Limit laws in Anticipated Rejection algorithms

paper: Anticipated rejection algorithms and the Darling–Mandelbrot distribution

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An algorithm of exact sampling is a randomised algorithm that outputs configurations \( X \in \mathcal{X}_n \) according to a given measure \( \mu_n(X) \) (e.g., the uniform measure \( \mu_n(X) = 1/|\mathcal{X}_n| \)).

Thus, it comes with a probability distribution \( p_n(T) \) for (e.g.) the time-complexity \( T \).

If \( p_n(T) \) is asymptotically normal, \( p_n(T) \sim \exp \left( -\frac{(T-\tau n^\gamma)^2}{2\sigma^2 n^\gamma} \right) \)
and you can prove it (as it is often the case), it suffices to determine the average rescaled complexity \( \tau = \lim_{n \to \infty} \mathbb{E}(T/n^\gamma) p_n \)

This will NOT be the case here!

We will consider a large family of exact sampling algorithms. We will prove linearity (\( \gamma = 1 \)), and convergence to an (almost) new family of distributions, the Darling–Mandelbrot distributions, with rather unusual analytic properties.
Exact sampling in linear time

An algorithm of exact sampling is a randomised algorithm that outputs configurations $X \in \mathcal{X}_n$ according to a given measure $\mu_n(X)$ (e.g., the uniform measure $\mu_n(X) = 1/|\mathcal{X}_n|$)

Thus, it comes with a probability distribution $p_n(T)$ for (e.g.) the time-complexity $T$

If $p_n(T)$ is asymptotically normal, $p_n(T) \sim \exp \left( -\frac{(T - \tau n^\gamma)^2}{2\sigma^2 n^\gamma} \right)$

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We will prove linearity ($\gamma = 1$), and convergence to an (almost) new family of distributions, the Darling–Mandelbrot distributions, with rather unusual analytic properties
Consider a trivial problem: let $B_n$ the set of length-$n$ random walks $\omega$ on $\mathbb{Z}^2$, starting at the origin.

Of course, we can sample uniformly from $B_n$. 
Now, let $\mathcal{A}_n \subseteq \mathcal{B}_n$ the set of walks staying within a region $\Omega_n \subseteq \mathbb{Z}^2$

We have an obvious rejection algorithm:

while $\omega \notin \mathcal{A}_n$ { sample $\omega$ from $\mathcal{B}_n$ } ; return $\omega$ ;

Of course, if $\rho_n := |\mathcal{A}_n|/|\mathcal{B}_n| = \Theta(1)$, this naïve algorithm is linear, while if $\rho_n = o(1)$, it is slower...

You can save some time if you can interrupt the construction of $\omega$ as soon as you certify that $\omega \notin \mathcal{A}_n$ (anticipated rejection)

In this case, a surprising phenomenon may occur: you can have linear complexity even when $\rho_n = o(1)$ (e.g., $\rho_n \sim n^{-\frac{1}{2}}$)
example 1: $\Omega_n$ is a centered box of side $2\ell(n)$

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If $\ell(n) = O(\sqrt{n})$, $\rho_n = O(1)$.

However, even a box as big as $\ell(n) \sim a\sqrt{n}\ln n$ makes $\rho_n \sim n - \frac{\pi}{2}a^2$.

Anticipated rejection does not save much.

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If $\ell(n) = \mathcal{O}(\sqrt{n})$, $\rho_n = \mathcal{O}(1)$.

However, even a box as big as $\ell(n) \sim a\sqrt{\frac{n}{\ln n}}$ makes $\rho_n \sim n^{-\frac{\pi^2}{2a^2}}$

Anticipated rejection does not save much...
example 2: $\Omega_n$ is the half-plane

$\rho_n \sim 1/\sqrt{n}$

However, now the anticipated rejection strategy is quite effective: most of the rejects are $O(1)$, the average size is $O(\sqrt{n})$ thus the average overall size of the rejected paths is linear.
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However now the anticipated rejection strategy is quite effective:
most of the rejects are $O(1)$, the average size is $O(\sqrt{n})$
thus the average overall size of the rejected paths is linear
How could this happen?

In example 1, we have two competing scales, $\sqrt{n}$ and $\ell$. This ultimately causes the typical reject size to be $O(\ell^2)$ (when $\ell \lesssim \sqrt{n}$).

In example 2, the domain is scale invariant: $\omega$ is asymptotically a self-similar fractal, just like the unconstrained path. This makes the model interesting and induces an algebraic (fat) tail in the distribution of $|\omega|$ before exiting $\Omega$. Which ultimately makes anticipated rejection effective.

Thus we are lucky: the sets of systems which are interesting, efficient for anticipated rejection and investigable by our methods tend to coincide...
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Anticipated Rejection: some history

One of the first applications of the Anticipated Rejection strategy was for the sampling of Motzkin meanders, i.e. directed walks, with steps \{-1, 0, +1\}: (1) starting at zero; (2) constrained to stay non-negative; (3) arriving anywhere.

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It could be determined that:

- On average, \( \sqrt{n \frac{\pi}{3}} \) runs were required;
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The transcendental constant \( \sqrt{\frac{\pi}{3}} \) has disappeared from mean and variance. The exponents for number of runs and size of a run sum up to 1 … just two lucky accidents?
Consider an anticipated rejection algorithm. Call \( s(n) \) the survival probability at size \( n \) in a run. Let \( s(n) \sim c n^{-\alpha} \), with \( 0 < \alpha < 1 \).

Then

The average complexity of failed runs is linear. The asymptotic rescaled probability distribution of this quantity, \( g_\alpha(x) \), has Laplace transform \( \tilde{g}_\alpha(z) \)

\[
\tilde{g}_\alpha(z) = \frac{z^{-\alpha}}{-\alpha \gamma(-\alpha, z)} \quad \text{with} \quad \gamma(s, z) = \int_0^z du \ u^{s-1} e^{-u}
\]

**Remark:** we can write more explicitly

\[
\tilde{g}_\alpha(z) = \left( 1 - \sum_{n \geq 1} \frac{\alpha}{n - \alpha} \frac{(-z)^n}{n!} \right)^{-1}
\]
Darling–Mandelbrot distribution: some history

This family of distributions coincides with the one that Lew defines in a different context (ratio largest summand vs. sum, in Lévy theory of stable distributions), and calls Darling–Mandelbrot distribution

Darling, 1952; Lew, 1994

Louchard determined the convergence to a distribution and a form for the Laplace transform, for the “Florentine Algorithm”

Louchard, 1999

... thus, we know overall only three papers that, in some way, analyse such a universal distribution
And only the very basic analytic properties were studied
Consider \( \{x_i\}_{i \in \mathbb{N}} \) i.i.d. random variables, with distribution \( f(x) \)

**Generalized Central Limit Theorem:**

Study the distribution of \( y = \lim_{n \to \infty} n^{-\gamma}(x_1 + \cdots + x_n) \)

Interesting when \( f(x) \sim c \cdot x^{-\alpha-1} \), with \( 0 \leq \alpha \leq 2 \) (and \( \gamma = 1/\alpha \))

Leads to Lévy (skew) \( \alpha \)-stable distributions, up to a scaling by \( c \)

Lévy skew stable distributions have algebraic tails, and are \( C^\infty \) on \( \mathbb{R}^+ \)

Gnedenko and Kolmogorov, 1954

**The “Threshold Sum Process” involved in our analysis**

\( y = \lim_{n \to \infty} n^{-\gamma}(x_1 + \cdots + x_{i^*} - 1) \), where \( i^* \) is the smallest \( i \) with \( x_i > n \)

Interesting when \( f(x) \sim c \cdot x^{-\alpha-1} \), with \( 0 < \alpha < 1 \) (and \( \gamma = 1 \))

Leads to Darling–Mandelbrot distributions, no dependence from \( c \)

These distributions have exponential tails, and are not \( C^\infty \) at all \( x \in \mathbb{N} \)
Heuristic derivation

The proof requires a careful analysis based on Lévy’s Continuity Theorem
A good idea of what goes on here comes from the following:

- The number of failed runs is geometrically distributed, 
  $s(n)$ gives the rate.
- Let $\tilde{h}_{\alpha,n}(z)$ the Laplace Transform of one failed run, we have
  \begin{align*}
  \tilde{g}_{\alpha,n}(z) &= \frac{s(n)}{1 - \tilde{h}_{\alpha,n}(z)} \\
  \end{align*}

- The series of moments of $\tilde{h}_{\alpha,n}(z)$ converges to the naïve corresponding integrations of the tail behaviour
  \begin{align*}
  \tilde{h}_{\alpha,n}(z) &\sim 1 - s(n) + \sum_{k \geq 1} \frac{\alpha}{k - \alpha} c n^{k-\alpha} \left(-z\right)^k \frac{1}{k!} \\
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Series of moments

Consider the expression \( \tilde{g}_\alpha(z) = \left(1 - \sum_{n \geq 1} \frac{\alpha}{n - \alpha} \frac{(-z)^n}{n!}\right)^{-1} \)

Note the independence of \( \tilde{g}_\alpha(z) \) (and \( g_\alpha(x) \)) from the constant \( c \)

Moments are extracted through derivatives of \( \tilde{g}_\alpha(z) \), and thus are rational functions of \( \alpha \)
(mean and variance are \( \frac{1}{1-\alpha} \) and \( \frac{\alpha}{(2-\alpha)(1-\alpha)^2} \))

Conversely, the average number of runs is \( 1/s(n) \sim c^{-1} n^\alpha \)
and the average size of a failed run is
\[ \sum_{m<n} m (s(m) - s(m+1)) \sim c \frac{\alpha}{1-\alpha} n^{1-\alpha} \]

This explains the disappearence of transcendental constants, and the fine-tuning of the exponents.
Laplace Transform is not enough!

How do our distributions *really* look like?
We shall anti-transform our Laplace Transform…

…unluckily, this is impossible…
(and this plot was never done before)

Too bad, as the peculiar non-analyticities at all integers would have been evident!

The investigation of $g_{\alpha}(x)$ is rather done through various *détours* and alternate characterisations. In particular, we prove:

- An expansion of Lauricella type
- A piecewise ODE on $[k, k + 1]$ intervals (+ boundary conds)
- A “holonomic” cancellation property
Analytic properties 1: series expansion

\[ g(x) = \sum_{k \geq 0} g_k(x) \quad g_k(x) \text{ analytic with support on } ]k, +\infty[ \]

\[ g_k(x) = (a \ast b \ast \cdots \ast b)(x), \quad \text{with} \]

\[ a(x) = C x^{\alpha - 1} \quad b(x) = -C \frac{(x-1)^\alpha}{x} 1_{x \geq 1} \quad C = \frac{\sin(\pi \alpha)}{\pi} = \frac{1}{\Gamma(\alpha)\Gamma(1-\alpha)} \]

which gives (let \( \beta_k = (\alpha - 1) + k(\alpha + 1) \))

\[ g_k(x) = \frac{1}{\Gamma(1-\alpha)\Gamma(-\alpha)^k\Gamma(\beta_k)}(x - k)^{\beta_k} 1_{x \geq k} \quad \left[ 1 + O(x - k) \right] \]

leading singular behaviour at \( x = k \)  

Lauricella-type series (\( \star \))

\[ (\star): \sum_{n_1, \ldots, n_k \geq 0} \frac{\prod_i (1 + \alpha)^{n_i}}{(\beta_k)^{n_1 + \cdots + n_k}} (k - x)^{n_1 + \cdots + n_k} \]
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Analytic properties 2: the differential equation

\[ g(x) \text{ satisfies the relation} \]

\[ (1 - \alpha) g(x) + x g'(x) = -\alpha (g \ast g)(x - 1) \]

non-linearity, convolution and translation of the argument make the RHS apparently ugly…

however, as \( g(x) \) has support on \( ]0, +\infty[ \),
this is trivially solved on \( ]0, 1[ \) (this determines \( g_0(x) \)),
then, on \( ]k, k + 1[ \) makes a non-homogeneous linear ODE for \( g_k(x) \),
(\text{which only appears on the LHS})
given that the \( g_h(x)'s \) (for \( h < k \)) are known

This gives a quite effective numerical way of evaluating \( g(x) \)
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This gives a quite effective numerical way of evaluating $g(x)$
Let $D_k$ the linear differential operators

$$D_k = (x - k) \frac{d}{dx} + 1 - (k + 1)\alpha$$

Let $E_k = D_k \cdots D_0$

Then $E_k g_h(x) = 0$ for all $h \leq k$.

Note that, from the degree of $E_k$, this implies that $g_0, \ldots, g_k$ are a basis of the linear space of solutions to $E_k f(x) = 0$ on $]k, +\infty[$
More domains of applications

To which models/algorithms does our analysis apply?

- We mentioned the “Florentine Algorithm”, and variations. This gives a variety of “meander problems”.

- Meanders are in bijection with several other interesting structures, most notably families of planar trees, and of directed lattice animals. All these examples have $\alpha = 1/2$.

- The “constrained random walk” paradigm of our example generalizes to walks constrained to a cone in generic dimension. Remarkably, this gives the full range of exponents $0 < \alpha < 1$.

- Special cases include celebrated combinatorial problems such as Gessel and Kreweras walks.

- More advanced examples include Vicious walkers, and $k$-uples of mutually avoiding random walks...
Directed Lattice Animals

Motzkin

Dyck

Schröder

\[ \alpha = 1/2 \] in all these cases

<table>
<thead>
<tr>
<th>Motzkin</th>
<th>square lattice</th>
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<td>Dyck</td>
<td>Triangular lattice</td>
<td>Bétréma and Penaud, 1991</td>
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<td>Schröder</td>
<td>“Chess king” lattice</td>
<td>Bacher, 2014</td>
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</tbody>
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The classical Rémy Algorithm for the uniform sampling of binary trees has been recently generalised to the unary-binary case, and improved in order to have linear bit-complexity (with no logs)

**Bacher**, Bodini and Jacquot, 2014

This new approach involves a dynamics for a marked position $\star$ on the tree, and a reject if this position reaches the root.

As the tree grows, the $\star$ tends to stay at large distance from the root

(just like the endpoint of a meander tends to stay away from the $x$-axis)

The resulting anticipated rejection has $\alpha = 1/2$
Random Walks in conical domains

Recall our initial “running example” of constrained random walks

The main reason for an algebraic tail in survival probability was the scale invariance of the process

The most general context in which this occurs are conical domains in arbitrary dimension $d$, an analysis pioneered by Sommerfeld, 1896
Random Walks in conical domains

Recall our initial “running example” of constrained random walks

The main reason for an algebraic tail in survival probability was the scale invariance of the process

The most general context in which this occurs are conical domains in arbitrary dimension $d$, an analysis pioneered by Sommerfeld, 1896

Passing to the continuum Heat Equation and radius/angle coordinates gives $s(n) \sim c \, n^{-\frac{\nu}{2}}$, where $\lambda = \nu(\nu + d - 2)$, and $\lambda$ is the smallest eigenvalue for the reduced angular problem

In $d = 2$, $\alpha = \frac{\pi}{2\theta}$. We get a range $\frac{1}{4} < \alpha < 1$ for $\pi/2 < \theta < 2\pi$

In $d = 3$, for circular cones of angle $\theta$, $\nu$ is determined by $P_{\nu}(\theta) = 0$, where $P_{\nu}$ is the Legendre function. We get the full range $0 < \alpha < 1$ for $\arccos \frac{1}{\sqrt{3}} < \theta < \pi$
Kreweras and Gessel walks

- Effective angle: $\theta = \frac{2\pi}{3}$
- Thus $\alpha = \frac{\pi}{2\theta} = \frac{3}{4}$
- Number of runs $\sim c N^{3/4}$
- Size of a run $\sim 3c^{-1}N^{1/4}$
- Complexity $\sim 4N$

- Effective angle: $\theta = \frac{3\pi}{4}$
- Thus $\alpha = \frac{\pi}{2\theta} = \frac{2}{3}$
- Number of runs $\sim c N^{2/3}$
- Size of a run $\sim 2c^{-1}N^{1/3}$
- Complexity $\sim 3N$

Bousquet-Mélou, 2005; Bostan and Kauers, 2010
Mutually avoiding random walks

Yet another combinatorial structure amenable to anticipated rejection are $k$-uples of mutually avoiding lattice walks. Here it is hard to establish $\alpha$ rigorously, but arguments of Conformal Field Theory and the Knizhnik–Polyakov–Zamolodchikov relation led Duplantier to infer an asymptotic behaviour implying $\alpha = \frac{5}{8}$ for $k = 2$.