Well labeled paths and the volume of a polytope

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2. Paths, trees and matchings.
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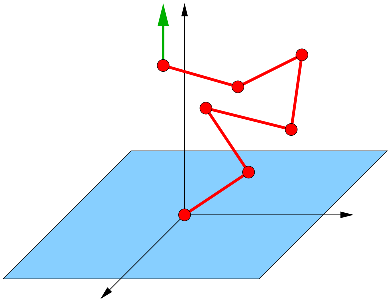
The polytope Π_n

In his study of a polypeptide model, Bertrand Duplantier discovered a certain polytope describing the configuration space of the model.



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The polytope Π_n

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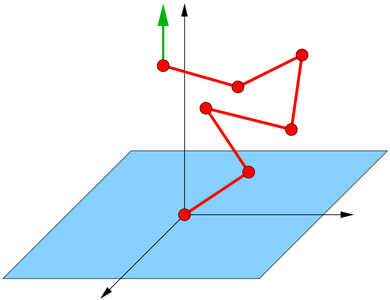

The polypeptide is composed of n line segments of unit length, and is attached to the ground. Now we consider the possible heights h_i of the extremities of the line segments.

The polytope Π_n

The polytope obtained is the following

Definition

We let Π_n be the set of points $x = (x_i)_i$ in $\mathbb{R}^n$ such that for all i,

$$x_i \geqslant 0 \quad \textit{and} \quad |x_i - x_{i-1}| \leqslant 1$$

with the convention $x_0 = 0$.

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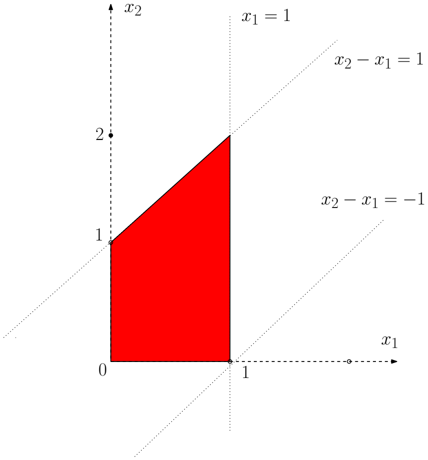
This is a bounded region (note that $0 \leqslant x_i \leqslant i$ for all i), and is formed by an intersection of half spaces in $\mathbb{R}^n$.

The polytope Π_n

For $n = 2$ we have for instance



Elementary polytopes

Let $\mathbf{h}$ be a point of $\mathbb{Z}^n$, and let σ be a permutation of $[n] := \{1, \ldots, n\}$.

Definition

We define the elementary polytope $E(\boldsymbol{h}, \sigma)$ *as the set of* $y = (y_i)_i$ *in* $\mathbb{R}^n$ *such that*

- $h_i \leqslant y_i \leqslant h_i + 1$ *and*
- $\epsilon(y_{\sigma^{-1}(1)}) \leqslant \epsilon(y_{\sigma^{-1}(2)}) \leqslant \ldots \leqslant \epsilon(y_{\sigma^{-1}(n)})$

where $\epsilon(t) \in [0, 1[$ *is the fractional part of* t *(i.e.* $t - \epsilon(t) \in \mathbb{Z}$*).*

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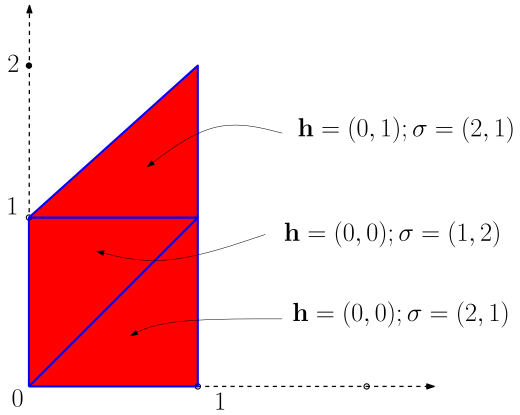
All elementary polytopes have the same volume $\frac{1}{n!}$. Then we have the following proposition :

Proposition

The interior of a given elementary polytope $E(\mathbf{h}, \sigma)$ is either included in Π_n or disjoint from Π_n.

Subpolytopes for $n = 2$



3 subpolytopes $E(\mathbf{h}, \sigma)$

So, in order to compute the volume of Π_n, it suffices to count the number of elementary subpolytopes $E(\mathbf{h}, \sigma)$ inside it, and divide by $n!$. For this, we will encode $(h_i, \sigma_i), i \in [n]$ as the point $(i-1, h_i)$ labeled by the integer σ_i. Then the condition for a polytope $E(\mathbf{h}, \sigma)$ to be included in Π_n is the following :

Definition

A well-labelled positive path of size n is a pair $(\mathbf{h}, \sigma)$ made of a integer vector $\mathbf{h} = (h_1, h_2, \dots, h_n) \in \mathbb{Z}^n$ and a permutation $\sigma = \sigma_1\sigma_2 \dots \sigma_n$ of $[n]$ such that :

1. $h_1 = 0$, $h_i \geqslant 0$, *and* $h_i - h_{i-1} \in \{-1, 0, 1\}$ *for all* i
2. $h_i > h_{i+1}$ *implies* $\sigma_i < \sigma_{i+1}$, *while* $h_{i+1} < h_i$ *implies* $\sigma_i > \sigma_{i+1}$.

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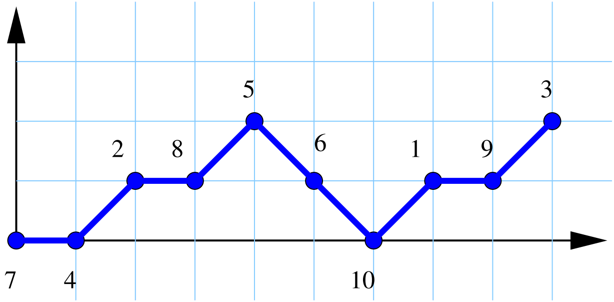
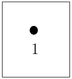
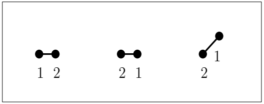


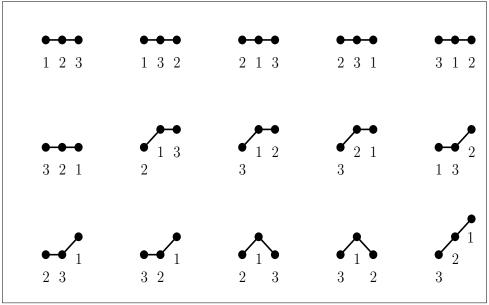
Positive paths for $n = 1, 2, 3$



$P_1 = 1$



$P_2 = 3$



$P_3 = 15$

Definition

A *well-labelled Motzkin path* *of size n is a pair* $(\boldsymbol{h}, \sigma)$ *made of a integer vector* $\boldsymbol{h} = (h_1, h_2, \dots, h_n) \in \mathbb{Z}^n$ *and a permutation* $\sigma = \sigma_1\sigma_2 \dots \sigma_n$ *of* $[n]$ *such that :*

1. $h_1 = 0$*,* $h_i \geqslant 0$*,* $h_{i+1} - h_{i-1} \in \{-1, 0, 1\}$ *for* $i = 1 \dots n-1$*,and.. .*
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1. $h_1 = 0$, $h_i \geqslant 0$, $h_{i+1} - h_{i-1} \in \{-1, 0, 1\}$ *for* $i = 1 \ldots n-1$, *and* $h_n = -1$.
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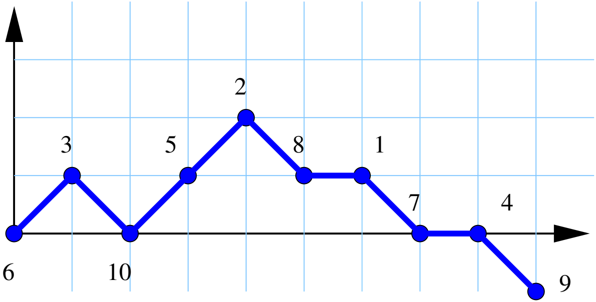

We defined the classes of well-labeled Motzkin paths and positive paths, which we will denote by $\mathcal{M}$ and $\mathcal{P}$.

To compute the volume of Π_n, we need to enumerate $\mathcal{P}_n$, the class of positive paths of size n. Still, we will focus on the class $\mathcal{M}_n$, which is easier to enumerate and is an essential step in the enumeration of $\mathcal{P}_n$.

A matching of size n is a partition of $[2n]$ with all blocks of size 2 ; equivalently, it is an involution on $[2n]$ without fixed points.

Main Results

Theorem

There are explicit bijections between the classes $\mathcal{P}_n$ and $\mathcal{M}_{n+1}$ and the matchings on $[2n]$.

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We have as immediate corollaries :

Corollary

1. *For all n we have* $|\mathcal{P}_n| = |\mathcal{M}_{n+1}| = (2n-1)!! := (2n-1)\cdot(2n-3)\cdots 3\cdot 1.$
2. *The volume of the polytope Π_n is equal to* $\frac{(2n-1)!!}{n!}$

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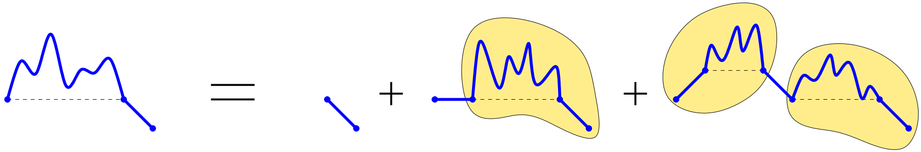
We will now exhibit the bijections announced in the main theorem above : in both cases, they will use a certain class of trees as an intermediate object.

Recursive decomposition of the class $\mathcal{M}$

Let us decompose the paths $(\mathbf{p}, \sigma)$ according to its second point h_1, which can be equal to $-1, 0$ or 1. Then we can write the following symbolic equation :



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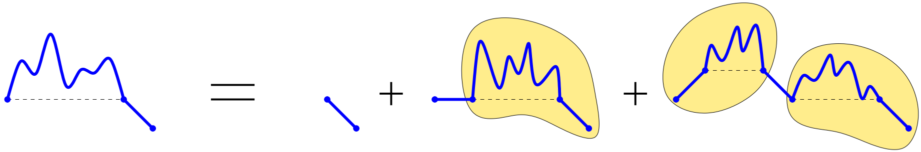


Notice that this is easily translated in the following equation :

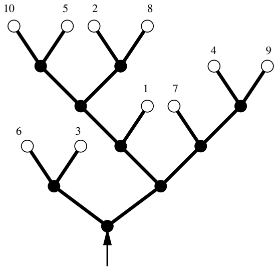
$$M(z) \;=\; \frac{z^2}{2} + zM(z) + \frac{M(z)^2}{2},$$

where $M(z) = \sum_n |\mathcal{M}_n| \frac{z^n}{n!}$ is the exponential generating function of the class $\mathcal{M}$. From this we can already deduce the enumeration $|\mathcal{M}_{n+1}| = (2n-1)!!$ by solving the equation, or by Lagrange inversion formula.

From paths to trees

Definition

A *labelled binary tree* *of size n is a rooted tree with n leaves having n different labels in $[n]$ and such that each (unlabelled) internal vertex has exactly two unordered children.*

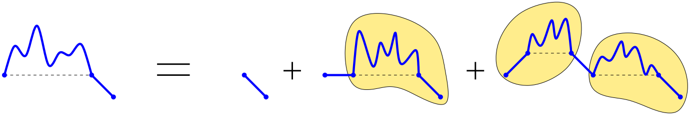


Proposition

There is a recursive bijection between $\mathcal{M}_n$ and $\mathcal{T}_n$.

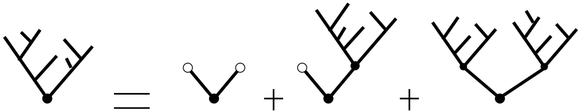
From paths to trees

Now remember the decomposition of $\mathcal{M}$:

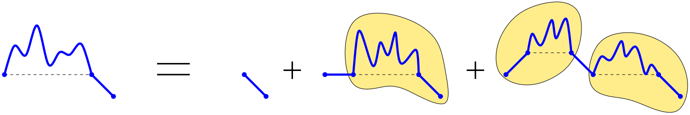


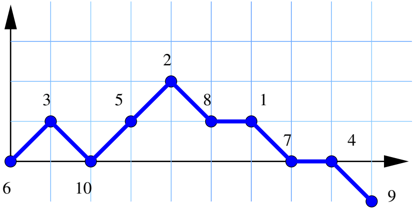
We will recursively attach to the three cases :

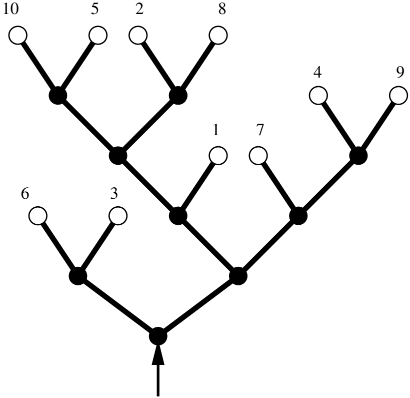
- The tree with one root, and two leaves labelled σ_1 and σ_2.
- The tree with one root, one leaf (labeled by σ_1) and one nontrivial subtree
- The tree with one root and two non trivial subtrees.



From paths to trees : example







From trees to matchings

This is a bijection due to Bill Chen.

First, number all internal non root vertices of the tree by $m = n+1, n+2, \dots, 2n-2$ in this order, as follows :

- Consider all unlabelled internal vertices that have both of their children labelled.
- Among these, choose the one which has the child with the smallest label.
- Label this vertex by m.

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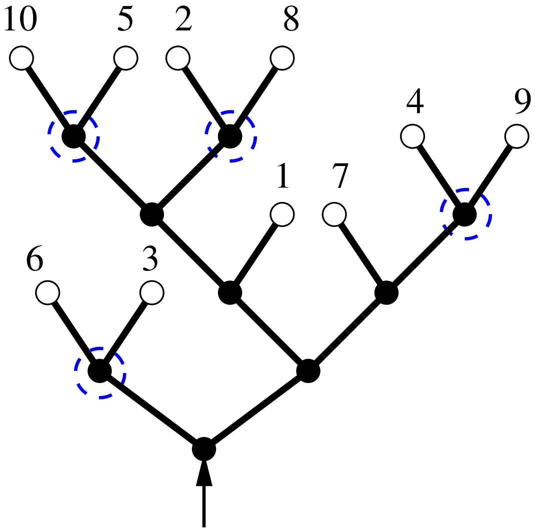
Once the tree is fully labeled, define a matching M on $[2n-2]$ by letting $\{i, j\}$ be a block of M if i and j are the labels of siblings.

From trees to matchings



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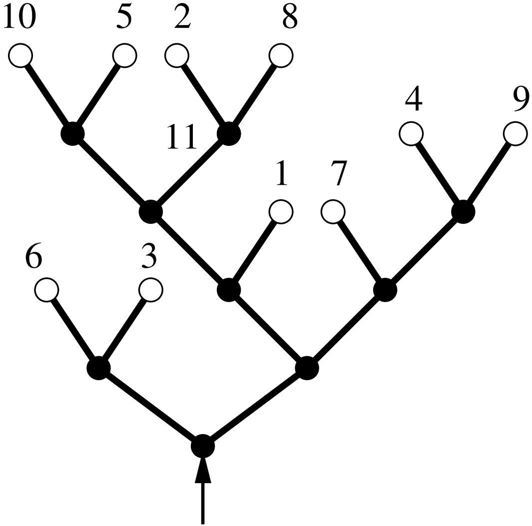

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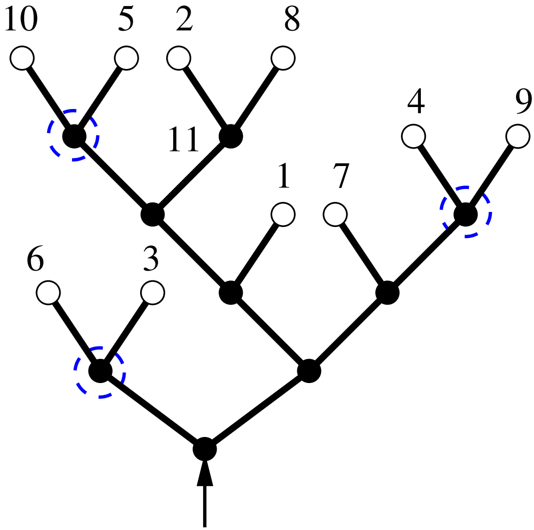

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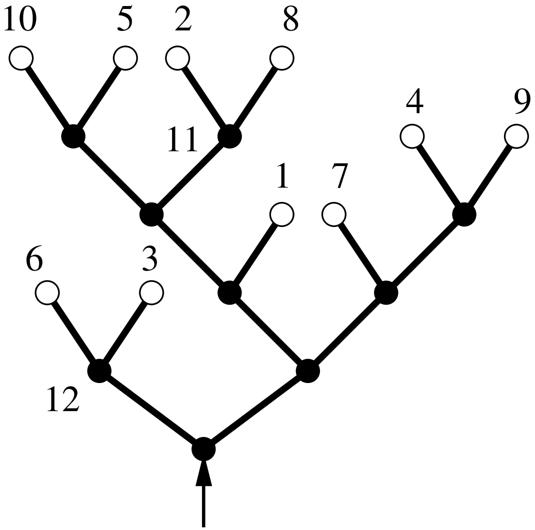

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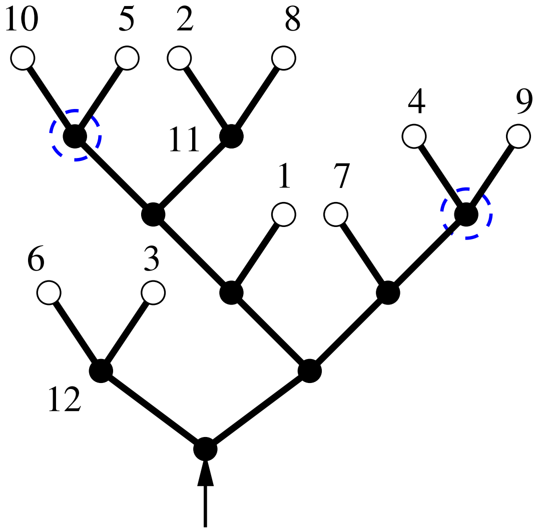

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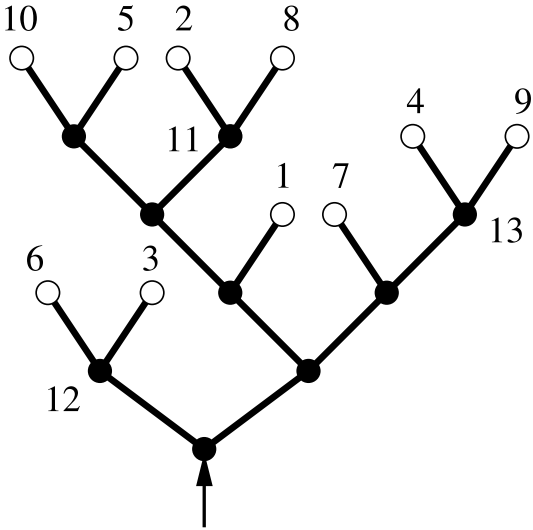

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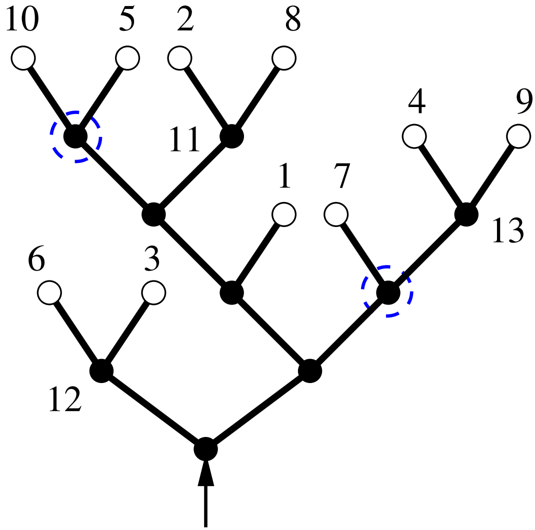

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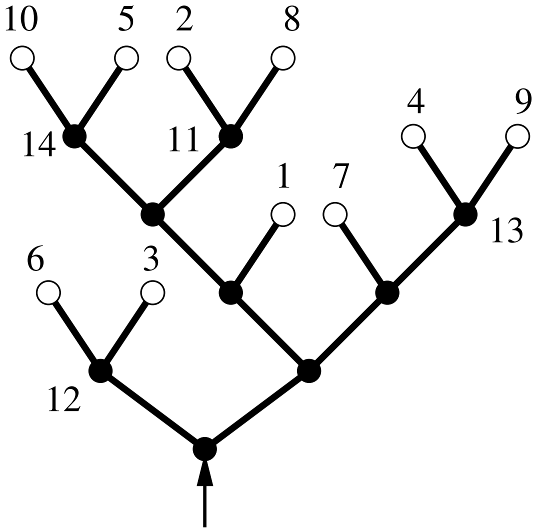

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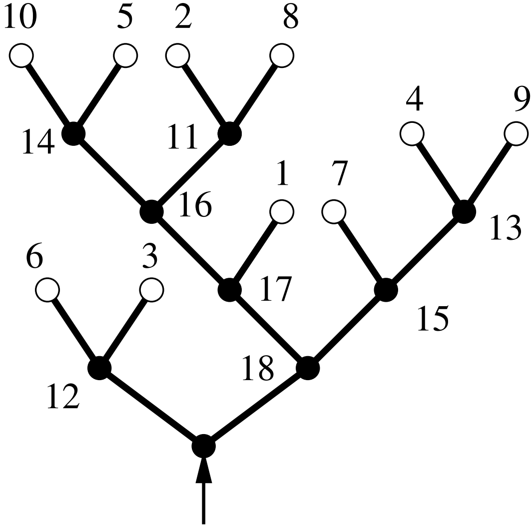

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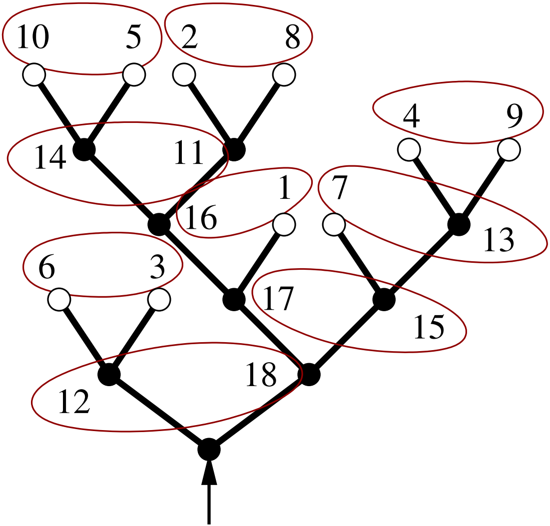

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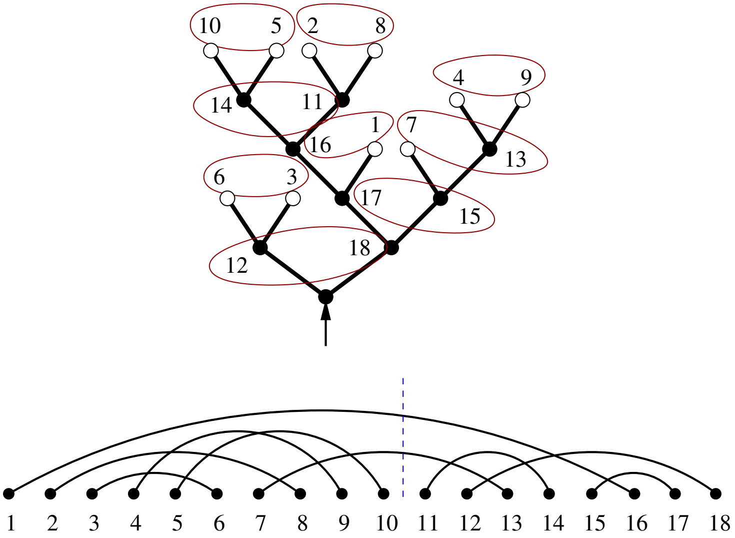
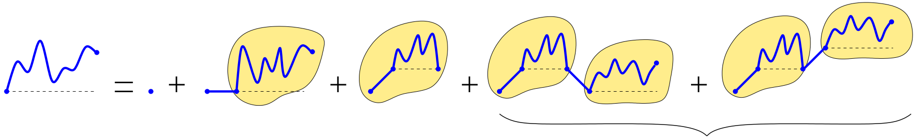


What about positive paths ?

They admit the following decomposition, based on $\mathcal{M}$.



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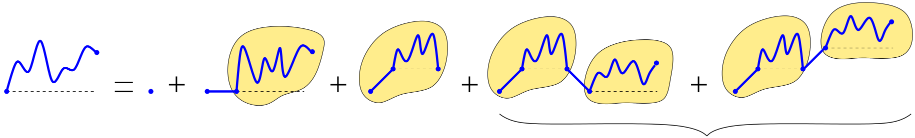
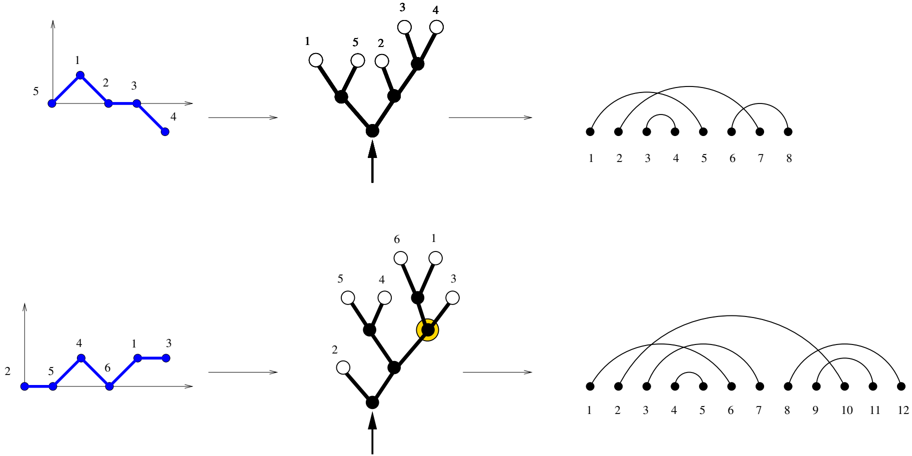


From this, one can define a bijection between $\mathcal{P}_n$ and marked labeled binary trees.They are the same trees but with a distinguished vertex.

Then it is easy to give a bijection between marked trees with n leaves and matchings on $[2n]$. It is a simple modification of Bill Chen´s bijection.

Summary of bijections



Refinement

A leaf in a binary tree is single if its sibling is an internal node.

Theorem

For all integers n, k, we have bijections between

1. *well-labelled Motzkin paths of size n with k horizontal steps,*
2. *labelled binary trees with n leaves, k of which are single leaves, and*
3. *matchings on $[2n-2]$ having k pairs $\{i, j\}$ such that $i \in \{1, \ldots, n\}$ and $j \in \{n+1, \ldots, 2n-2\}$.*

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Corollary

The number of well-labelled Motzkin paths of size n having k horizontal steps is 0 if $n-k$ is odd, and otherwise

$$\binom{n}{k}\binom{n-2}{k} k!\,(n-k-1)!!\,(n-k-3)!!$$

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We have a similar result for positive paths :

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Corollary

The number of well-labelled positive paths of size n having k horizontal steps is

$$\begin{cases} \binom{n}{k}\binom{n-1}{k} k!\,[(n-k-1)!!]^2 & \text{if } n-k \text{ is even,} \\ \binom{n}{k+1}\binom{n-1}{k} (k+1)!\,[(n-k-2)!!]^2 & \text{otherwise.} \end{cases}$$

Application to permutation enumeration

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Theorem

For any integer n, the number of permutations of size n having a positive up-down sequence is $[(n-1)!!]^2$ *if n is even and* $[(n-2)!!]^2$ *otherwise. The number of permutations of size n having a Dyck up-down sequence is* $(n-1)!!\,(n-3)!!$ *if n is even and 0 otherwise.*