiplying by the probability \( 3/4 \) of reaching the line instead of jumping over (or, equivalently, omitting the denominator), gives on average \( \sqrt{8/3} \) tries for accepting a run of the algorithm. This completes our proof, and (given the optimality of BBHl shuffling, and of sampling i.i.d. random values from \( \mu_{\infty}^{(c)} \)) tells us that our algorithm has average bit complexity \( \sim \sqrt{8/3}S[\mu_0] \).

## 3 Irreducible context-free structures and coloured trees

As explained in detail in the Analytic Combinatorics book \( \left[ 5 \right] \), several interesting combinatorial structures admit a recursive \textit{context-free} definition, that is, for every structure \( y \), weighted with the
measure of choice \( p(y) \), one can choose canonically two integers \( h \) and \( k \), such that \( y \) is decomposed into \( h \) "atoms" and \( k \) sub-structures \( y_1, \ldots, y_k \), with \( p(y) = \phi_{h,k} \prod_j p(y_j) \) and \(|y| = h + \sum_j |y_j| \). In the symbolic framework described in \([5]\) (generalised in the natural way for dealing with weighted objects instead of just counting, see e.g. \([31]\)), this reads

\[
\mathcal{Y} = \sum_{h,k} \phi_{h,k} Z^{\otimes h} \times \mathcal{Y}^{\otimes k},
\]

for \( \phi_{h,k} \) real non-negative, and, at the level of generating functions,

\[
Y(z) = \sum_{h,k} \phi_{h,k} z^h Y(z)^k.
\]

The \( \phi_{h,k} \)‘s must satisfy certain technical conditions, mostly of summability (no fat tails), and non-triviality. Calling \( \Phi(z,y) = \sum_{h,k} \phi_{h,k} z^h Y^k \), the equation above reads

\[
Y(z) = \Phi(z,Y(z)).
\]

This is the situation called \emph{tree-like structures and implicit functions} in \([5]\). Many concrete examples are of the form \( \Phi(z,y) = z \phi(y) \), that is, every decomposition involves a single extra elementary node. This is the case of simply-generated (rooted planar) trees, when each node counts as an unit, and of Lukasiewicz excursions \([5, \text{p. 74}]\), that is lattice paths in the upper-half plane with steps of \( \pm 1 \) (these two families are in simple bijection, where the path describes the depth-first search countour of the tree). This is the special case called \emph{context-free structures and polynomial systems} in \([5]\), and, for what concerns exact sampling, if \( \phi(y) \) is a polynomial, is covered by Devroye algorithm, while more general paths or trees (for example paths in the upper-half plane with steps in \( (1,\pm1) \) and \( (3,0) \)) are in the more general framework (in the example, with \( \Phi(z,y) = zy^2 + z^3 y + z \)).

An even more general framework is one in which we have more than one (but finitely many, say \( m + 1 \)) types of combinatorial structures \( \mathcal{Y}^{(\alpha)} \), with \( \alpha = 0, 1, \ldots, m \). Again, for every structure \( y \) of type \( \alpha \), weighted with the measure of choice, one can choose canonically \( m + 2 \) integers, \( h, k_0, k_1, \ldots, k_m \), such that \( y \in \mathcal{Y}^{(\alpha)} \) is decomposed into \( h \) “atoms” and \( k_\beta \) structures \( y_1^{(\beta)}, \ldots, y_{k_\beta}^{(\beta)} \in \mathcal{Y}^{(\beta)} \), for all \( \beta = 0, 1, \ldots, m \), with \( p_\alpha(y) = \phi_{h,k_0,k_1,\ldots,k_m} \prod_{j=1}^{k_\beta} p_\beta(y_j^{(\beta)}) \) and \(|y| = h + \sum_\beta \sum_j |y_j^{(\beta)}| \). In the symbolic framework described in \([5]\), this reads

\[
\mathcal{Y}^{(\alpha)} = \sum_{h,k_0,k_1,\ldots,k_m} \phi_{h,k_0,k_1,\ldots,k_m} Z^{\otimes h} \times (\mathcal{Y}^{(0)})^{\otimes k_0} \times (\mathcal{Y}^{(1)})^{\otimes k_1} \times \cdots \times (\mathcal{Y}^{(m)})^{\otimes k_m},
\]

and, at the level of generating functions,

\[
Y^{(\alpha)}(z) = \sum_{h,k_0,k_1,\ldots,k_m} \phi_{h,k_0,k_1,\ldots,k_m} z^h \prod_\beta Y^{(\beta)}(z)^{k_\beta}.
\]

Calling \( \tilde{Y} = (Y^{(0)}, Y^{(1)}, \ldots, Y^{(m)}) \) and \( \tilde{\Phi} = (\Phi^{(0)}, \Phi^{(1)}, \ldots, \Phi^{(m)}) \), and introducing the functions \( \Phi^{(\alpha)}(z,\tilde{y}) = \sum_{h,k_0,k_1,\ldots,k_m} \phi_{h,k_0,k_1,\ldots,k_m} z^h \prod_\beta y_\beta^{(\beta)} \), the equation above is just the natural multi-component version of \((13)\), that is

\[
\tilde{Y}(z) = \tilde{\Phi}(z,\tilde{Y}(z)).
\]

This is the situation called \emph{context-free structures and polynomial systems} in \([5]\), and the main object of interest in this paper. By convention (see e.g. \([5]\ \text{ex. I.54, pg. 82}\)), the combinatorial class to which we are interested is the one represented by the first component of our vector.

Just like equations of the form \( Y = z \phi(Y) \) describe trees counted with the number of nodes, and more generally equations of the form \( Y = \Phi(z,Y) \) can be related to trees where internal nodes and leaves are distinguished, counted with the number of leaves\(^5\) configurations associated to a

\(^5\)In order to have finitely many configurations for each given size, we require that no unary node can have an internal child, i.e., that \( \Phi(z,Y) \) has no monomial \( z^0 Y^1 \).
Figure 1: Example of trajectory for the stochastic rewriting rules associated to the specification $A = A z + B^2 + z$; $B = A^3 + z^2$. In blue, the node in the stack that is being processed at the present step of the process; in black, the other nodes in the stack; in gray, nodes that have already been processed.

context-free structure can be put in bijection with certain ‘weighted coloured trees’, in which the size is the number of leaves, and the internal nodes can be ‘coloured’ with the indices from 0 to $m$, and an internal node of colour $\alpha$, with $k_\beta$ children of colour $\beta$ and $h$ children leaves comes with a factor $\varphi_h^{(\alpha)}$ in the weight.

The specification given by the system can be interpreted as a stochastic rewriting rule, of which every trajectory can be translated into a coloured tree (see Figure 1). The process is parametrised by a solution $(\rho, \vec{\tau})$ of the system $\vec{\Phi}(\rho, \vec{\tau}) = \vec{\tau}$. It starts with a node of label 0 at the root, which is the only node in a stack of ‘boundary nodes’. Then, for a node in the stack with label $\alpha$, we choose the composition of its offspring according to the probability distribution

$$p_\alpha(h; k_0, k_1, \ldots, k_m) = \tau_\alpha^{-1} \varphi_h^{(\alpha)} \rho^h \prod_\beta \tau_\beta^{k_\beta}.$$ (17)

(Note that, indeed, these probabilities are normalised.) Then, the node leaves the stack, and all of its $k_0 + \cdots + k_m$ non-leaf descendents are put in the stack. We continue the process, picking up nodes from the stack, e.g. in random order or in a breath-first search. The process stops when the stack is empty (or doesn’t stop at all). The order of the operations does not affect the probability distribution of the outcome, as long as it is guaranteed that, for each finite height $h$, almost surely every node in the stack, at height $h$ in the tree, is processed at some point, and in particular this is the case when the process stops almost surely. The resulting process, besides the minor complicancies coming from the colouring, is essentially a Galton–Watson (GW) process. In particular, it is well known that we have a critical Galton–Watson process whenever these parameters correspond to the solution of the characteristic system [5, pg. 483], i.e., the solution to the system of $m + 2$ equations

$$\vec{\Phi}(\rho, \vec{\tau}) = \vec{\tau} \quad \det (I - K) = 0 \quad K_{\alpha\beta} := \frac{\partial}{\partial \tau_\beta} \Phi^{(\alpha)}(\rho, \vec{\tau})$$ (18)

in $(\mathbb{R}^+)^{m+2}$ with smallest value of $\rho$, while we have a subcritical GW process whenever the spectrum of the matrix $K$ is strictly contained in the disk of radius 1 (or, equivalently, the Frobenius eigenvalue of the matrix $K$ is strictly smaller than 1). Indeed, the Frobenius eigenvalue of $K$ corresponds to the average number of children, in the GW process in which the nodes of the stack are taken randomly. Subcritical GW processes lead to a probability distribution on the extensive parameters

---

6Now, in order to have finitely many configurations for each given size, we require that the linear part of $\Phi(0, Y)$ is a nilpotent matrix.
Figure 2: Top left: the rewriting rules for two-terminal graphs with no \( W_5 \) minor. As said in the text, letters \( A, P, S \) and \( W \) denote “all”, “series”, “parallel” and “Wheatstone bridge” subclasses. Letters \( S^* \) and \( P^* \) denote \( A \setminus S = z + P + W \) and \( A \setminus P = z + S + W \), respectively. Bottom: an example of configuration. The two terminals are the left-most and right-most vertices. Top right: the decomposition tree associated to the example.

of the tree (such as the number of nodes of a given type) which has exponential tails, while, if the combinatorial system is also “irreducible”, critical GW processes lead to a probability distribution with tail \( p(n) \sim C \cdot n^{-3} \), with \( C \) determined by the DLW Theorem (the precise notion of irreducibility is presented in the context of this theorem, we refer to [5] for the details). Supercritical GW processes, associated to the case in which the Frobenius eigenvalue is larger than 1, lead to trees which have a finite probability of being of infinite size. In this case, the measure described by the parameters \((\rho, \vec{\tau})\), and conditioned to produce finite trees, is well-defined, and interesting in several respects, however we do not need this notion in this paper, so we do not discuss further the supercritical case.

4 Examples of irreducible context-free structures

A nice example of context-free structure is the class of (two-terminal) series-parallel graphs, described for example in [5, p. 72, ex. I.46], and more in detail in [32]. Another, slightly more complex example (but also more “typical”, as, contrarily to series-parallel graphs, does not have colourings alternating along the layers of the tree, and is irreducible and aperiodic), is the class of (two-terminal) graphs with no \( W_5 \) minor. To our knowledge, this class has been discussed so far only in a seminar of ours,

\[ W_5 \] is the wheel graph with five vertices.
on the very same topic of this paper. This class is described by the system of equations

\[
\begin{align*}
A &= z + S + P + W \\
S &= \sum_{k \geq 2} (z + P + W)^k \\
P &= \sum_{k \geq 2} \frac{1}{k!} (z + S + W)^k \\
W &= \frac{1}{2} A^5
\end{align*}
\]

where letters \(A, P, S\) and \(W\) have been chosen to denote “all”, “series”, “parallel” and “Wheatstone bridge” subclasses of these graphs. See Figure 2 for a description of the specification as a rewriting system (left), a typical example of configuration (bottom), and its representation as a coloured tree (right).

Strictly speaking, these classes are not context-free structures, because the functions \(\Phi^{(n)}\) are not polynomial. Nonetheless, they can be treated on a similar ground, as in fact the DLW Theorem has several extensions (see the discussion in [5, pg. 493], in particular the Remark VII.29).

Another example is constituted by recursive topological subdivisions of a rectangle by straight lines. This is a new model, somewhat pictorially similar to ‘quadtrees’ (cf. [5, Ex. VII.23, pg. 523]), and, if we trade rectangles for triangles, to ‘stack-triangulations’ [33]. In this problem, every rectangle can be subdivided either horizontally, or vertically, or in both directions. However we impose a further condition, that in a sense avoids multiple countings of the same configuration: if we have divided a rectangle horizontally, we cannot divide horizontally any of the two resulting rectangles, and similarly for vertical subdivisions. See a typical example in Figure 4. The size of a configuration is the number of rectangles in the subdivision. If we call \(R(z)\) the generating function for these configurations, and \(H(z)\) (resp. \(V(z)\)) the ones for rectangles that come from a horizontal (resp. vertical) subdivision, these functions satisfy the system of equations

\[
\begin{align*}
R &= z + H^2 + V^2 + R^4 \\
H &= z + V^2 + R^4 \\
V &= z + H^2 + R^4
\end{align*}
\]

which is illustrated by Figure 3. If we use the symmetry induced by (say) 90-degree rotations, we can identify the generating functions \(H\) and \(V\), and reduce the system to two equations

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*See [https://library.cirm-math.fr/Record.htm?idlist=2&record=19286312124010045949](https://library.cirm-math.fr/Record.htm?idlist=2&record=19286312124010045949), recorded during the meeting AofA: Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms, on June 24th, 2019, at the Centre International de Rencontres Mathématiques (CIRM), Marseille, France. Slides are available at [https://www.cirm-math.fr/RepOrga/1940/Slides/Sportiello.pdf](https://www.cirm-math.fr/RepOrga/1940/Slides/Sportiello.pdf), and the system (19) is on page 65. Note that in this document there is a typo (\(W_4\) in place of \(W_5\)) in the excluded-minor description of the class of graphs.

---
Figure 4: Typical example of ‘recursive topological subdivision’ of the unit square, of size 100.

\[
\begin{align*}
R &= z + 2H^2 + R^4 \\
H &= z + H^2 + R^4
\end{align*}
\]

(21)

We can further eliminate \( H \), to get the algebraic relation

\[
1 + 4R = (1 + z + R + R^4)^2,
\]

(22)

that is, the inverse of the generating function, \( z(R) \), is given by

\[
z(R) = \sqrt{1 + 4R - 1 - R - R^4}.
\]

(23)

The critical values \( (z^*, R^*, H^*, V^*) \) are thus given as the roots of integer-valued polynomials (e.g., \( R \) is determined by the equation \( z'(R) = 0 \), identified by the constraint of being real-positive, and
At this point, we recall the Cyclic Lemma and, rephrased in terms of lists of subtrees $z$ being the smallest real-positive root:
\begin{align}
    z^* & : 0.1868943725 \ldots & 16777216 z^7 + 113311744 z^6 + 276168704 z^5 + 277020672 z^4 \\
    & & + 166353408 z^3 - 146027008 z^2 + 69783040 z - 9433303 = 0 \\
    R^* & : 0.3945155166 \ldots & 64R^7 + 16R^6 + 32R^4 + 8R^3 + 4R - 3 = 0 \\
    H^* & : 0.3028172374 \ldots & 8H^7 + 28H^6 + 36H^5 + 20H^4 + 4H^3 + 2H - 1 = 0 \quad (V^* = H^*)
\end{align}

5 From trees to walks, and the cyclic lemma

From this point onward, we assume that our context-free structure is irreducible and aperiodic in the sense of the DLW Theorem. We also use $A(z)$ as a synonym of $Y(0)(z)$, as this first component, besides being associated to the combinatorial class that we want to sample, plays a distinct role in the whole construction of the algorithm.

As we described above, the combinatorial structures we shall sample are in bijection with rooted planar trees $T \in T_n$, whose root index is $A$, and which have $n$ leaves. The number of internal nodes is not fixed, however it is bounded by $Kn$ for some constant $K$ (as we have required that the linear part of $\Phi$ is a nilpotent matrix).

Several algorithms for the exact sampling of trees, including the Devroye Algorithm among various others, make use of a bijection with suitable lattice paths, and the cyclic lemma. However, as we said above, this strategy does not apply immediately to coloured trees.

A better idea is to decompose the trees into subtrees, by breaking it at all the internal nodes with label $A$. Each tree is thus described by a list of subtrees, $T = (t_1, \ldots, t_k)$, where a subtree $t_j$ has root index $A$, leaves of two types ($A$ and $z$), and all other internal nodes with labels in $\{1, \ldots, m\}$. We call $T_{v,\ell}$ the class of such subtrees having $v$ leaves with label $z$, and $\ell$ leaves with label $A$, and $T^{(\text{sub})} = \bigcup_{v,\ell \geq 0} T_{v,\ell}$ the class off all subtrees altogether. Let us adopt the shortcuts $v_i = v(t_i)$ and $\ell_i = \ell(t_i)$, and $k = k(t)$. A set of necessary and sufficient conditions for a list $t$ to determine a tree is the following:
\begin{enumerate}
    \item $\sum_{j=1}^k v_j = n$;
    \item $\sum_{j=1}^k (\ell_j - 1) = -1$;
    \item $\sum_{j=1}^{k'} (\ell_j - 1) \geq 0$ for all $k' < k$.
\end{enumerate}

In other words, the concatenation of the vectors $\vec{u}_j := (v_j, \ell_j - 1)$ must constitute a generalisation of the notion of Lukasiewicz path, in which the steps can go forward by an amount different from $+1$. In lack of a name that has already been fixed in the literature, we will call them generalised Lukasiewicz excursions.

This construction has traded the complicacy of coloured steps, and non-local correlations, with the (comparatively minor) complicancy of steps with variable horizontal length. In particular, if we remove the constraint of remaining in the upper-half plane, the corresponding generalised Lukasiewicz walks have exchangeable steps.

If we call $A_n$ the partition function at size $n$, i.e. $A_n = [z^n]A(z)$, we have
\begin{align}
    \mu_n(T) & = \frac{W(T)}{A_n} \mathbb{1}\left(T \in T_n\right) \quad W(T) = \prod_{v \in V(T)\text{ internal}} \phi_{h(v),k_0(v),k_1(v),\ldots,k_m(v)}^{(\alpha(v))} \tag{27}
\end{align}

and, rephrased in terms of lists of subtrees
\begin{align}
    \mu_n(t) & = \frac{\prod_j W(t_j)}{A_n} \mathbb{1}\left(t \text{ satisfies the conditions (1), (2) and (3) above}\right). \tag{28}
\end{align}

At this point, we recall the Cyclic Lemma.
Lemma 1 (Cyclic Lemma) Let $U$ be a set of steps in $\mathbb{Z}^2 \setminus (0,0)$, strictly contained in a half-plane $\mathbb{H}_{a/b} = \{(x,y) \mid ya + xb > 0\}$. Let $w_0 = (u_1, \ldots, u_k) \in U^k$ be a walk from the origin to the point $(n_x, n_y) \in \mathbb{H}_{a/b}$. For $0 \leq j < k$, call $w_j = (u_{j+1}, \ldots, u_k, u_1, \ldots, u_j)$ the cyclic shifts of $w_0$. If $n_x$ and $n_y$ are coprime, there exists exactly one index $0 \leq j < k$ such that the walk $w_j$ is contained in the half-plane $\mathbb{H}_{-n_y/n_x}$.

We shall call Cyc the operator such that, applied to a walk $w_0$, gives the only cyclic shift $w_j$ of $w_0$ with the property above. An immediate and crucial consequence of this lemma (also based on the fact that our generalised Lukasiewicz excursions reach the point $(n, -1)$ and all integers are coprime with $-1$), is that we can rewrite equation (28) getting rid of the complicated condition (3):

$$\mu_n(t) = \sum_{t' : Cyc(t) = t} \frac{1}{A_n} \prod_j W(t'_j) k(t') \mathbb{1}(t' \text{ satisfies the conditions (1) and (2) above}) \quad (29)$$

We will call generalised Lukasiewicz bridges the corresponding family of directed lattice walks, that is, the same walks as the excursions, without the constraint of remaining in the upper half-plane. As a consequence, if we are able to exactly sample lists $t'$ with the measure $\mu_n^{\text{(cyc)}}(t)$ above, we are able to exactly sample our combinatorial structures with complexity $T(n) + \Theta(n)$.

In the remaining of this paper we will concentrate on the problem of exactly sample lists $t$ from the measure $\mu_n^{\text{(cyc)}}(t)$ above. At this point, the pertinence of our toy-model problem of Section 2 dealing with the simplest possible family of lattice bridges which is not Dyck bridges (for which the problem reduces to random shuffles), should be apparent.

6 Further analytic preliminaries

Having renamed $A(z)$ our generating function $Y^{(0)}(z)$, our system (16) reads

$$\begin{cases}
Y^{(0)}(z) & \equiv A(z) = \Phi^{(0)}(z, A(z), Y^{(1)}(z), \ldots, Y^{(m)}(z)) \\
Y^{(1)}(z) & = \Phi^{(1)}(z, A(z), Y^{(1)}(z), \ldots, Y^{(m)}(z)) \\
& \vdots \\
Y^{(m)}(z) & = \Phi^{(m)}(z, A(z), Y^{(1)}(z), \ldots, Y^{(m)}(z))
\end{cases} \quad (31)$$

Similarly the generating function for the subtrees

$$A(z, u) = \sum_{t \in T^{(m)}} W(t) z^{v(t)} u^{f(t)} = \sum_{v, \ell \geq 0} z^v u^\ell \sum_{t \in T^{cyc}} W(t) \quad (32)$$

is given by

$$A(z, u) = \Phi^{(0)}(z, u, Y^{(1)}(z, u), \ldots, Y^{(m)}(z, u)) \quad (33)$$

where the $Y^{(\alpha)}(z, u)$’s satisfy the reduced system

$$\begin{cases}
Y^{(1)}(z, u) & = \Phi^{(1)}(z, u, Y^{(1)}(z, u), \ldots, Y^{(m)}(z, u)) \\
& \vdots \\
Y^{(m)}(z, u) & = \Phi^{(m)}(z, u, Y^{(1)}(z, u), \ldots, Y^{(m)}(z, u))
\end{cases} \quad (34)$$

\footnote{Here $\delta(n)$ denotes the Kronecker delta $\delta_{n0}$, and not the Dirac delta. This choice is based on the fact that here $n$ is replaced by large expressions, which would be poorly rendered as indices, and also there is no risk of confusions, as there are no Dirac delta’s in this paper.}
As a check, let us verify that the measure in (30) is indeed normalised. At this aim we should have, for all \( n \geq 0 \),

\[
1 = \sum_{\ell \in \mathbb{C}^2} \rho_n^{(cyc)}(t) = \frac{1}{A_n} \left[ z^n u^{-1} \right] \frac{1}{k} \left( \sum_{\ell} W(t) z^\ell u^{\ell(t)-1} \right)^k
= -\frac{1}{A_n} \left[ z^n u^{-1} \right] \ln \left( 1 - \frac{A(z, u)}{u} \right)
= -\frac{1}{A_n} \left[ z^n \right] \oint_{2\pi i} \frac{du}{2\pi i} \ln \left( 1 - \frac{A(z, u)}{u} \right),
\]

where the integral is on a contour encircling the origin, and no other pole of the integrand. Or, in other words, taking the generating function for an arbitrary value of \( z \) in the interval \([0, \rho_i]\),

\[
A(z) = -\oint_{2\pi i} \frac{du}{2\pi i} \ln \left( 1 - \frac{A(z, u)}{u} \right).
\]

However, the logarithm has a cut discontinuity on an interval starting from the origin, along the positive real axis, and this cut ends at the point \( u(z) \) such that \( A(z, u(z)) = u(z) \). If we deform the contour of integration as to encircle this cut discontinuity, the integral is exactly (minus) the length of the interval (factors \( 2\pi i \) simplify exactly as in the classical proof of the Cauchy Theorem), so we get that our check is equivalent to the relation \( A(z) = u(z) \) for all \( z \in [0, \rho_i] \), whenever \( A(z, u(z)) = u(z) \).

Indeed, on the manifold \((z, u) \in \mathcal{M} \subset \mathbb{C}^2\) where the latter holds, any solution of the bivariate reduced system is also a solution of the original univariate system, i.e., \( \mathcal{Y}^{(\alpha)}(z, u(z)) = \mathcal{Y}^{(\alpha)}(z) \) for all \( 0 \leq \alpha \leq m \), and in particular for \( m = 0 \), so that our claim is verified.

There is a two-parameter family of natural measures on the set of possible subtrees \( t \), where the two parameters are the Lagrange multipliers for the number of \( A \)- and \( z \)-leaves:

\[
\mu(t; z, u) := \left( \frac{A(z, u)}{u} \right)^{-1} z^u u^{\ell(t)-1}.
\]

One point \((\zeta, \theta) \in (\mathbb{R}^+)^2\), that we shall call the critical point, has a crucial role in the following. These two values are defined by

\[
\frac{A(\zeta, \theta)}{\theta} = 1; \quad \frac{\partial}{\partial \theta} A(\zeta, \theta) = 0.
\]

The first condition corresponds to \((\zeta, \theta) \in \mathcal{M}\), i.e., to the fact that the weight \( \theta \) associated to the \( A \)-leaves coincides with the generating function of trees with root-index \( A \). The second condition is a rewriting of the equation \( \frac{\partial}{\partial \theta} \ln A(\zeta, \theta) = 0 \) in light of \((\zeta, \theta) \in \mathcal{M}\), and this equation describes the fact that our generalised Lukasievicz paths have average zero drift, as to be expected for optimising the efficiency of the Boltzmann sampling of paths from \((0, 0)\) to \((n, -1)\), when \( n \gg 1 \). If we had to perform a Boltzmann sampling of our generalised Lukasievicz bridges, the optimality strategy suggested by singularity analysis would tell that we have to sample the subtrees \( t_j \) of the walk exactly with the measure \( \mu(t; \zeta, \theta) \). However, this first algorithm would have a rather poor efficiency: not only we have a factor \( \sim 1/\sqrt{n} \) for the probability of reaching the point \((n, -1)\), but also we have a crude acceptance rate of order \( \sim 1/n \) on the typical cases, because our acceptance rate must reproduce the factor \( 1/k(t) \) in the cyclic lemma up to a multiplicative constant, but this factor, in general, may be as large as \( 1 \) (in the exponentially rare case in which the root is the only node of the tree with label \( A \)). Note that we did not have this problem in our toy model of Section 2, as in that case the possible steps of the walk have bounded length. As we will see, we will need to come up with two different ideas, for dealing with these two different problems.

There is a second remarkable characterisation of the critical point \((\zeta, \theta)\), which is the following:

**Lemma 2** The values \((\zeta, \theta)\) satisfying (38) are the components \((\rho, \tau_0)\) of the solution \((\rho, \tau)\) of the characteristic system (18). Furthermore, the vector \((1, \frac{\partial}{\partial \theta} \mathcal{Y}^{(1)}(\zeta, \theta), \ldots, \frac{\partial}{\partial \theta} \mathcal{Y}^{(m)}(\zeta, \theta))\) is the Frobenius vector of the matrix \( K \).
Proof. Indeed, the first equation of (38) coincides with the component 0 of the first equation of (18). For the second equation of (38), the explicit calculation of  
\[
\frac{\partial}{\partial \theta} A(\zeta, \theta) = \frac{\partial}{\partial \theta} \Phi^{(0)}(\zeta, \theta, Y^{(1)}(\zeta, \theta), \ldots, Y^{(m)}(\zeta, \theta)) 
\]
\[
= \frac{\partial}{\partial \theta} \Phi^{(0)}(\zeta, \theta, Y^{(1)}(\zeta, \theta), \ldots, Y^{(m)}(\zeta, \theta)) 
\]
\[
+ \sum_{\beta=1}^{m} \frac{\partial}{\partial Y^{(\beta)}} \Phi^{(0)}(\zeta, \theta, Y^{(1)}(\zeta, \theta), \ldots, Y^{(m)}(\zeta, \theta)) \frac{\partial}{\partial \theta} Y^{(\beta)}(\zeta, \theta) 
\]
\[
= K_{00} + \sum_{\beta=1}^{m} K_{0\beta} \frac{\partial}{\partial \theta} Y^{(\beta)}(\zeta, \theta). 
\]
(39)

Similarly, for the other components we have
\[
\frac{\partial}{\partial \theta} Y^{(\alpha)}(\zeta, \theta) = K_{\alpha 0} + \sum_{\beta=1}^{m} K_{\alpha \beta} \frac{\partial}{\partial \theta} Y^{(\beta)}(\zeta, \theta). 
\]
(40)

That is, introducing the shortcuts
\[
\vec{v} = \left( \frac{\partial}{\partial \theta} A(\zeta, \theta), \frac{\partial}{\partial \theta} Y^{(1)}(\zeta, \theta), \ldots, \frac{\partial}{\partial \theta} Y^{(m)}(\zeta, \theta) \right); 
\]
\[
\vec{v}' = \left( 1, \frac{\partial}{\partial \theta} Y^{(1)}(\zeta, \theta), \ldots, \frac{\partial}{\partial \theta} Y^{(m)}(\zeta, \theta) \right); 
\]
(41) (42)

we have
\[
K \vec{v}' = \vec{v}. 
\]
(43)

If both equations (38) hold, we have
\[
0 = \frac{\partial}{\partial \theta} A(\zeta, \theta) = \frac{\theta}{\partial \theta} \frac{\partial}{\partial \theta} A(\zeta, \theta) - A(\zeta, \theta) = \frac{1}{\theta} \left( \frac{\partial}{\partial \theta} A(\zeta, \theta) - 1 \right), 
\]
(44)

that is, \(\vec{v} = \vec{v}'\), which thus is an eigenvector of \(K\), with eigenvalue 1. Now, the fact that the coefficients \(\phi\) defining the system are real-positive implies that \(K\) has a Frobenius eigenvector, and also that the entries of \(\vec{v}\) are all positive, so \(\vec{v}\) must be the Frobenius eigenvector of \(K\), and \((\zeta, \theta, Y^{(1)}(\zeta, \theta), \ldots, Y^{(m)}(\zeta, \theta))\) coincides with the solution \((\rho, \tau_0, \tau_1, \ldots, \tau_m)\) of the characteristic system. \(\square\)

One consequence of this lemma is that, in lack of a more direct strategy specific for the structure at hand, we can always determine \((\zeta, \theta)\) by using general-purpose libraries already developed for the ordinary Boltzmann Method, as explained in [32], or, when we will deal with multi-parametric Boltzmann sampling, in [35] (see also https://paganini.readthedocs.io/en/latest/).

A further analytic ingredient that we will need in the following is:

Lemma 3 There exists a radius \(\delta > 0\) such that the measure \(\mu(t; z, u)\) is associated to a subcritical GW process, for all \((z, u) \in B(\zeta, \theta, \delta)\).

\[16\]
7 The algorithm

Let us define the support $U$ of the combinatorial specification as the set of vectors $\vec{u} = (v, \ell - 1) \in \{0, 1, \ldots\} \times \{-1, 0, 1, \ldots\}$ such that $\mathcal{T}_{v, \ell} \neq \emptyset$. Note that $(0, 0)$ and $(0, -1)$ cannot be elements of $U$ (because every tree must have some leaves, and we have required the linear part of $\vec{\Phi}$ to be nilpotent, so we cannot have only one leaf, and of $A$ type). Let us also call $v_0 \geq 1$ the smallest integer such that $(v_0, -1) \in U$, i.e. such that $\mathcal{T}_{v_0, 0} \neq \emptyset$. This integer must exist, otherwise there would exist no generalised Lukasiewicz excursions associated to our combinatorial class. Call

$$T_0 = \sum_{t \in \mathcal{T}_{v_0, 0}} W(t),$$

the generating function of our objects in $\mathcal{T}_{v_0, 0}$ (which is a finite polynomial in the phi’s), and call $\mu_0(t)$ the natural measure on $\mathcal{T}_{v_0, 0}$

$$\mu_0(t) = \frac{W(t)}{T_0}$$

(note that it is also the restriction of $\mu(t; \zeta, \theta)$ to $\mathcal{T}_{v_0, 0}$, although, in fact, it does not depend on $\zeta$ and $\theta$).

Let $\mu(t)$ be some measure, still to be determined, with support on $\mathcal{T}^{(sub)} \setminus \mathcal{T}_{v_0, 0}$.

Let us call the landing diagonal $D_n$ as the set of points in $\mathbb{N} \times \mathbb{Z}$ on the line with slope $-1/v_0$ passing through $(n, -1)$, and with ordinate above $-1$:

$$D_n = \{(i, j) \mid j \geq -1, i + v_0 j = n - v_0\}.$$ \hspace{1cm} (47)

Let us call the final region $F_n$ as the set of points in $\mathbb{N} \times \mathbb{Z}$ beyond the landing diagonal:

$$F_n = \{(i, j) \mid i + v_0 j \geq n - v_0\}.$$ \hspace{1cm} (48)

Our algorithm for random (generalised Lukasiewicz) bridges induced by an irreducible context-free structure has the same idea outlined in our toy model of Section 2, that is, for a suitable measure $\mu(t)$ and a suitable acceptance-rate function $r_n(\{\vec{u}_j\}_{1 \leq j \leq k(t)})$.

Algorithm 4: Accelerated Boltzmann Method, for generalised Lukasiewicz bridges.

```
beg
repeat
  $\vec{u} = (0, 0)$;
  $k = 0$;
  $t = ()$;
  while $\vec{u} \not\in F_n$ do
    $k \rightarrow k + 1$;
    $t_k \leftarrow \mu_{\infty}$;
    $\vec{u}_k = (v(t_k), \ell(t_k) - 1)$;
    $\vec{u} \rightarrow \vec{u} + \vec{u}_k$;
    Append $t_k$ to $t$;
  until $\vec{u} \in D_n$ and rand$_{[0, 1]} < r_n(\{\vec{u}_j\})$;
  $m = \vec{u}_2 + 1$;
  for $i = 1 \ldots m$ do
    $t_{k+i} \leftarrow \mu_0$;
    Append $t_{k+i}$ to $t$;
    $\sigma \leftarrow \text{BBHL}(k, m)$;
    $t = \sigma \circ t$;
  return $t$
end```

The algorithm for excursions, and thus for (coloured) trees and for irreducible context-free structures, is identical to the previous one, in which the last instruction $t = \sigma \circ t$ is replaced by $t = \text{Cyc} \circ \sigma \circ t$. 

At this point we have to guess which measure \( \mu_\neq(t) \) is more adapted at this aim. Let us call \( \mu_\neq(t; z, u) \) the restriction of \( \mu(t; z, u) \) to \( T \setminus T_{0,0} \). If we believe in the Boltzmann Method paradigm, we should be induced to choose, as measure \( \mu_\neq(t) \), the critical measure \( \mu_\neq(t; \zeta, \theta) \). However, in the past, experience has shown that small modifications of the critical parameters, scaling algebraically with \( n \), may improve the performance of the algorithm (see the papers cited in the introduction, or also, e.g., [34] Sec. 4.4), and, as we will see later on, this is the case also here.

Let us then introduce a larger family of measures. At fixed \( n \), let \( X = \{ (\pi_a, z_a, u_a) \}_{1 \leq a \leq q} \) be a finite set of parameters, where \( \pi_a \) is a discrete probability distribution \((\pi_a > 0 \text{ for all } a, \text{ and } \pi_1 + \cdots + \pi_q = 1)\), and \((z_a, u_a)\) are points in the ball introduced in Lemma 3. We will define the measure \( \mu_\neq(t) \) associated to \( X \) as

\[
\mu_\neq(t) = \sum_{a=1}^{q} \pi_a \mu_\neq(t; z_a, u_a).
\]

Sampling from these measures is immediate: you should just first sample \( a \), with distribution \( \pi \), and then sample from \( \mu(t; z_a, u_a) \), using the stochastic rewriting system, possibly repeating the procedure (with the same \( a \)) if the subtree \( t \) is in \( T_{0,0} \) (both this event and its complementary happen with a probability \( \Theta(1) \), so the average number of runs is also \( \Theta(1) \)). More explicitly, the measure above reads

\[
\mu_\neq(t) = \sum_{a=1}^{q} \pi_a \frac{u_a}{A(z_a, u_a) - T_0 z_a^\omega} W(t)^{\pi_a(t) u_a^{(t)}(t) - 1} = \sum_{a=1}^{q} \pi_a \theta \frac{\pi_a}{A(\zeta, \theta) - T_0 \zeta^\omega} W(t)^{\pi_a(t)^{(t)} u_a^{(t)}(t) - 1},
\]

where the parameters \( \pi_a \) have been introduced for later convenience, but are in general not normalised.

We can re-formulate a set of parameters \( X \) in the form \( z_a = \zeta \exp(\xi_a) \), \( u_a = \theta \exp(\eta_a) \). Call \( \bar{\zeta} = \sum a \bar{\pi}_a \zeta_a / \sum a \bar{\pi}_a \), and \( \bar{\eta} = \sum a \bar{\pi}_a \eta_a / \sum a \bar{\pi}_a \). In this reparametrisation we have

\[
\mu_\neq(t) = \frac{\theta}{A(\zeta, \theta) - T_0 \zeta^\omega} W(t)^{\pi_a^{(t)} u_a^{(t)}(t) - 1} \sum_{a=1}^{q} \bar{\pi}_a \exp(\xi_a v(t) + \eta_a (\ell(t) - 1)).
\]

We say that a set \( X \) is balanced if \( \bar{\xi} = \bar{\eta} = 0 \). Of course, the critical sampler \( X = \{ (1, \zeta, \theta) \} \) is also balanced.

In the second part of the algorithm we must repeatedly sample from \( \mu_0 \). This is algorithmically is immediate, as in fact the set \( T_{0,0} \) contains finitely many elements, which can be found in constant time in a preprocessing procedure, together with their weights \( W(t) \).

So, all that is left to do is repeating our analysis of the acceptance-rate function, along the same lines presented in Section 2, but in this more complicated setting. We do this analysis in the next sections.

8 Analysis of the acceptance ratio

The conditions on the acceptance-rate function read in this case:

1. the algorithm samples according to the desired measure;
2. \( r_n(\{ \bar{u}_j \}) \in [0,1] \) for all \( n,k \geq 1 \) and lists \( \{ \bar{u}_j \}_{1 \leq j \leq k} \) with \( \sum_j \bar{u}_j \in D_n \);
3. the function \( r_n(\{ \bar{u}_j \}) \) can be calculated efficiently, i.e., in average time at most \( \Theta(n) \);
4. \( \mathbb{E}(r_n(\{ \bar{u}_j \})) = \Theta(1) \).

Again, we start by analysing the probability of getting any given output string \( t \). Recall that we have called \( m \) the integer corresponding to the ordinate of the point on the landing diagonal that we reached, plus 1. In other words, if we label the points of the landing diagonal with the non-negative
integers, we have landed on the \( m \)-th point. We also called \( k \) the number of subtrees generated in the first part of the algorithm, thus the complete list \( t \) obtained at the end of the algorithm has \( k + m \) items, and, for \( n > v_0 \), has \( 1 \leq k \leq n - v_0 \) and \( 0 \leq m \leq \lfloor n/v_0 \rfloor - 1 \). Indeed, the points \( \bar{u} \in \mathbb{N} \times \mathbb{Z} \) are partitioned into diagonals according to the integer \( \hat{n}(\bar{u}) := u_1 + v_0 u_2 = \bar{u} \cdot (1, v_0) \). By definition of \( v_0 \), for all the points \( \bar{u} \) in the support \( U \), this combination is a positive integer, except for \((v_0, -1)\), for which it is zero. The origin is on the diagonal with parameter zero, and the landing diagonal has parameter \( n' := n - v_0 \). The case with largest possible values of \( k \) and \( m \) is when only the steps \((0, 1)\) and \((v_0, -1)\) are used, in the first and second part of the algorithm, respectively, which occurs, for example, in the case of binary trees counted by number of leaves, \( A = z + A^2 \) (which, from the point of view of our algorithm, is trivial, as the core of the operations is fully contained in the BBHL shuffling procedure). We anticipate that we will only consider functions \( r_n(\{\bar{u}_j\}) \) that only depend on the parameters \( \bar{u}_j = \hat{u}(\bar{u}_j) \).

Introduce the shortcuts
\[
A_0 = \frac{T_0}{\theta} \zeta_0; \quad A_\theta = \frac{A(\zeta, \theta)}{\theta} - A_0.
\] (52)

Call
\[
\bar{v} := \zeta \frac{\partial}{\partial \zeta} \frac{A(\zeta, \theta)}{\theta}.
\] (53)

This quantity is the average horizontal length of the steps of our Lukasiewicz walks, if these are sampled with the critical measure \( \mu(t; \zeta, \theta) \). That is, for critical steps,
\[
E(\bar{u})_{\mu(t; \zeta, \theta)} = (\bar{v}, 0).
\] (54)

As the GW process associated to the subtrees is subcritical, this quantity is of order 1.

It is also easy to calculate the analogous quantity for \( \mu_\theta(t; \zeta, \theta) \), as
\[
(\bar{v}, 0) = E(\bar{u})_{\mu(t; \zeta, \theta)} = A_\theta E(\bar{u})_{\mu_\theta(t; \zeta, \theta)} + A_0 E(\bar{u})_{\mu_0(t)} = A_\theta E(\bar{u})_{\mu_\theta(t; \zeta, \theta)} + A_0 (v_0, -1),
\] (55)

that is
\[
E(\bar{u})_{\mu_\theta(t; \zeta, \theta)} = \frac{(\bar{v} - A_0 v_0, A_0)}{1 - A_0}.
\] (56)

This has two important consequences. First, the initial part of the algorithm makes walks with a positive drift. Second, the average amount of diagonals by which these walks do jump at each step is \( 1/(v_0 + A_0) \), \((v_0, -1) = \bar{v}/A_\theta = \Theta(1) \). This is an aspect of the fact that the probability of reaching the landing diagonal is of order 1. More precisely, if \( p(\bar{u}) \) is the probability distribution of \( \bar{u} \) for steps in a walk, and \( \hat{p}(x) = \sum_{\bar{u}} p(\bar{u}) x^{\bar{u}} \) is the corresponding generating function, the asymptotic probability of reaching the landing diagonal is \( (\frac{\partial}{\partial x} \hat{p}(x))^{-1} \big|_{x=1} \), and the corrections are exponentially small in the length of the walk. So, in our case,
\[
P(\text{reaching } D_n) = \left( \frac{\partial}{\partial x} x^{-v_0} A(\zeta x, \theta x^{v_0}) - \theta A_0 \right)^{-1} \big|_{x=1} + O(\exp(-\alpha n)) = \Theta(1).
\] (58)

This is an important check, as \( P(\text{reaching } D_n) = \Theta(1) \) is a necessary condition for an algorithm of our form to reach complexity optimal up to a multiplicative constant. The inverse of the quantity evaluated above enters as a factor in this complexity multiplicative constant.

---

10More generally, in a Markov chain in which we jump by \( a \) with probability \( p_a \) (with \( a \in \mathbb{N}^+ \)), the asymptotic probability \( q \) that a site \( n \) is not occupied is given by the sum over \( k, j \geq 0 \) of the probability that we have a jump of length \( k + j + 2 \), from \( n - k - 1 \) (which must be occupied), to \( n + j + 1 \):
\[
q = \sum_{j,k \geq 0} (1 - q) p_{j+k+2} = \sum_{\ell \geq 2} (1 - q) (\ell - 1) p_{\ell} = (1 - q) (\hat{p}'(1) - 1)
\] (57)

that is, the probability that a site is occupied is \( 1 - q = 1/\hat{p}'(1) \).
Now, let \( t \) be a list that, in the first part of our algorithm, has reached the landing diagonal. The probability of getting this, with parameters \( k \) and \( m \) as defined above, before the shuffling, is

\[
p(t) = \left( \prod_{j=1}^{k} \mu_{\neq}(t_j) \right) \left( \prod_{j=1}^{m} \mu_0(t_{k+j}) \right) r_n(\{\tilde{u}_j\}).
\]  

(59)

After the shuffling, we get a further factor \( 1/\binom{k+m}{k} \). The resulting probability must be proportional to the measure \( \mu_n^{(\text{cyc})}(t) \) in (30), that is

\[
\left( \prod_{j=1}^{k} \mu_{\neq}(t_j) \right) \left( \prod_{j=1}^{m} \mu_0(t_{k+j}) \right) r_n(\{\tilde{u}_j\}) \propto \binom{k+m}{k} \prod_{j=1}^{k+m} W(t_j).
\]  

(60)

Note that we can rewrite (51) as

\[
\mu_{\neq}(t) = \frac{W(t)\zeta^{v(t)}\theta^{(t)-1}}{A_0} f(v(t), \ell(t)); \quad F(v, \ell) = \sum_{a=1}^{q} \tilde{\pi}_a \exp(\xi_a v + \eta_a(\ell - 1)).
\]  

(61)

More simply, (46) reads

\[
\mu_0(t) = \frac{W(t)\zeta^{v(t)}\theta^{-1}}{A_0},
\]  

(62)

thus, substituting in (60),

\[
\zeta^n \theta^{-1} \left( \prod_{j=1}^{k+m} W(t_j) \right) \left( \prod_{j=1}^{k} F(v_j, \ell_j) \right) r_n(\{\tilde{u}_j\}) \propto \binom{k+m}{k} \prod_{j=1}^{k+m} A_0^m \prod_{j=1}^{k+m} W(t_j).
\]  

(63)

That is, there must exist a function \( K_n \) such that

\[
r_n(\{\tilde{u}_j\}) = K_n \binom{k+m-1}{k} A_0^m \prod_{j=1}^{k+m} F(v_j, \ell_j)^{-1},
\]  

(64)

which can be calculated efficiently, and such that \( r \) is valued in \([0,1]\), and its average is \( \Theta(1) \).

In particular, we have required that \( r_n \) is a function of the \( \tilde{u}_j \)'s only, that is, we must have that \( F \) is a function of \( \tilde{u} \) only. This happens if and only if \( \eta_a = u_0 \xi_a \) for all \( a \), and in this case we have

\[
F(\tilde{u}) = \sum_{a=1}^{q} \tilde{\pi}_a \exp(\xi_a \tilde{u}).
\]  

(65)

We have anticipated that “critical sampling”, that is, performing the sampling in the first part of the algorithm with the critical measure \( \mu_{\neq}(t) = \mu_{\neq}(t; \zeta, \theta) \), does not lead to an optimal complexity in general. Nonetheless, it is instructive to first analyse this simpler case, and understand the reason why we need the more complicated combinations in equation (49).

In the critical case, the function \( F(\tilde{u}) \) is just 1, and we have

\[
r_n(\{\tilde{u}_j\}) = K_n \binom{k+m-1}{k} A_0^m.
\]  

(66)

Recall that, from the definition of \( A_0 \) and \( A_0 \), and the equation (38), we have \( A_0 = A_0 = 1 \), so that the combination \( \frac{k+m}{k+m} A_0^k A_0^m \) is a binomial distribution. At fixed \( k+m \), it is maximised at \( k/(k+m) \simeq A_0 \). The further factor coming from the cyclic lemma gives only a small perturbation. Analytic Combinatorics predicts that, for lists \( t \) which are typical in the seeked measure \( \mu_n^{(\text{cyc})}(t) \), we have \( (k+m)\bar{v} \simeq n \). Thus, Stirling approximation gives \( r_n(\{\tilde{u}_j\}) \sim K_n C/n^2 \) on typical lists, with \( C \) a finite constant that can be easily evaluated.
However, this result is not satisfactory. Indeed, unless the reduced system is specially simple, there exist trees \( T \) in \( \mathcal{T} \) with root of label \( A \), no other node with this label, and arbitrarily large number of \( z \)-leaves. In this case, we can have lists \( \mathbf{t}(T) \) of subtree decompositions with values of \((k, m)\) as small as \((1, 0)\), and in this case we have

\[
r_n(\{n - v_0\}) = K_n A_{\theta}.
\]

As we must have \( \max(\tilde{u}_j) r_n(\{\tilde{u}_j\}) \leq 1 \), we have \( K_n \leq 1 / A_{\theta} \), and the acceptance rate on typical lists is only \( O(n^{-2}) \). This is the ‘second problem’ of the two mentioned on page \( \ref{section:two-problems} \).

This suggests to explore the more general class of measures in equation \( \ref{eq:measures} \), where the function \( F(\tilde{u}) \) may enter the expression \( \ref{eq:expression} \) in a way that solves this problem. In the following we shall consider only balanced sets \( X \). The conceptually simplest choice is to take a set \( X \) composed of only two points, \( a \in \{+, -\} \), with \( \tilde{\pi}_+ = \tilde{\pi}_- \) and \( \xi_+ = -\xi_- \). We anticipate that the appropriate scaling is of the form \( \xi_+, \eta_+ = \Theta(n^{-\frac{1}{2}}) \), and, for definiteness, we choose once and for all

\[
\xi_+ = \pm \frac{\varepsilon}{\sqrt{n - v_0}}; \quad \eta_+ = \pm \frac{\varepsilon}{\sqrt{n - v_0}} v_0;
\]

with \( \varepsilon \) a constant to be determined later on. (In fact, optimising \( \varepsilon \) is not crucial, as it only affects the overall constant in the complexity, not the scaling exponent.) Of course, using \( n \) and \( n' = n - v_0 \) is essentially equivalent for large \( n \), and our choice is driven by the fact that the combination \( n' \), the index of the landing diagonal, appears repeatedly in the analysis.

This scaling in \( n \) implies, by continuity, that the considerations above (e.g. on the drift of the first part of the walk), leading to the fact that we have a positive probability of reaching the landing diagonal, remain valid in this more general framework, by continuity, for \( n \) large enough. Also, for \( n \) large enough, the points \((z_{\pm}, u_{\pm})\) are contained in the disk of Lemma \( \ref{lemma:disks} \).

Consider the function

\[
f(\varepsilon) = \ln \left( \frac{e^{-xv_0} A(\varepsilon^x, \theta e^{xv_0}) - A_0}{A(\varepsilon, \theta) - A_0} \right).
\]

We have \( \tilde{\pi}_+ = \tilde{\pi}_- \exp(\pm f(\frac{\varepsilon}{\sqrt{n}})) \). As we have required \( \pi_+ + \pi_- = 1 \) and \( \tilde{\pi}_+ = \tilde{\pi}_- \), we have

\[
\tilde{\pi}_+ + \tilde{\pi}_- = \frac{1}{\cosh(f(\frac{\varepsilon}{\sqrt{n}}))} = 1 - \Theta(n^{-1}).
\]

As a result, the factors \( F(\tilde{u}) \) appearing in \( \ref{eq:expression} \) take the simple form

\[
F(\tilde{u}) = \frac{\cosh(\frac{n}{\sqrt{m}} \tilde{u})}{\cosh(f(\frac{\varepsilon}{\sqrt{n}}))}.
\]

From the convexity of the hyperbolic cosine (that is, \( \min \cosh(p \varepsilon) \cosh((1 - p) \varepsilon) \) is attained at \( p = \frac{1}{2} \)) we have that, for any value of \( k \), the maximum of the combination \( \prod_{j=1}^{k} F(\tilde{u}_j)^{-1} \) appearing in \( \ref{eq:expression} \) is bounded from above by the \( k \)-th power of the analytic continuation of the function \( F \), valued at \( k^{-1}\tilde{u}(n, -1) = n' / k \), that is

\[
r_n(\{\tilde{u}_j\}) \leq K_n \frac{(k + m - 1)!}{k! m!} A_{\theta}^k A_0^m \left( \frac{\cosh(f(\varepsilon / \sqrt{n}))}{\cosh(f(\varepsilon / \sqrt{n}))} \right)^k.
\]

As \( k \) is bounded by \( n' \), for all lists \( \mathbf{t} \) the factor \( \cosh(f(\varepsilon / \sqrt{n})) \) is in a range \([1, C]\), for some \( C = \Theta(1) \) that can be evaluated easily, and we can omit this factor in the analysis of an upper bound (up to include a factor \( C \) at the end of the calculation), i.e. search a value \( K_n \) that satisfies the bound

\[
r_n(\{\tilde{u}_j\}) \leq K_n C \frac{(k + m - 1)!}{k! m!} A_{\theta}^k A_0^m \cosh(\frac{\varepsilon \sqrt{n}}{k})^{-k}.
\]

Indeed, it can be seen that non-balanced sets \( X \) lead to weights of the form \( \exp(\xi(n - v_0) + \eta(m - 1) + ck) \) times the one associated to the balanced set, in which the \( \xi_\alpha \)’s and \( \eta_\alpha \)’s are translated by their weighted averages, and the \( \pi_\alpha \)’s are modified as to produce the same set \( \tilde{\pi}_\alpha \) up to an overall factor \( e^{\varepsilon} \), and factors of this form are not the best choice for correcting the \( \sim n^{-\frac{1}{2}} \) term in the acceptance rate.

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Now, if \( k \sim n^\gamma \) we have

\[
\left( \cosh(\varepsilon \sqrt{n'}) / k \right)^{-k} \sim \begin{cases} 
\exp(-\Theta(\sqrt{n})) & \gamma \leq \frac{1}{2} \\
\exp(-\Theta(n^{1-\gamma})) & \frac{1}{2} < \gamma < 1 \\
\exp(-\varepsilon^2/(2\kappa)) & \gamma = 1, \, k \sim \kappa n 
\end{cases} \tag{74}
\]

so, as for lists with \( k \sim n \) we have a bound of order \( n^{-\frac{1}{2}} \), while for lists with \( k \sim n^\gamma = o(n) \) we have a bound not larger than \( \exp(-\Theta(n^{1-\gamma})) \). We can perform our analysis under the assumption that \( k = \Theta(n') \). At \( k \) fixed and large, the maximum in \( m \) is achieved for \( m = \lfloor (kA_0 - 1)/A_\phi \rfloor \), we have that also \( m = \Theta(n') \).

So we have proven that the worst case of the bound is achieved for \( k = \kappa n' \), \( m = \mu n' \), and \( \kappa, \mu = \Theta(1) \). Furthermore, the saddle-point approach predicts \( \kappa/\mu = A_\phi/A_0 + o(1) \), and the bound above reads

\[
r_n(\{\tilde{u}_j\}) \lesssim K_nC \frac{1}{n^2} \frac{A_\phi}{\sqrt{2\pi A_0}} \frac{1}{\kappa} \exp\left( -\frac{\varepsilon^2}{2\kappa} \right). \tag{75}
\]

The maximum of the last factor, \( \exp(-\varepsilon^2/(2\kappa))/\kappa^2 \) is achieved for \( \kappa = \varepsilon^2/3 \), and is valued \( \left( \frac{3}{\varepsilon^2} \right)^2 \).

We still have a choice of \( \varepsilon = \Theta(1) \). This tuning is not crucial for the complexity, however, it is easy to just choose the optimal value. As the saddle-point calculation predicts \( \kappa(1 + \frac{A_\phi}{A_0})n' = \mathbb{E}(k + m) = n'/\bar{v} \), we have

\[
\frac{\varepsilon^2}{3} = \kappa = \frac{A_\phi}{\bar{v}}, \tag{76}
\]

and thus, for this value,

\[
r_n(\{\tilde{u}_j\}) \lesssim K_nC \frac{1}{n^2} \frac{A_\phi}{\sqrt{2\pi A_0}} \left( \frac{\bar{v}}{\varepsilon A_\phi} \right)^{\frac{3}{2}} = K_nC \frac{1}{n^2} \frac{\sqrt{\bar{v}^3}}{2\pi e^{3} A_0 A_\phi}. \tag{77}
\]

It is relatively easy to produce a value \( K_n \sim C'n^2 \) which certifies that \( r_n(\{\tilde{u}_j\}) \leq 1 \) for all \( t \), and that can be evaluated efficiently. More details are given in Appendix \[ Using this value of \( K_n \), the values \( k \) and \( m \) which are the worst case, and also, up to small corrections, the ones predicted by the saddle point, and the bound on the product of cosh’s given by \( \tilde{u}_j = \frac{n'}{\sqrt{n'}} \), gives \( r_n(\{\tilde{u}_j\}) \lesssim C'' \) for some constant \( C'' < 1 \).

At this point the function \( r_n \) has been chosen, and we are left with the evaluation of \( \mathbb{E}(r_n(\{\tilde{u}_j\})) \).

At this aim we do not need anymore rigorous bounds, but the large-\( n \) asymptotics is sufficient to determine the asymptotic complexity.

The random values of \( k \) and \( m \) entering this average are asymptotically Gaussian, with a quadratic form scaling with \( n' \), that is \( k \sim k^*, m \sim m^* \sim \sqrt{n'} \). In order to determine that the algorithm is optimal up to a multiplicative constant, we only need to know this factor. If we want to evaluate this constant, we have to evaluate the quadratic form precisely. The quadratic form \( Q_{(n,m)} \) associated to the fluctuations of \( n \) and \( m \) at fixed \( k \), so that we have (here and below the notation \( X^* \), or \( \mathbb{E}(X) \), stands for the saddle-point expectation of the random variable \( X \))

\[
p_k(\delta n, \delta m) \propto \exp\left( -\frac{1}{2k} (\delta n, \delta m) Q_{(n,m)}^{-1} (\delta n, \delta m) \right) \tag{78}
\]

is given by

\[
Q_{(n,m)} = \begin{pmatrix}
\mathbb{E}((u_1 + v_0 u_2)^2) & \mathbb{E}((u_1 + v_0 u_2)(u_2 - v_0 u_1)) \\
\mathbb{E}((u_1 + v_0 u_2)(u_2 - v_0 u_1)) & \mathbb{E}((u_2 - v_0 u_1)^2)
\end{pmatrix} - \begin{pmatrix}
\mathbb{E}(u_1 + v_0 u_2)^2 & \mathbb{E}(u_1 + v_0 u_2)(u_2 - v_0 u_1) \\
\mathbb{E}(u_1 + v_0 u_2)(u_2 - v_0 u_1) & \mathbb{E}(u_2 - v_0 u_1)^2
\end{pmatrix} \tag{79}
\]
where expectations of \((u_1, u_2) = (v, \ell - 1)\) are w.r.t. the measure \(\mu_{\phi}\). This is a direct consequence of the CLT. The quadratic form \(Q^{(k,m)}\) associated to the fluctuations of \(k\) and \(m\) at fixed \(n\) are obtained through a change of variables at leading order, described by a matrix \(B\)

\[
Q_{(k,m)}^{-1} = \frac{n}{k^2} B^{-T} Q_{(n,m)}^{-1} B^{-1}; \quad B = \begin{pmatrix} -\frac{k}{n} & 0 \\ -\frac{m}{n} & 1 \end{pmatrix}. \tag{80}
\]

That is, asymptotically,

\[
p_n(\delta k, \delta m) \simeq \frac{1}{2\pi n \sqrt{\det Q_{(k,m)}}} \exp \left( -\frac{1}{2n} (\delta k, \delta m) Q_{(k,m)}^{-1} \left( \begin{array}{c} \delta k \\ \delta m \end{array} \right) \right). \tag{81}
\]

The simple binomial factor

\[
K_n \frac{(k + m - 1)!}{k!m!} A_k^{(k,m)} A_0^m \sim C_n \exp \left( -\frac{1}{2n} (\delta k, \delta m) R \left( \begin{array}{c} \delta k \\ \delta m \end{array} \right) \right); \quad R = \frac{n}{k} \begin{pmatrix} A_n & 1 \\ A_x & 0 \end{pmatrix}. \tag{82}
\]

Note that the matrix \(R\) has rank 1, so it is only positive semi-definite, with zero eigenvalue w.r.t. the infinitesimal transformation \(k/n \to k/n + \varepsilon A_{\phi}, m/n \to m/n + \varepsilon A_0\).

The most complicated correction factor is due to the product

\[
\Pi_j \cosh \left( \frac{3A_{\phi}}{\sqrt{\pi n^3}} \tilde{u}_j \right)^{-1} \cosh \left( \frac{3A_{\phi}}{\sqrt{\pi n^3}} n' \right)^{-k^*} \tag{83}
\]

As said above, this quantity has been bounded by its evaluation at \(\tilde{u}_j = \mathbb{E}(\tilde{u}) = \tilde{u}' = \frac{6}{A_{\phi}}\), and the overall constant coming from dealing with simplifications of the bound is the constant \(C_n\) appearing above in \(\text{(83)}\).

The typical lists of \(\tilde{u}_j\)’s, however, have entries which are different, and follow some distribution with all moments (and all cumulant moments) of order 1, and all joint moments almost factorised, i.e., for \(j_\alpha\) distinct indices and \(\sum_\alpha \nu_\alpha\) of order 1,

\[
\mathbb{E}(\tilde{u}_{j_1}' \cdot \cdot \cdot \tilde{u}_{j_\alpha}'') = M_{\nu_1} \cdot \cdot \cdot M_{\nu_\alpha} + O(n^{-1}); \quad M_1 = \frac{n'}{k^*} = \frac{\tilde{v}}{A_{\phi}}. \tag{85}
\]

Let us start our analysis with some heuristics. As we have \(k = \Theta(n)\), we are in a regime in which we can approximate the functions \(\cosh(\alpha/\sqrt{n})\) by \(\exp(-\alpha^2/(2n))\), which gives (recalling that \(\mathbb{E}(\tilde{u}) k^* = n'\))

\[
\mathbb{E} \left( \Pi_j \cosh \left( \frac{3A_{\phi}}{\sqrt{\pi n^3}} \tilde{u}_j \right)^{-1} \cosh \left( \frac{3A_{\phi}}{\sqrt{\pi n^3}} n' \right)^{-k^*} \right) \approx \mathbb{E} \left( \Pi_j \exp \left( -\frac{3A_{\phi}}{2n^2} \tilde{u}_{j'}^2 \right)^{-1} \exp \left( -\frac{3A_{\phi}}{2n^2} n' \right)^{-k^*} \right) \approx \mathbb{E} \left( \exp \left( -\frac{3A_{\phi}}{2n^2} \frac{1}{n'} \sum_j \tilde{u}_{j'}^2 \right) \right) \approx \exp \left( -\frac{3A_{\phi}}{2n} \frac{1}{n'} \sum_j \mathbb{E}(\tilde{u}) \tilde{u}_{j'}^2 \right) \tag{86}
\]

\[
\approx \exp \left( -\frac{3A_{\phi}}{2n} \frac{1}{n'} \left[ \mathbb{E}(\tilde{u}^2) - \mathbb{E}(\mathbb{E}(\tilde{u}))^2 \right] \right). \]

\[23\]
Some of the passages above, and especially the last one, are hard to justify, as in principle we should consider possible correlations between joint moments (that can be relevant even if they are of order $1/n$, because, for example, in the expansion of an expression of the form $\mathbb{E}(\exp(\sum_{j=1}^{\bar{n}} x_j))$ there are $\sim n^2$ moments of the form $\mathbb{E}(x_i x_j)$, and only $\sim n$ moments $\mathbb{E}(x_i^2)$), and correlations between moments of the $\tilde{u}_j$’s and the random variable $k$.

However it is clear that these correlations may only affect the overall constant, and cannot change the fact that the result is of order 1.

In order to perform a more rigorous calculation, we shall revert to the Markov Chain approach that we have already used for the evaluation of $\mathbb{P}(\text{reaching } D_n)$ in (58). Now we rather approximate the functions $\cosh(\alpha/\sqrt{n})^{-1} \approx \cos(\alpha/\sqrt{n})$, and assume that, for a probability distribution $p_a$,

$$\mathbb{E}_{\sum_j a_j = n} \left( \prod_j \cos \left( \frac{\sqrt{n}}{N} a_j \right) \right) \sim \exp(-n\xi_N) \quad (87)$$

for some $\xi_N$ of order $1/N$. Self-consistency gives

$$\exp(-n\xi_N) = \sum_a p_a \exp(-(n-a)\xi_N) \cos \left( \sqrt{\frac{n}{N}} a_j \right) \quad (88)$$

that is

$$1 = \frac{1}{2} \left( \tilde{p} \left( \exp \left( \xi_N + i\sqrt{\frac{n}{N}} \right) \right) + \tilde{p} \left( \exp \left( \xi_N - i\sqrt{\frac{n}{N}} \right) \right) \right) \quad (89)$$

This is consistent with the ansatz $\xi_N = \xi/N$, and the result, obtained from Taylor expansion at first non-trivial order,

$$\xi = \frac{\epsilon^2}{2} \frac{\tilde{p}'(1) + \tilde{p}''(1)}{\tilde{p}'(1)} = \frac{\epsilon^2}{2} E_p(a^2) \quad (90)$$

Our sought quantity at numerator is thus

$$\exp(-n\xi_n) = \exp(-\xi) = \exp \left( -\frac{\epsilon^2}{2} \frac{E_p(a^2)}{E_p(a)} \right) \quad (91)$$

while the quantity at denominator is, using $k^* E_p(a) = n'$,

$$\exp \left( -\frac{\epsilon^2}{2n} k^* E_p(a)^2 \right) = \exp \left( -\frac{\epsilon^2}{2} \frac{E_p(a^2)}{E_p(a)} \right) \quad (92)$$

Taking the ratio, and using the definition of $\epsilon^2$, gives back the quantity obtained in (86).

As a result, the product of cosh’s, at leading order, does not interfere with the Gaussian average over $\delta k$ and $\delta m$, and the overall acceptance ratio is given by

$$\mathbb{E}(r_n) \simeq \frac{C''}{\sqrt{\det(\mathbb{I} + Q_{(k,m)})}} \exp \left( -\frac{3\epsilon^2}{2n^2} \left[ E(\tilde{a}^2) - E(\tilde{u}^2) \right] \right) \quad (93)$$

The three factors above are all real values in $[0,1]$, and of order 1. This average rate, multiplied by the quantity $\mathbb{P}(\text{reaching } D_n)$ in (58), gives the inverse of the multiplicative factor in the complexity, w.r.t. the Shannon bound.

### A A simple fact in Perron–Frobenius Theory

This section is devoted to the proof of the following fact:

**Lemma 4 (Monotonicity of the Frobenius eigenvalue)** For $x \in \mathbb{R}^+$ and $K = (\bar{a}B)$ an irreducible non-negative square matrix, let $K(x)$ be the matrix $K(x) = (x\bar{a}B)$, and $\lambda_1(x)$ its Frobenius eigenvalue. The function $\lambda_1(x)$ is strictly increasing.
Proof. Call \( \vec{v}_i(x) \), \( \vec{v}_i(x)^* \) and \( \lambda_i(x) \) the right-eigenvectors, left-eigenvectors and eigenvalues of \( K(x) \), respectively, with index 1 reserved to the Frobenius one (which is unique). At first order in \( \varepsilon \) we have

\[
\vec{v}_1(x + \varepsilon) = \vec{v}_1(x) + \varepsilon \sum_j \gamma_j(x) \vec{v}_j(x); \quad \lambda_1(x + \varepsilon) = \lambda_1(x) + \varepsilon \delta. \tag{94}
\]

Decompose the vector \( \vec{a} \) in the eigenbasis:

\[
\vec{a} = \sum_j \alpha_j(x) \vec{v}_j(x); \quad \alpha_j(x) = \frac{(\vec{v}_j(x)^*, \vec{a})}{(\vec{v}_j(x)^*, \vec{v}_j(x))}. \tag{95}
\]

Note that, as \( \vec{a} \) is positive and \( \vec{v}_1(x)^* \) is Frobenius, \( \alpha_1(x) > 0 \) for all \( x > 0 \). The defining equation

\[
K(x + \varepsilon)\vec{v}_1(x + \varepsilon) = \lambda_1(x + \varepsilon)\vec{v}_1(x + \varepsilon) \tag{96}
\]

gives, at first order in \( \varepsilon \),

\[
\sum_j \lambda_j(x) \gamma_j(x) \vec{v}_j(x) + (\vec{v}_1(x)) = \sum_j \alpha_j(x) \vec{v}_j(x) - \delta \vec{v}_1(x) - \lambda_1(x) \sum_j \gamma_j(x) \vec{v}_j(x) = 0. \tag{97}
\]

Taking a scalar product with \( \vec{v}_1(x)^* \) (and using the unicity of the Frobenius vector for orthogonality) gives

\[
\delta = (\vec{v}_1(x)^*)_1 \alpha_1(x) > 0. \tag{98}
\]

□

B The BalancedShuffle algorithm

Here we describe an algorithm, given by Bacher, Bodini, Hollender and Lumbroso in [11, sec. 1.1], for the uniform sampling of strings \( \nu = (\nu_1, \ldots, \nu_n) \in \{0, 1\}^n \) with \( \sum_i \nu_i = k \). As stated in the text, this algorithm is ‘optimal’ for the randomness resource, in the sense that the random-bit complexity at leading order coincides with the Shannon bound.

Call \( \beta = k/n \). The idea is that you sample the \( \nu_i \)’s one by one, as if \( \nu \) were to be sampled with the measure \( \mu(\nu) = \text{Bern}^n_\beta \) (this costs \( \Theta(1) \) per variable), and, as soon as you have an excess of \( \nu_i \) equal to 0 or to 1, complete with a sequence of Fisher–Yates random swaps. These swaps cost \( \sim \ln n \) each, but are performed on average only \( \sim \sqrt{n} \) times, so the swap part of the algorithm has subleading complexity, and the overall complexity is genuinely linear, with no logarithmic factors.

For completeness, we give in Algorithm 5 a summary of the main features. In this algorithm RndInt\(_n\) returns a uniform random integer in \( \{1, \ldots, n\} \).

**Algorithm 5: BBHL-shuffling.**

begin
\[ a = k, \ b = n - k, \ i = 0; \]
repeat
\[ i++; \]
\[ \nu_i \leftarrow \text{Bern}_\beta; \]
\[ \text{if } \nu_i = 1 \text{ then } a--; \]
\[ \text{else } b--; \]
until \( a < 0 \) or \( b < 0; \)
if \( a < 0 \) then \( \nu = 0; \)
else \( \nu = 1; \)
for \( j \leftarrow i \) to \( n \) do
\[ \nu_j = \nu; \]
\[ h \leftarrow \text{RndInt}_j; \]
\[ \text{swap } \nu_j \text{ and } \nu_h; \]
return \( \nu \)
Note that, if $\beta$ is almost a 2-adic number, namely $\beta = \frac{a}{2^b} + \varepsilon$ for some integers $a$ and $d$, and $\varepsilon = o(n^{-\gamma}(\ln n)^{-\gamma})$, it may be convenient to just use the value $\beta = \frac{a}{2^b}$, which speeds up the main part of the algorithm, at the price of slowing down the subleading part.

**C Certification of the constant $K_n$**

In Section 8, equation (73), we need to produce an explicit expression $K_n$, as large as possible, and such that we can certify

$$K_n \max_{k,m} C \frac{(k + m - 1)!}{k! m!} A^k A^m_0 \cosh \left( \frac{\varepsilon \sqrt{n}}{k} \right)^{-k} \leq 1. \tag{99}$$

(In this section, for simplicity of notation, we replace $n'$ by $n$, so it is intended that $K_n$ here corresponds to $K_{n+v_0}$ in the body of the paper). Here $C$ and $\varepsilon = \sqrt{3A_\beta/\bar{v}}$ are explicit constants, and $A_0$, $A_\beta$, are parameters in $[0,1]$, with $A_0 + A_\beta = 1$. All of these quantities are $\Theta(1)$, in a scaling where $k, m, n$ are large.

In that section we anticipated the conclusion that, as needed for our algorithm to reach optimal complexity up to a multiplicative constant, we can choose $K_n$ as large as $\sim n^2$, which is optimal up to a multiplicative constant as it is the scaling that this quantity would have if we restricted the analysis to the sole position of the saddle-point prediction, that is, calling $k = \kappa n$, $m = \mu n$ (with $\kappa, \mu = \Theta(1)$)

$$K_n = n^2 C^{-1} \sqrt{\frac{2\pi e^3 A_0 A_\beta}{\bar{v}^3}}. \tag{101}$$

This section is devoted to the description of a method by which we can produce a constant $C' = \Theta(1)$, and a certification that, by choosing $K_n \sim C'n^2$, equation (99) is satisfied.

First of all, while the original domain of maximisation is constituted by $k, m$ integers, with $k \geq 1$ and $m \geq 0$, we can first extend it to $m \in \mathbb{R}^+$ (as this produces an upper bound, which is the appropriate bound direction). In this case convexity in $m$, at given $k$, is immediate, and we have a rather explicit equation for the optimal value $m^*(k)$:

$$\psi(m + k) - \psi(m + 1) + \ln A_0 = 0, \tag{102}$$

where $\psi(x) = \frac{d}{dx} \ln \Gamma(x)$ is the digamma function, which, for $x$ large, goes as $\psi(x) = \ln x + \frac{1}{2x} + \ldots$, this justifying one of the two saddle-point equations, $m/(k + m) = A_0$. So we can rewrite (99) as the stronger condition

$$K_n \max_{k \geq 1} C \frac{\Gamma(k + m^*(k))}{k! \Gamma(m^*(k) + 1)} A^k A^{m^*(k)}_0 \cosh \left( \frac{\varepsilon \sqrt{n}}{k} \right)^{-k} \leq 1. \tag{103}$$

This is an equation of the form $K_n \max_k g(k, m(k)) \leq 1$. Now, suppose that we can certify that, for some integers $a \leq b$, $\frac{d}{dk} g(k, m(k)) > 0$ for all $k \leq a$ and and $\frac{d}{dk} g(k, m(k)) < 0$ for all $k \geq b$. This implies that the maximum $m^* = m^*(n)$ is attained for $k \in \{a, a + 1, \ldots, b\}$. As the evaluation of any single value of $g$, or derivative, with $\mathcal{O}(\ln n)$ digits of precision, takes a time of order $\mathcal{O}((\ln n)^{\gamma})$ for some $\gamma$, under the assumptions above finding the maximum has complexity of order $\mathcal{O}((\ln n)^{\gamma})$ (by just trying out all the values in the potential interval of integers.

In general, we have

$$\frac{d}{dk} g(k, m(k)) = \frac{\partial}{\partial k} g(k, m(k)) + \frac{\partial}{\partial m} g(k, m(k)) \frac{\partial m(k)}{\partial k}. \tag{104}$$
However, in our application the function \( m(k) \) is defined by the equation \( \frac{\partial}{\partial m} g(k, m(k)) = 0 \), so the expression above simplifies into
\[
\frac{d}{dk} g(k, m(k)) = \frac{\partial}{\partial k} g(k, m(k)).
\] (105)

The quantity of interest, \( \frac{d}{dk} g(k, m(k)) \), is thus, up to overall positive factors,
\[
(\psi(m^*(k) + k) - \psi(k + 1) + \ln A_\varphi) + \left(- \ln \cosh \left(\frac{\sqrt{n}}{k}\right) + \frac{\sqrt{n}}{k} \tanh \left(\frac{\sqrt{n}}{k}\right)\right)
\] (106)

This quantity is of order \( 1/n \), as it can be seen by setting \( k = \kappa n \) and \( m^*(k) = \kappa n A_0/A_\varphi + \delta \), which defines \( \delta \) in terms of \( \kappa \) through \( |\delta| \leq 2 \). At leading order in \( 1/n \), it changes sign where it is expected to do so, i.e. at the position of the saddle point. So, if we can bound the involved functions with absolute errors of order \( 1/n^2 \) (i.e., relative errors of order \( 1/n \)), we can have a bound on the position of the point(s) where the derivative changes sign, which is of order \( 1/n \) on the scale of \( \kappa \), that is, of order \( 1 \) on the scale of \( k \), or, in other words, \( b - a + 1 = \Theta(1) \).

One involved function is \( \psi(m + k) - \psi(m + 1) \). This expression is bounded at arbitrary order, by using (the analytic continuation of) \( \psi(x + N) - \psi(x) = \sum_{k=0}^{N-1} \frac{1}{x+k} \), and then the Euler–Maclaurin formula at the desired order, with the customary simplest bound on the error term,
\[
\sum_{i=m}^{n} f(i) \leq \int_{m}^{n} dx f(x) + \frac{f(n) + f(m)}{2} + \sum_{k=1}^{p} \frac{B_{2k}}{(2k)!} (f^{(2k-1)}(n) - f^{(2k-1)}(m)) + |R_p|.
\] (107)

This gives in particular, already at \( p = 1 \),
\[
\psi(x + y + 1) - \psi(x) \leq \ln \frac{x+y}{x} + \frac{2x+y}{2x(x+y)} + \left(- \frac{1}{12} \pm \frac{2\zeta(2p)}{(2\pi)^{2p}} \frac{y(2x+y)}{x^2(x+y)^2}\right),
\] (109)

which is of the desired form. A second special function that appears in our estimates is
\[
c(x) := - \ln \cosh \sqrt{x} + \sqrt{x} \tanh \sqrt{x}.
\] (110)

This is a rather regular function, that behaves as \( c(x) \sim x/2 \) for \( x \) small and \( c(x) \sim \ln 2 \) for \( x \) large. We can find, for example
\[
\frac{3x(12 + x)}{(6 + x)(12 + 5x)} \leq c(x) \leq \frac{3x(6 + x)}{4(3 + x)^2}
\] (111)

and the difference between the two bounds is of order \( \sim x^4/864 \), which, in our case \( x = \mathcal{O}(1/n) \), scales as \( n^{-4} \) and is far sufficient at our aims.

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