More Phylogenetic polytopes: poset associahedra.

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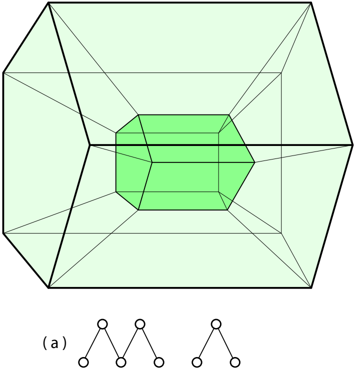
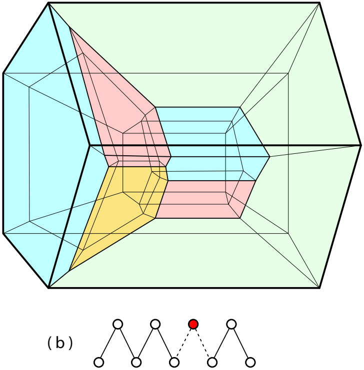


(a)



(b)

Tubes

A *lower set* L is a subset of a poset P such that if $y \preceq x \in L$, then $y \in L$. The *boundary* of an element x is $\partial x := \{y \in P \mid y \prec x\}$.

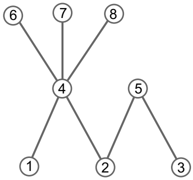
Definition

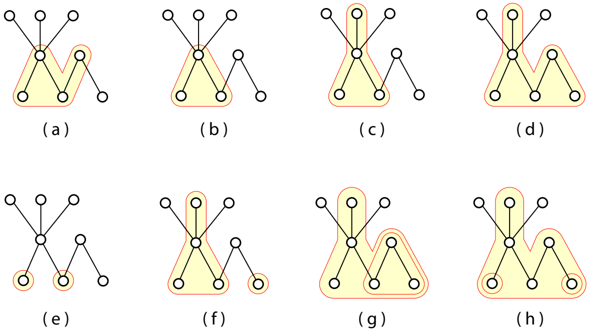
Let $\mathfrak{b}_x := \{y \in P \mid \partial y = \partial x\}$ *be the bundle of the element* x*.*

Definition

A lower set is filled if, whenever it contains the boundary ∂x *of an element* x*, it also intersects the bundle* $\mathfrak{b}_x$ *of that element. A tube is a filled, connected lower set.*

Tubes





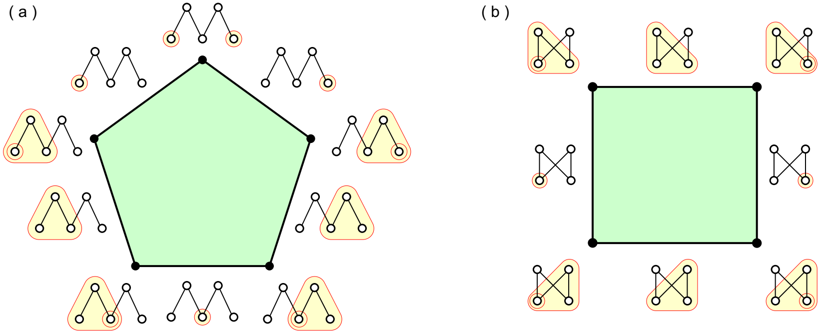
A *tubing* T is a collection of tubes (not containing all of P) which are pairwise disjoint or pairwise nested, and for which the union of every subset of T is filled.

Tubes

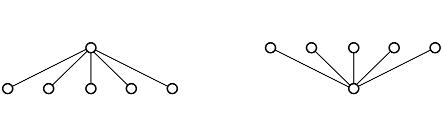
Theorem

Let P be a poset with n elements partitioned into b bundles. If $\pi(P)$ is the set of tubings of P ordered by reverse containment, the poset associahedron $\mathcal{KP}$ is a convex polytope of dimension $n - b$ whose face poset is isomorphic to $\pi(P)$.

posets.

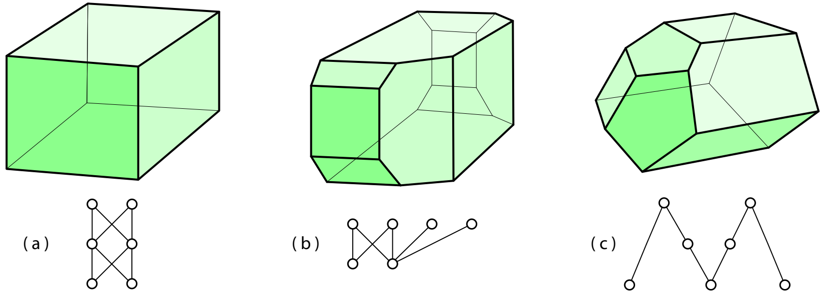


posets.

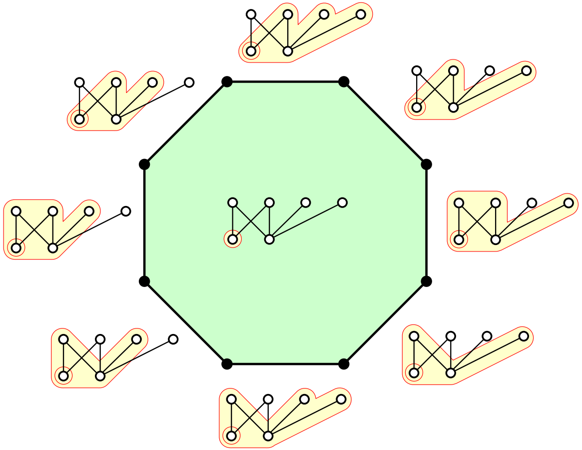


(a) *point* (b) *cube* (c) *simplex* (d) *permutohedron*

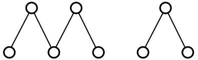
posets.

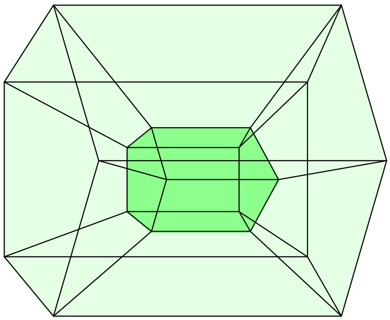


posets.

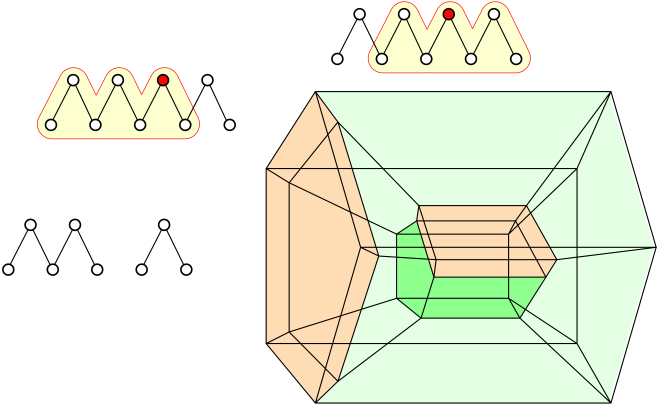


posets.

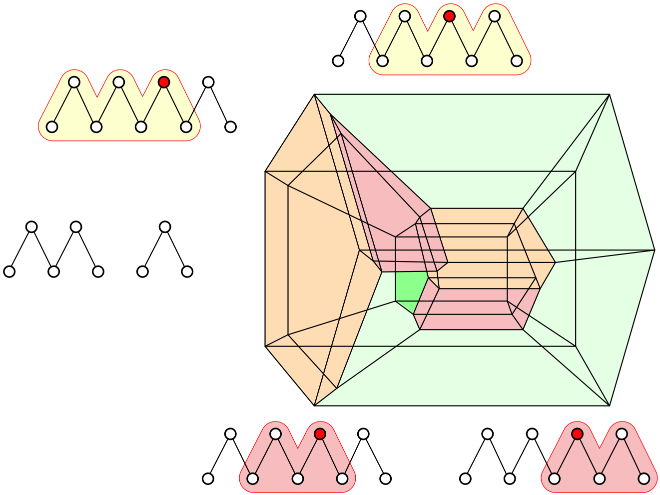




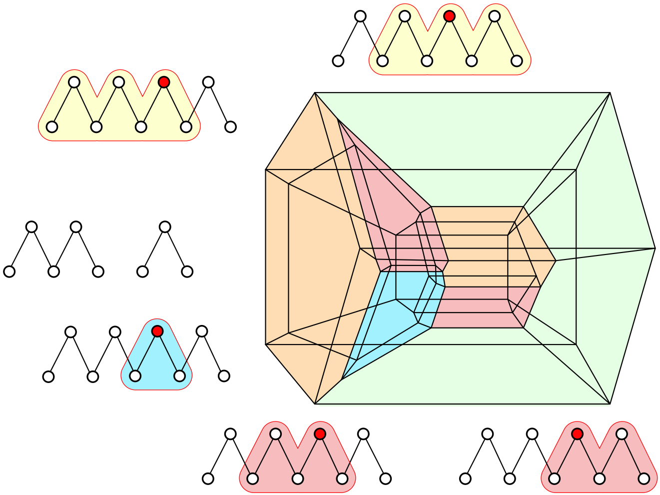
posets.



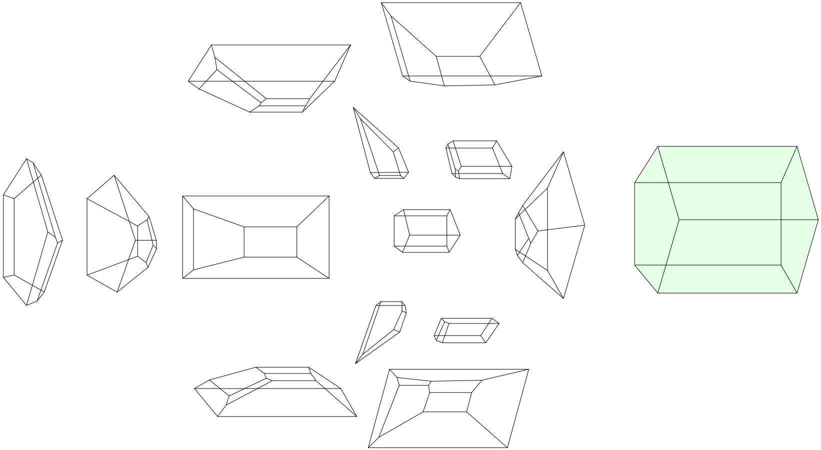
posets.



posets.



posets.



flips.

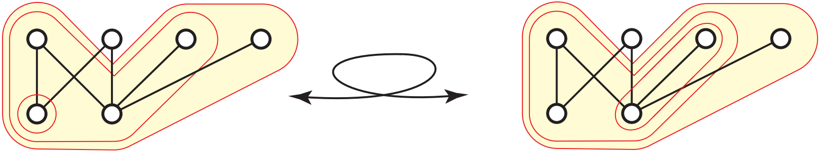
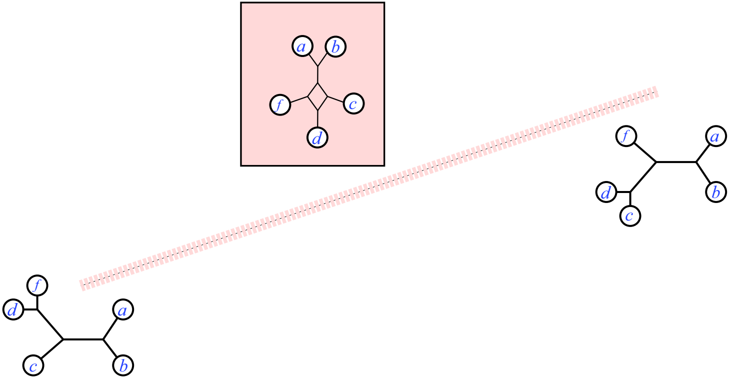


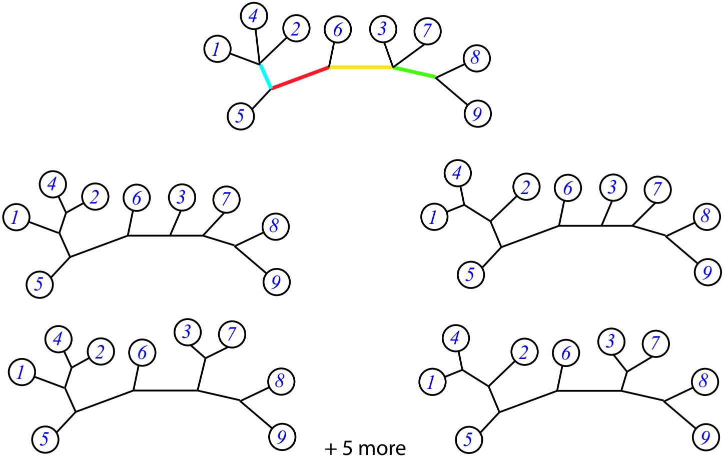
Figure: Each edge of a poset associahedron can be interpreted as a flip, where one tube is removed and another uniquely determined tube takes its place.

Back to BME

Question 1. Which split networks correspond to flips and faces in the Balanced Minimal Evolution polytope?

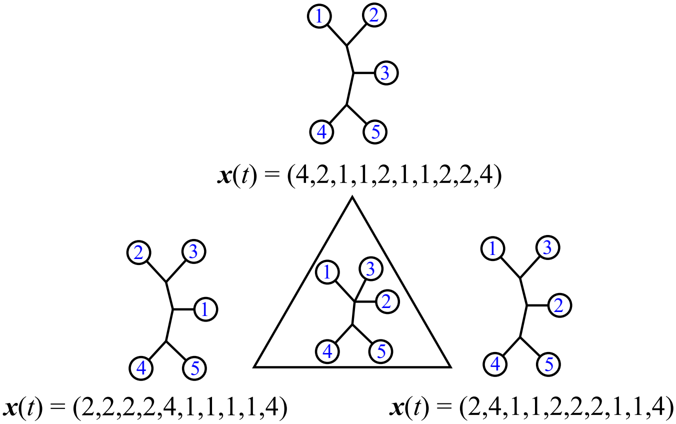


A1. any set of compatible splits.

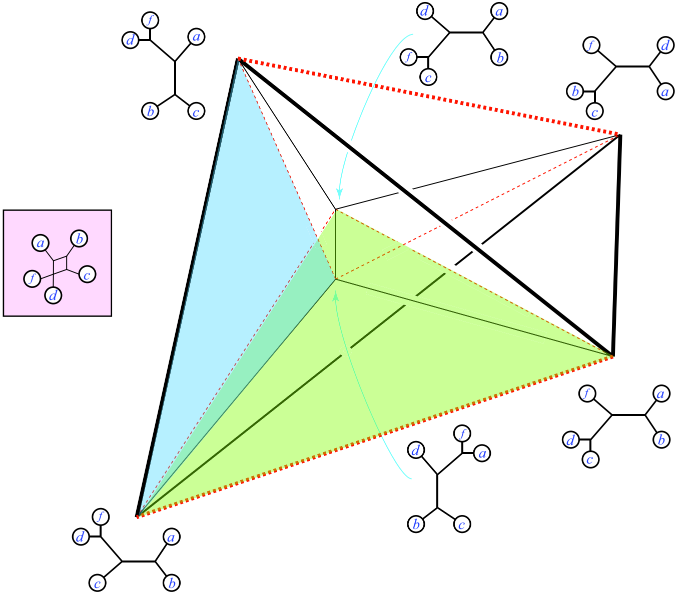


+ 5 more

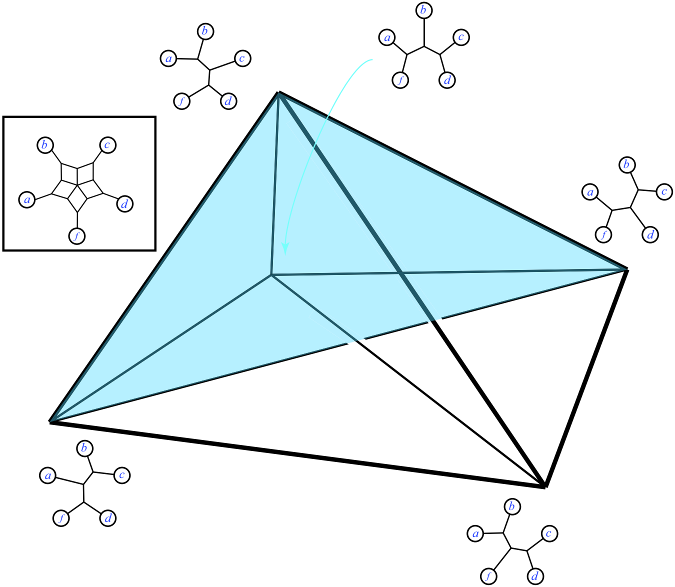
A1. any set of compatible splits.



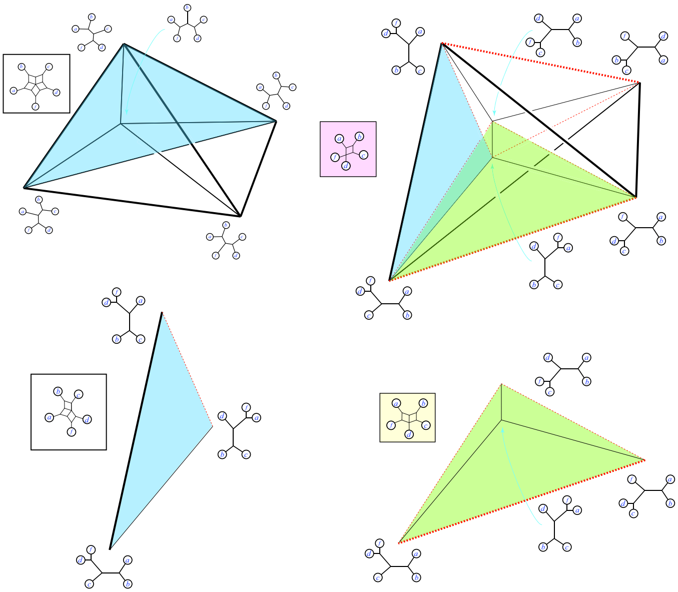
A1. Intersecting cherry splits



A1: Cyclic splits for $n = 5$

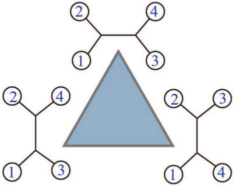


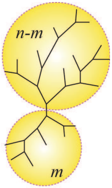
A1: Four split networks.



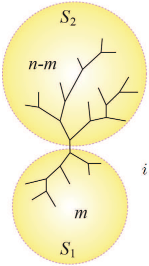
Q2: Split faces; split facets.

Question 2. If we use branch and bound to optimize on the region bounded by split faces of the BME polytope, are we guaranteed to get a valid tree?





Splitohedron.



$$\sum_{i<j,\ \text{leaves } i,j \in S_1} x_{ij} \leq (m-1)2^{n-3}$$

Theorem: the Splitohedron is a bounded polytope that is a relaxation of the BME polytope.

Proof: The split-faces include the cherries where the inequality is $x_{ij} \leq 2^{n-3}$, and the caterpillar facets have the inequality $x_{ij} \geq 1$, thus the resulting intersection of halfspaces is a bounded polytope since it is inside the hypercube $[1, 2^{n-3}]^{\binom{n}{2}}$.

Features of the BME polytope $\mathcal{P}_n$

number of species	dim. of $\mathcal{P}_n$	vertices of $\mathcal{P}_n$	facets of $\mathcal{P}_n$	facet inequalities (classification)	number of facets	number of vertices in facet
3	0	1	0	-	-	-
4	2	3	3	$x_{ab} \geq 1$	3	2
				$x_{ab} + x_{bc} - x_{ac} \leq 2$	3	2
5	5	15	52	$x_{ab} \geq 1$ (caterpillar)	10	6
				$x_{ab} + x_{bc} - x_{ac} \leq 4$ (intersecting-cherry)	30	6
				$x_{ab} + x_{bc} + x_{cd} + x_{df} + x_{fa} \leq 13$ (cyclic ordering)	12	5
6	9	105	90262	$x_{ab} \geq 1$ (caterpillar)	15	24
				$x_{ab} + x_{bc} - x_{ac} \leq 8$ (intersecting-cherry)	60	30
				$x_{ab} + x_{bc} + x_{ac} \leq 16$ $(3,3)$-split	10	9
n	$\binom{n}{2} - n$	$(2n-5)!!$	?	$x_{ab} \geq 1$ (caterpillar)	$\binom{n}{2}$	$(n-2)!$
				$x_{ab} + x_{bc} - x_{ac} \leq 2^{n-3}$ (intersecting-cherry)	$\binom{n}{2}(n-2)$	$2(2n-7)!!$
				$x_{ab} + x_{bc} + x_{ac} \leq 2^{n-2}$ $(m,3)$-split, $m \geq 3$	$\binom{n}{3}$	$3(2n-9)!!$
				$\sum_S x_{ij} \leq (m-1)2^{n-3}$ $(m, n-m)$-split S, $m > 2, n > 5$	$2^{n-1} - \binom{n}{2}$ $-n-1$	$(2(n-m)-3)!!$ $\times(2m-3)!!$

Splitohedron.

```
polytope > print $p->VERTICES;

1 1 2 1 4 2 4 1 2 2 1
1 1 2 4 1 2 1 4 2 2 1
1 1 4 2 1 1 2 4 2 1 2
1 1 1 2 4 4 2 1 2 1 2
1 1 1 4 2 4 1 2 1 2 2
1 1 4 1 2 1 4 2 1 2 2
1 2 1 4 1 2 2 2 1 4 1
1 8/3 4/3 8/3 4/3 4/3 4/3 8/3 8/3 8/3 4/3
1 2 1 1 4 2 2 2 4 1 1
1 4/3 4/3 8/3 8/3 8/3 8/3 4/3 4/3 8/3 4/3
1 4/3 8/3 4/3 8/3 8/3 8/3 4/3 4/3 4/3 8/3
1 4 1 2 1 1 2 1 2 4 2
1 4 2 1 1 2 1 1 2 2 4
1 8/3 4/3 4/3 8/3 4/3 8/3 4/3 8/3 8/3 4/3

1 2 2 2 2 1 1 4 4 1 1
1 2 2 2 2 1 4 1 1 4 1
1 4/3 8/3 8/3 4/3 8/3 4/3 8/3 4/3 4/3 8/3
1 4/3 8/3 8/3 4/3 4/3 8/3 8/3 4/3 8/3 4/3
1 4 1 1 2 1 1 2 4 2 2
1 8/3 4/3 4/3 8/3 8/3 4/3 4/3 8/3 4/3 8/3
1 8/3 4/3 8/3 4/3 8/3 4/3 4/3 4/3 8/3 8/3
1 2 2 2 2 4 1 1 1 1 4
1 8/3 8/3 4/3 4/3 4/3 8/3 4/3 4/3 8/3 8/3
1 8/3 8/3 4/3 4/3 4/3 4/3 8/3 8/3 4/3 8/3
1 2 4 1 1 2 2 2 1 1 4
1 4/3 4/3 8/3 8/3 8/3 4/3 8/3 8/3 4/3 4/3
1 4/3 8/3 4/3 8/3 4/3 8/3 8/3 8/3 4/3 4/3
```

Splitohedron.

```
polytope > print $p->VERTICES;

1 1 2 1 4 2 4 1 2 2 1
1 1 2 4 1 2 1 4 2 2 1
1 1 4 2 1 1 2 4 2 1 2
1 1 1 2 4 4 2 1 2 1 2
1 1 1 4 2 4 1 2 1 2 2
1 1 4 1 2 1 4 2 1 2 2
1 2 1 4 1 2 2 2 1 4 1
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1 2 1 1 4 2 2 2 4 1 1
1 4/3 4/3 8/3 8/3 8/3 8/3 4/3 4/3 8/3 4/3
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1 4 1 2 1 1 2 1 2 4 2
1 4 2 1 1 2 1 1 2 2 4
1 8/3 4/3 4/3 8/3 4/3 8/3 4/3 8/3 8/3 4/3

1 2 2 2 2 1 1 4 4 1 1
1 2 2 2 2 1 4 1 1 4 1
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```
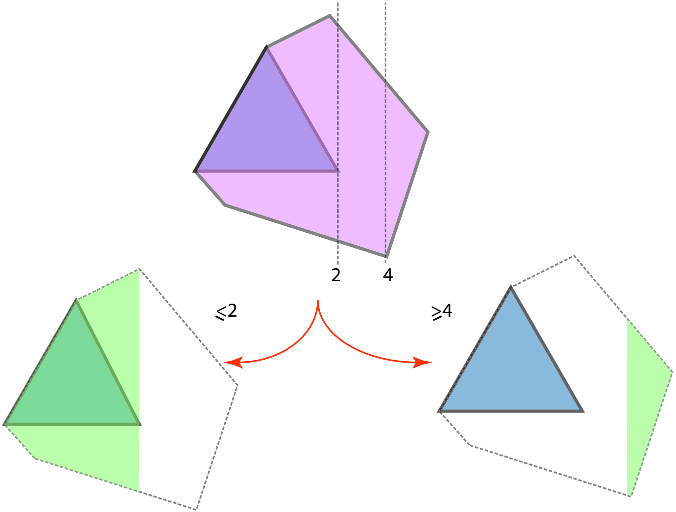

BnB.

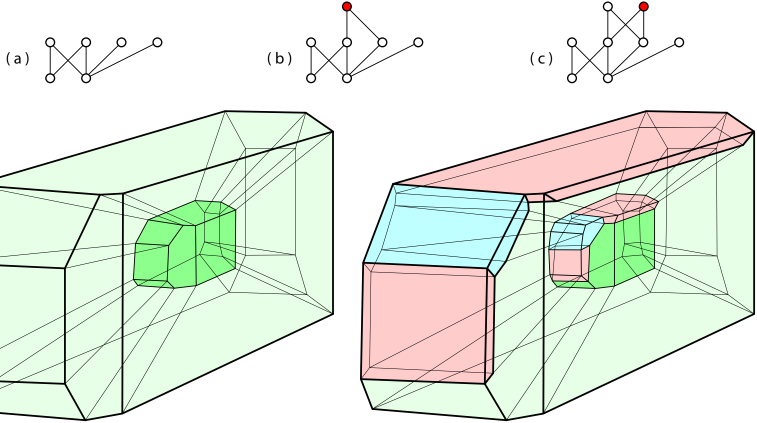


A2: So far so good!

- We tested up to $n = 10$, with and without noise.
- Results are completely accurate...
- We need to find a way to break it! MatLab code available: `http://www.math.uakron.edu/~sf34/class_home/research.htm`

Thanks!

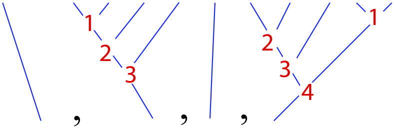
Questions and comments?



Advertisement:

`http://www.math.uakron.edu/~sf34/hedra.htm`

An open question.



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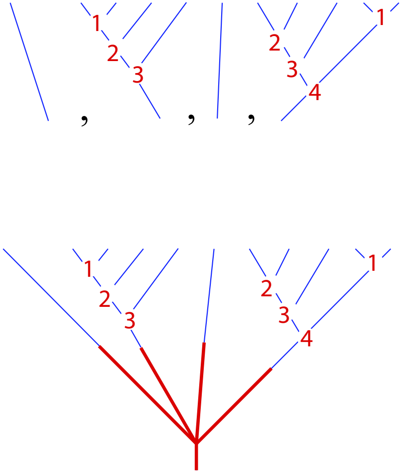

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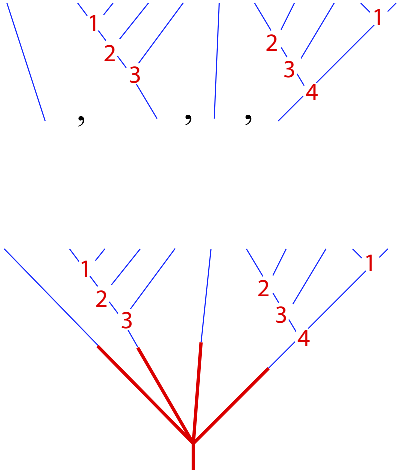

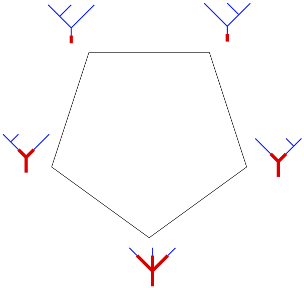

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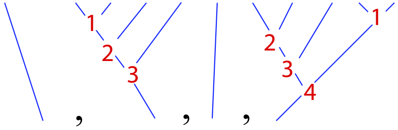

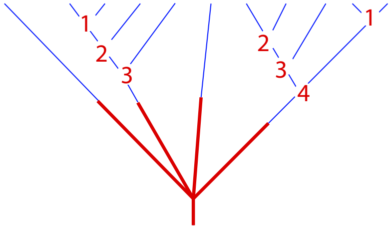

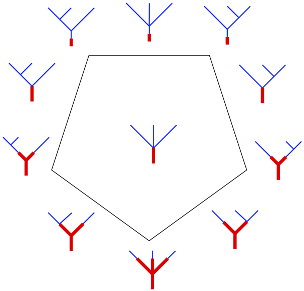

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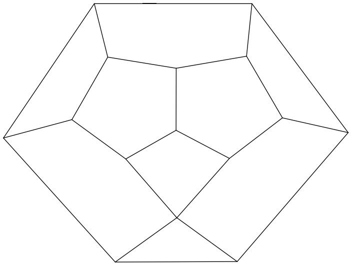

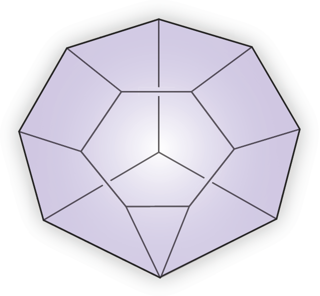

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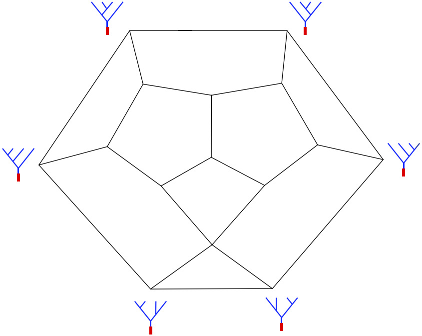

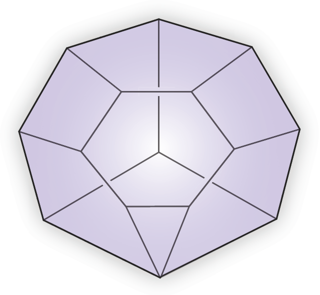

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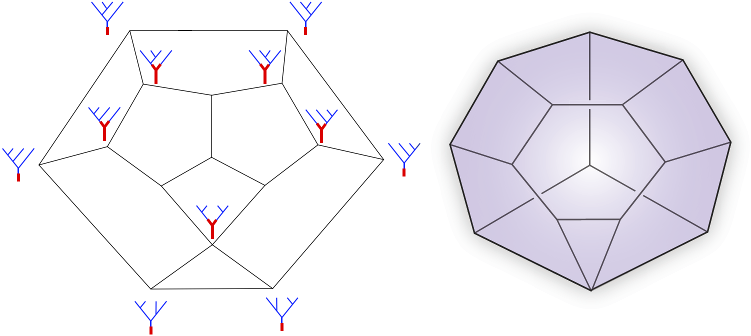

1,2,6,15,...Invert transform of the factorials.