Well labeled paths and the volume of a polytope

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2. Paths, trees and matchings.
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3. Refined enumeration ; application to permutations.
The polytope $\Pi_n$

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 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 $\Pi_n$

The polytope obtained is the following

**Definition**

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

$$x_i \geq 0 \text{ and } |x_i - x_{i-1}| \leq 1$$

with the convention $x_0 = 0$. 


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

For $n = 2$ we have for instance:

\[ x_2 - x_1 = 1 \]
\[ x_2 - x_1 = -1 \]
\[ x_1 = 1 \]

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Elementary polytopes

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

**Definition**

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

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

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

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

**Definition**

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

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All elementary polytopes have the same volume $\frac{1}{n!}$. 
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where \( \epsilon(t) \in [0, 1[ \) is the fractional part of \( t \) (i.e. \( t - \epsilon(t) \in \mathbb{Z} \)).

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

**Proposition**

The interior of a given elementary polytope \( E(h, \sigma) \) is either included in \( \Pi_n \) or disjoint from \( \Pi_n \).
Subpolytopes for $n = 2$

3 subpolytopes $E(h, \sigma)$

$h = (0, 0); \sigma = (0, 1)$

$h = (0, 1); \sigma = (2, 1)$

$h = (0, 0); \sigma = (1, 2)$

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Well labeled paths

So, in order to compute the volume of $\Pi_n$, it suffices to count the number of elementary subpolytopes $E(h, \sigma)$ 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 $\sigma_i$. Then the condition for a polytope $E(h, \sigma)$ to be included in $\Pi_n$ is the following:

**Definition**

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

1. $h_1 = 0$, $h_i \geq 0$, 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 $\sigma_i > \sigma_{i+1}$.
Well labeled paths

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![Diagram of a well-labelled positive path](image-url)
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 $(h, \sigma)$ made of an integer vector $h = (h_1, h_2, \ldots, h_n) \in \mathbb{Z}^n$ and a permutation $\sigma = \sigma_1\sigma_2\ldots\sigma_n$ of $[n]$ such that:

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

2. $h_i > h_{i+1}$ implies $\sigma_i < \sigma_{i+1}$, while $h_{i+1} < h_i$ implies $\sigma_i > \sigma_{i+1}$. 


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

1. $h_1 = 0$, $h_i \geq 0$, $h_{i+1} - h_{i-1} \in \{-1, 0, 1\}$ for $i = 1 \ldots n - 1$, and $h_n = -1$.
2. $h_i > h_{i+1}$ implies $\sigma_i < \sigma_{i+1}$, while $h_{i+1} < h_i$ implies $\sigma_i > \sigma_{i+1}$.
We defined the classes of well-labeled Motzkin paths and positive paths, which we will denote by $M$ and $P$.

To compute the volume of $\Pi_n$, we need to enumerate $P_n$, the class of positive paths of size $n$. Still, we will focus on the class $M_n$, which is easier to enumerate and is an essential step in the enumeration of $P_n$.

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 \( P_n \) and \( M_{n+1} \) and the matchings on \([2n]\).

We have as immediate corollaries:

**Corollary**

For all \( n \) we have

\[
|P_n| = |M_{n+1}| = (2n - 1)!! = (2n - 1) \cdot (2n - 3) \cdot \ldots \cdot 3 \cdot 1.
\]

The volume of the polytope \( \Pi_n \) is equal to

\[
(2n - 1)!! \cdot n!
\]

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.
Main Results

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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 $\Pi_n$ is equal to $\frac{(2n-1)!!}{n!}$.
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2. The volume of the polytope $\Pi_n$ is equal to $\frac{(2n-1)!!}{n!}$

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

$$M(z) = z^2 + zM(z) + M(z)^2,$$

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

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

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

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.
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 \( \mathcal{T}_n \).
Now remember the decomposition of $M$:

We will recursively attach to the three cases:

- The tree with one root, and two leaves labelled $\sigma_1$ and $\sigma_2$.
- The tree with one root, one leaf (labeled by $\sigma_1$) and one nontrivial subtree
- The tree with one root and two non trivial subtrees.
From paths to trees: example
This is a bijection due to Bill Chen.

First, number all internal non root vertices of the tree by \( m = n + 1, n + 2, \ldots, 2n - 2 \) 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 \( m \).
From trees to matchings

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First, number all internal non root vertices of the tree by \( m = n + 1, n + 2, \ldots, 2n - 2 \) 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 \( m \).

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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Well labeled paths and the volume of a polytope
From trees to matchings
What about positive paths?

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

$$
\begin{align*}
&= + + +
\end{align*}
$$

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.
What about positive paths?

They admit the following decomposition, based on $M$.

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 $j \in \{n+1, \ldots, 2n-2\}$.

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! \binom{n-k-1}{2} \binom{n-k-3}{2}!!.
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

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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

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

We have a similar result for positive paths:

**Theorem**

For all integers $n, k$, we have a bijection between

1. well-labelled positive paths of size $n$ with $k$ horizontal steps, and
2. matchings on $[2n]$ having $k$ pairs $(i, j)$ with $i \in \{1, \ldots, n\}$ and $j \in \{n + 1, \ldots, 2n - 1\}$.

**Corollary**

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

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

We have a similar result for positive paths:

**Theorem**

For all integers \( n, k \), we have a bijection between

1. well-labelled positive paths of size \( n \) with \( k \) horizontal steps, and
2. matchings on \([2n]\) having \( k \) pairs \((i, j)\) with \( i \in \{1, \ldots, n\} \) and \( j \in \{n + 1, \ldots, 2n - 1\} \).

**Corollary**

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

\[
\begin{cases}
\binom{n}{k} \binom{n-1}{k} k! \left[(n-k-1)!!\right]^2 & \text{if } n-k \text{ is even}, \\
\binom{n}{k+1} \binom{n-1}{k} (k+1)! \left[(n-k-2)!!\right]^2 & \text{otherwise}.
\end{cases}
\]
Application to permutation enumeration

Let \((p, \sigma)\) be a well-labelled path (in \(\mathcal{M}\) or \(\mathcal{P}\)). If it has no horizontal step, then the permutation \(\sigma\) determines \(p\).
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Let \((p, \sigma)\) be a well-labelled path (in \(M\) or \(P\)). If it has no horizontal step, then the permutation \(\sigma\) determines \(p\).

An ascent of a permutation \(\sigma = \sigma_1\sigma_2 \ldots \sigma_n\) is an index \(i < n\) such that \(\sigma_i < \sigma_{i+1}\); a descent is an index \(i < n\) such that \(\sigma_i > \sigma_{i+1}\). The up-down sequence of a permutation \(\sigma\) is given by \(p(\sigma) = p_1p_2 \ldots p_{n-1}\) where \(p_i = 1\) (respectively \(p_i = -1\)) if \(i\) is a descent (resp. an ascent). The up-down sequence is positive if it forms a positive path, and Dyck if it forms an extended Dyck path.

\[ \left\lfloor \frac{(n-1)!!}{2} \right\rfloor \text{ if } n \text{ is even} \]
\[ \left\lfloor \frac{(n-2)!!}{2} \right\rfloor \text{ otherwise.} \]

The number of permutations of size \(n\) having a Dyck up-down sequence is \(\frac{(n-1)!!(n-3)!!}{2}\) if \(n\) is even and 0 otherwise.
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The up-down sequence is positive if it forms a positive path, and Dyck if it forms an extended Dyck path.

**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.