A Combinatorial Framework for the Pons–Batle Identity: Young Tableaux, Lattice Paths, and Limit Laws

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Joint work with Michael Wallner (TU Wien, AT) and Guan-Ru Yu (NSYSU, TW)

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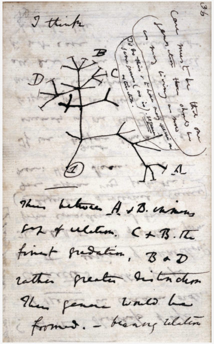
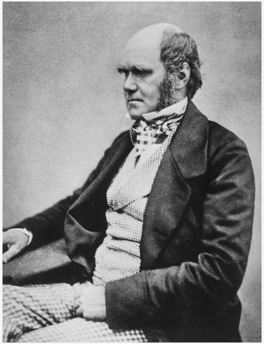
Evolutionary Biology

"The affinities of all the beings of the same class have sometimes been represented by a great tree. I believe this simile largely speaks the truth."

— Charles Darwin (On the Origin of Species, 1859)





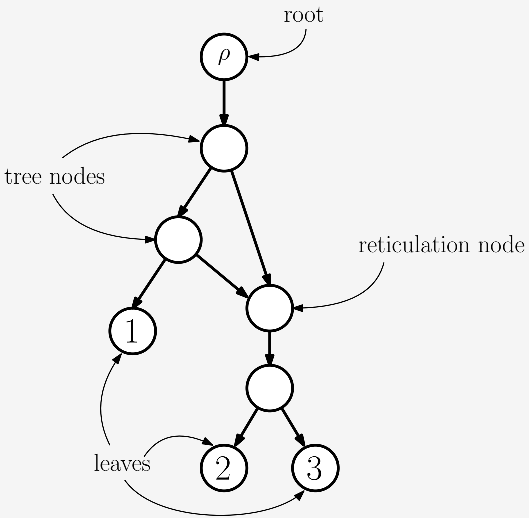
Source: darwin-online.org.uk

What are phylogenetic networks?

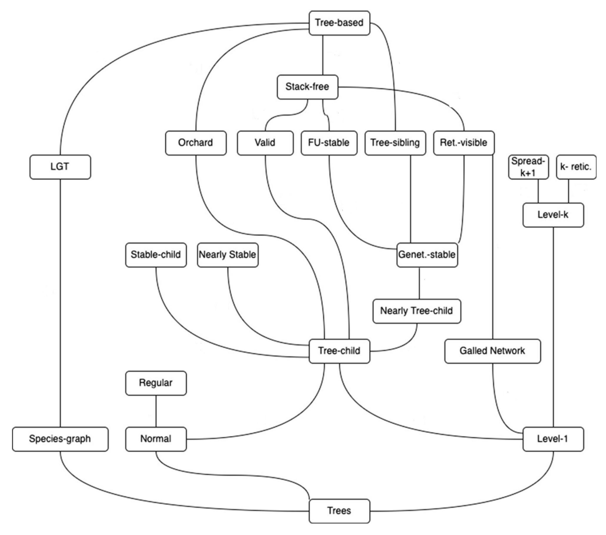
Definition (Phylogenetic Network)

A *phylogenetic network* is a root directed acyclic graph (DAG) that has the following properties:

node type	in-degree	out-degree
unique root	0	1
leaf	1	0
tree node	1	2
reticulation node	2	1



Hierarchy of phylogenetic networks



Source: Kong, Pons, Kubatko, Wicke, Classes of explicit phylogenetic networks and their biological and mathematical significance. J. Math. Biol. 84, 47 (2022)

Tree-child networks

Definition (Tree-child network)

A phylogenetic network is called *tree-child* if every non-leaf node has at least one child that is not a reticulation node.

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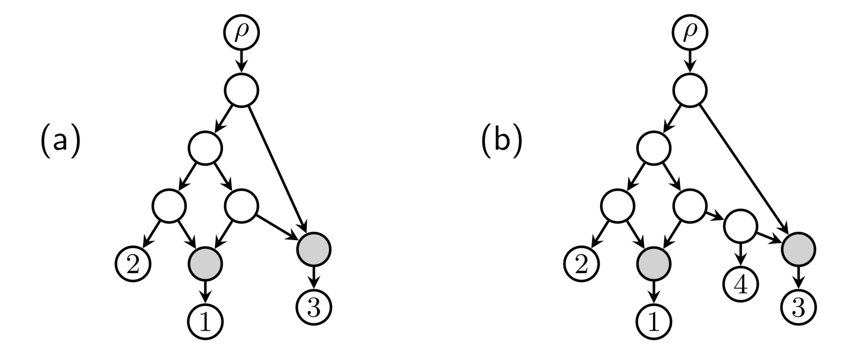

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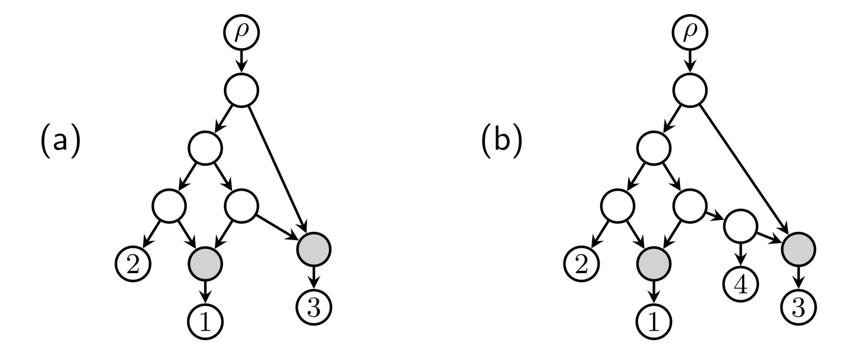

Figure: (a) is **not** tree-child, while (b) is tree-child.

Previous results of tree-child networks

Let TC_n be the number of tree-child networks with n leaves.

Theorem [McDiarmid, Semple, Welch 2015]

For constants $0 < c_1 < c_2$ such that we have

$$(c_1 n)^{2n} \leq \mathrm{TC}_n \leq (c_2 n)^{2n}.$$

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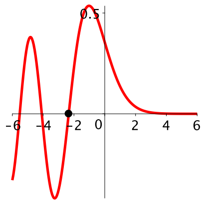
This result was considerably improved:

Theorem [Fuchs, Yu, Zhang 2021]

For $n \to \infty$ we have

$$\mathrm{TC}_n = \Theta\left(n^{-2/3} e^{a_1 (3n)^{1/3}} \left(\frac{12}{e^2}\right)^n n^{2n}\right),$$

where $a_1 \approx -2.3381$ is the largest root of the Airy function $\mathrm{Ai}(x)$ of the first kind.



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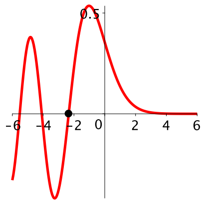

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Open problem: No efficient way to generate them!

The unexpected Pons–Batle Identity

Let $\mathrm{TC}_{n,k}$ be the number of tree-child networks with n leaves and k reticulation nodes.

Definition (Pons–Batle words)

Let $\mathcal{C}_{n,k}$ be the words over the alphabet $\{\omega_1, \ldots, \omega_n\}$, s.t.

1. $\omega_1, \ldots, \omega_k$ occur exactly **3 times**;
2. $\omega_{k+1}, \ldots, \omega_n$ occur exactly **2 times**;
3. **in every prefix:** $\#\omega_i = 0$ OR $\#\omega_i \geq \#\omega_j$ for all $j > i$.

Let $c_{n,k} = |\mathcal{C}_{n,k}|$.

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Let $c_{n,k} = |\mathcal{C}_{n,k}|$.

Example

- Consider $\mathcal{C}_{2,1}$ (i.e., $n = 2$ and $k = 1$)
- Alphabet $\{a, b\}$ (a comes before b)
- a: 3x, b: 2x
- $\#a \geq \#b$

$$\mathcal{C}_{2,1} = \{aabba, ababa, baaba, aaabb, aabab, abaab, baaab\}$$

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Simple recurrence:

$$\begin{cases} c_{1,1} = 1 \\ c_{n,k} = c_{n,k-1} + (2n + k - 1)c_{n-1,k}. \end{cases}$$

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Conjecture [Pons, Batle 2021]; Theorem [Lin, Liu, Liu, Liu, Xin 2026]

$$\mathrm{TC}_{n,k} = \frac{n!}{(n-k)!} c_{n,k}.$$

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Theorem [Chang, Fuchs, L., Wallner, Yu 2024]

$$\mathrm{TC}_{n,k} = \frac{n!}{2^{n-k-1}} b_{n,k}.$$

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Key observation implied by Pons–Batle Identity

$$\frac{b_{n,k}}{2^{n-k}} = \frac{c_{n,k}}{(n+1-k)!}.$$

But: Words are hard to build and count!

Young tableaux with walls

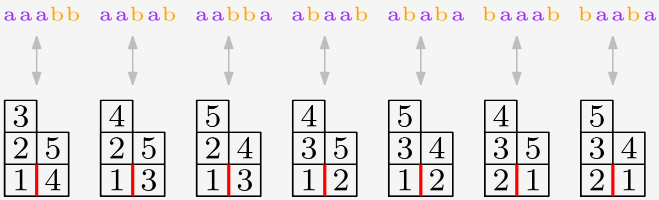
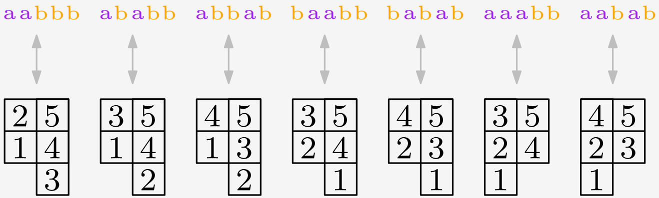


Figure: All words of the set $\mathcal{C}_{2,1}$ and their corresponding Young tableaux in $\mathcal{C}^*_{2,1}$.



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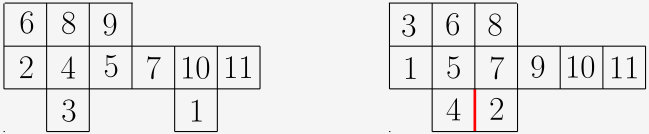
A general class of Young tableaux with walls

Let y_{k,ℓ_1,ℓ_2} denote the number of Young tableaux of type (k, ℓ_1, ℓ_2):

- top: k boxes (columns 1 $\sim$ k);
- middle: $n := \ell_1 + \ell_2 \geq k$ boxes (columns 1 $\sim$ n);
- bottom: ℓ_2 boxes in arbitrarily columns 1 $\sim$ n and adjacent boxes separated by walls.



(a) (b)

Figure: Two examples of Young tableaux with walls and holes of type $(k, \ell_1, \ell_2) = (3, 4, 2)$.

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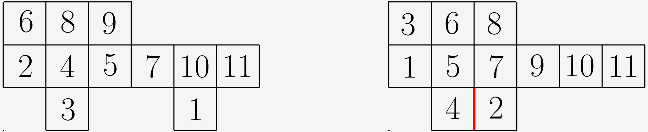
Filled with

- integers $1, 2, \ldots, k + \ell_1 + 2\ell_2$
- increasing along rows and columns
- but cells separated by **walls** have no order constraint.



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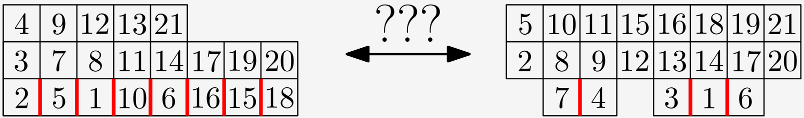
Advantage of these Young tableaux: a simple recurrence

The Pons–Batle Identity is equivalent to

$$\frac{b_{n,k}}{2^{n-k}} \overset{\text{(PB Id.)}}{=} \frac{c_{n,k}}{(n+1-k)!}.$$



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4	9	12	13	21			
3	7	8	11	14	17	19	20
2	5	1	10	6	16	15	18

$\overset{???}{\longleftrightarrow}$

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Lemma

The numbers y_{k,ℓ_1,ℓ_2} of Young tableaux with walls satisfy a simple recurrence:

$$y_{k,\ell_1,\ell_2} = y_{k-1,\ell_1,\ell_2} + y_{k,\ell_1-1,\ell_2} + (2\ell_2+\ell_1+k-1)y_{k,\ell_1,\ell_2-1}, \qquad \text{for } \ell_1+\ell_2 \geq k > 0,$$

such that $y_{0,0,0}=1$ and $y_{k,\ell_1,\ell_2}=0$ outside of the cone $\ell_1+\ell_2 \geq k > 0$.

An interpretation in terms of lattice paths

$$y_{k,\ell_1,\ell_2} = y_{k-1,\ell_1,\ell_2} + y_{k,\ell_1-1,\ell_2} + (2\ell_2+\ell_1+k-1)y_{k,\ell_1,\ell_2-1}, \qquad \text{for } \ell_1+\ell_2 \geq k > 0.$$

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Three different steps:

- $K = (1,0,0)$ and weight 1;
- $L_1 = (0,1,0)$ and weight 1;
- $L_2 = (0,0,1)$ and weight $2\ell_2+\ell_1+k-1$ when ending at (k,ℓ_1,ℓ_2).

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A bi-colored 2D lattice path problem

- $K \mapsto \ I = (1,0)$ and weight 1;
- $L_1 \mapsto J_1 = (0,1)$ and weight 1;
- $L_2 \mapsto J_2 = (0,1)$ and weight $i+j+k-1$ if the kth J_2-step ends at (i,j).

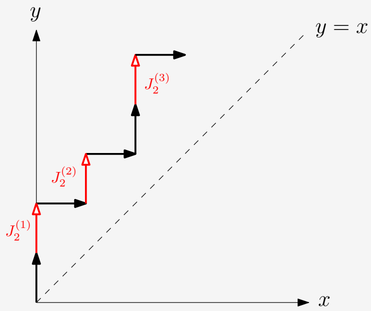
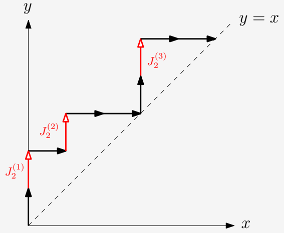


Figure: A projected 2D path of weight 90 staying in $y \geq x$. Non-trivial weights: $w(J_2^{(1)}) = 2$, $w(J_2^{(2)}) = 5$, $w(J_2^{(3)}) = 9$.

The classes of lattice paths enumerated by $b_{n,k}$ and $c_{n,k}$

$b_{n,k} = y_{n,n-k,k}$

- n steps $I = (1, 0)$
- $n - k$ steps $J_1 = (0, 1)$
- k steps $J_2 = (0, 1)$ (with non-trivial weight)
- From $(0, 0)$ to (n, n) never crossing $y = x$



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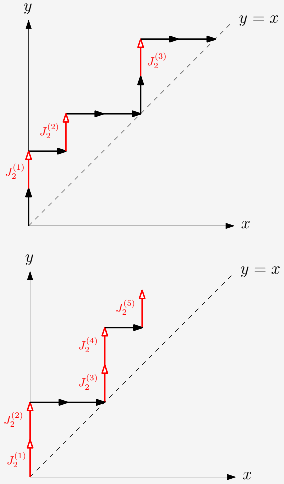

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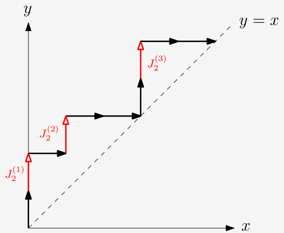

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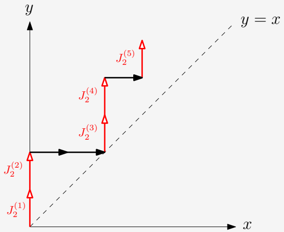

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Ordinary and exponential generating functions

Pons–Batle Identity

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Corollary

We define the ordinary and shifted exponential generating functions

$$B_k(z) = \sum_{n\geq 0} b_{n,k} z^{2n} \quad \text{and} \quad C_k(z) = \sum_{n\geq k} c_{n,k} \frac{z^{\,n-k+1}}{(n-k+1)!}.$$

For $k \geq 1$, the Pons–Batle Identity is equivalent to

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Example (case $k = 0$):

- $b_{n,0} = \frac{1}{n+1}\binom{2n}{n}$

$\Rightarrow$ $B_0(z) = \frac{1-\sqrt{1-4z^2}}{2z^2}$

- $c_{n,0} = (2n-1)!!$

$\Rightarrow$ $C_0(z) = 1 - \sqrt{1-2z}$

Therefore:

$$2B_0(z) = z^{-2} C_0(2z^2)$$

A recursive construction of B_k for $k \geq 1$

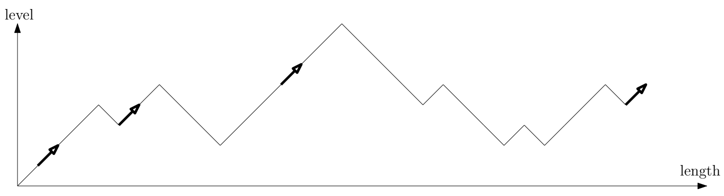
Generating functions:

1) $D(z) = \frac{1-\sqrt{1-4z^2}}{2z^2}$ *(Catalan)*
2) $E(z) = zD(z)$ *(shifted Catalan)*

A recursive construction of B_k for $k \geq 1$

Theorem (Recursive construction)

The generating function $F_k(z,u)$ of bicolored Dyck meanders with k J_2-steps that end with a J_2-step (z number of steps, u final level)



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$$F_k(z,u) = \frac{1}{z^{k-2}} \frac{d}{dz} \left(z^{k-1} \frac{uF_{k-1}(z,u) - E(z)F_{k-1}(z,E(z))}{u - E(z)} \frac{uE(z)}{1 - uE(z)} \right),$$

with $F_0(z) = 1$. The generating function $B_k(z)$ is then for $k \geq 0$ given by

$$B_k(z) = F_k(z, E(z))D(z).$$

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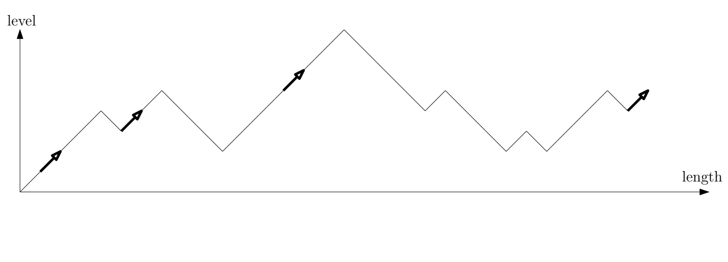

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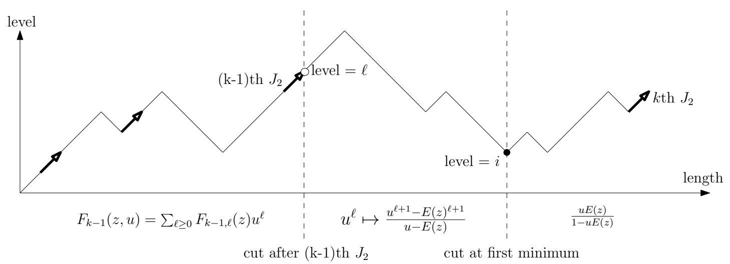

Explicit closed forms for B_k

We compute F_k and B_k efficiently by expressing them in E, using the algebraic equation $E = z(1+E^2)$.

$$\begin{aligned}
B_0(z) &= D(z) = 1 + E^2 \\
&= 1 + z^2 + 2\,z^4 + 5\,z^6 + O(z^8), && (A000108) \\
B_1(z) &= \frac{E^2(1+E^2)^2}{(1-E^2)^3} \\
&= z^2 + 7\,z^4 + 38\,z^6 + O(z^8), && (A000531) \\
B_2(z) &= \frac{E^4(1+E^2)^2(8E^4+15E^2+7)}{(1-E^2)^7} \\
&= 7\,z^4 + 106\,z^6 + 1010\,z^8 + O(z^{10}), \\
B_3(z) &= \frac{E^6(1+E^2)^2(175E^8+699E^6+979E^4+561E^2+106)}{(1-E^2)^{11}} \\
&= 106\,z^6 + 2575\,z^8 + 36080\,z^{10} + O(z^{12}).
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All B_k are algebraic functions of degree 2.

Explicit shape of C_k for $k \geq 1$

Theorem

For $k \geq 1$, the generating function $C_k(z)$ has the explicit shape

$$C_k(z) = \sum_{i=0}^{k} \gamma_{i,k} (1-2z)^{-\frac{i+3k-1}{2}},$$

where

$$\gamma_{i,k} = \frac{(i+3k-3)(i+3k-5)}{i} \gamma_{i-1,k-1} \qquad \text{for } 1 \leq i \leq k$$

with the initial terms $\gamma_{0,1} = -1$ and $\gamma_{1,1} = 1$, and $\gamma_{0,k} = -\sum_{i=1}^{k} \gamma_{i,k}$.

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<u>Proof idea:</u> Explicit *simple* recurrence for $c_{n,k}$:

$$c_{n,k} = c_{n,k-1} + (2n+k-1) c_{n-1,k}.$$

Gives a solvable linear differential equation for $C_k(z)$. □

Explicit closed forms for C_k

The first few terms of $C_k(2z^2)$ are given by

$$\begin{aligned} C_0(2z^2) &= 1-(1-4z^2)^{1/2} \\ &= 2\,z^2+2\,z^4+4\,z^6+10\,z^8+O(z^{10}), && (A284016) \\ C_1(2z^2) &= (1-4z^2)^{-3/2}-(1-4z^2)^{-1} \\ &= 2\,z^2+14\,z^4+76\,z^6+374\,z^8+O(z^{10}), && (A172060) \\ C_2(2z^2) &= \frac{15}{2}(1-4z^2)^{-7/2}-8(1-4z^2)^{-3}+\frac{1}{2}(1-4z^2)^{-5/2} \\ &= 14\,z^2+212\,z^4+2020\,z^6+15480\,z^8+O(z^{10}). \end{aligned}$$

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Using Maple, we can easily check that the PB-Identity

$$2B_k(z)=z^{2(k-1)}\,C_k(2z^2).$$

holds for $k \leq 250$ on our computer.

Limit laws for the case $k = 1$

- Overall goal: find a bijective interpretation between $b_{n,k}$ and $c_{n,k}$.
- Problem: But even for $k = 1$ we don't know how to do it.

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$\Rightarrow$ We study 3 different parameters to understand these structures better:

  - the position of the unique cell in the bottom row in $b_{n,1}$;
  - the value of the unique cell in the bottom row in $b_{n,1}$;
  - the value of the unique cell in the top row in $c_{n,1}$.

- In each case we get a **bivariate generating function** and the **limit law** for $n \to \infty$.

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GF of the position of the unique bottom cell in $\mathcal{B}^*_{n,1}$

$G(z,x) = \sum_{n,m\geq 0} g_{n,m} z^n x^m$, s.t. $g_{n,m}$ counts tableaux of $\mathcal{B}^*_{n,1}$ with the bottom cell in column m

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Proposition

$$G(z,x) = 2\,\frac{1-\sqrt{1-4\,xz}}{\sqrt{1-4\,xz}\left(\sqrt{1-4\,z}+\sqrt{1-4\,xz}\right)^2}$$
$$= xz + \left(5\,x^2+2\,x\right)z^2 + \left(21\,x^3+12\,x^2+5\,x\right)z^3 + O(z^4).$$

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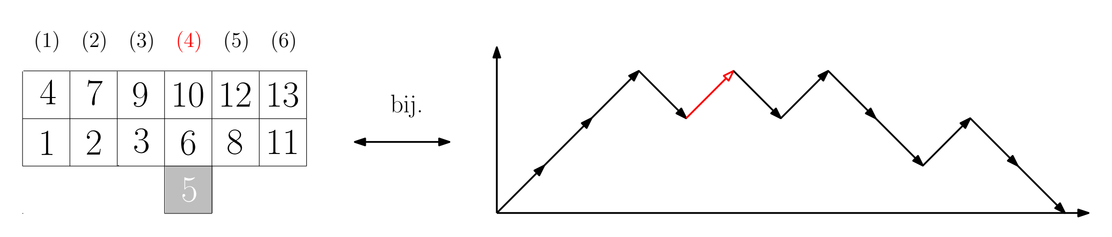
Proof idea: Use the lattice path interpretation:
Bottom cell in column m if and only if unique J_2-step is the m-th up step in the Dyck path. □



Limit law of the position of the unique bottom cell in $\mathcal{B}_{n,1}^*$

Define the random variable X_n of the position of the unique bottom cell in $\mathcal{B}_{n,1}^*$ drawn uniformly at random:

$$\mathbb{P}(X_n = m) = \frac{a_{n,m}}{\sum_k a_{n,k}} = \frac{[z^n x^m]\, G(z,x)}{[z^n]\, G(z,1)}.$$

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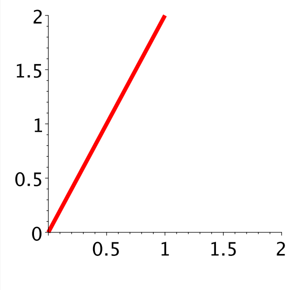
Theorem

$$\frac{X_n}{n} \xrightarrow{d} X \sim \mathrm{Beta}(2,1),$$

with density $f_X(x) = 2x$ *for* $x \in [0,1]$ *and* 0 *otherwise.*
The moments are given by $\mathbb{E}(X^r) = \frac{2}{r+2}$.



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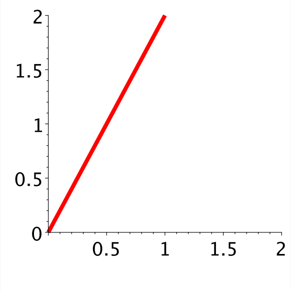


Therefore, on average,

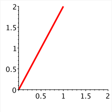
- the unique cell lies at column $\frac{2}{3}n$
- with standard deviation $\frac{\sqrt{2}}{6}n \approx 0.236n$.

Summary of limit laws

Random variables: always drawn uniformly at random.

1. X_n: position of the unique bottom cell in $\mathcal{B}^*_{n,1}$

$$\frac{X_n}{n} \xrightarrow{d} \mathrm{Beta}(2,1).$$



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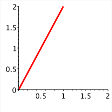
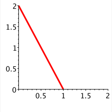


2. Y_n: value of the unique bottom cell in $\mathcal{B}^*_{n,1}$

$$\frac{Y_n}{2n} \xrightarrow{d} \mathrm{Beta}(1,2).$$



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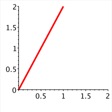

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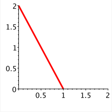
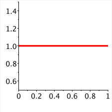


3. Z_n: value of the unique top cell in $\mathcal{C}^*_{n,1}$

$$\frac{Z_n}{2n} \xrightarrow{d} \mathrm{Beta}(1,1) = \mathrm{Unif}(0,1).$$



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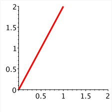

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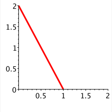

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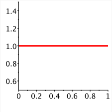

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