Faces of Balanced Minimal Evolution Polytopes and Linear Programming.

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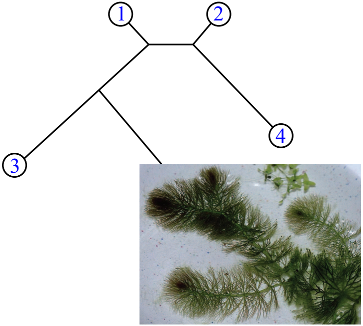
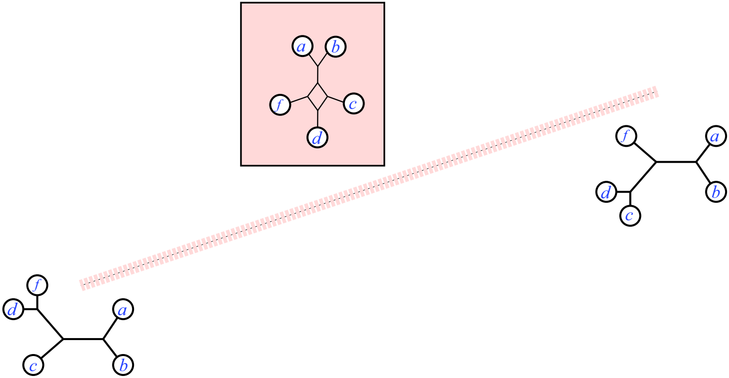
Satyan Devadoss. U. San Diego

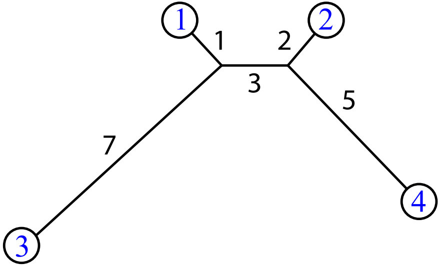


Q1: Split faces; split facets.

Question 1. Which split networks correspond to faces (and especially facets) of the Balanced Minimal Evolution polytope?



The Balanced minimal evolution method: ex. tree metric.



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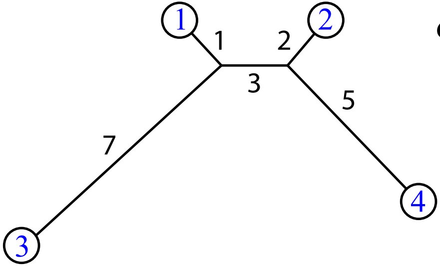
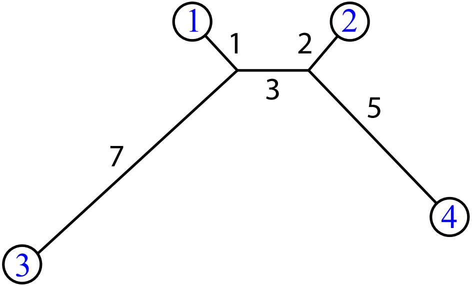


distance 1-2

$$\begin{bmatrix} 0 & 6 & 8 & 9 \\ 6 & 0 & 12 & 7 \\ 8 & 12 & 0 & 15 \\ 9 & 7 & 15 & 0 \end{bmatrix}$$

The Balanced minimal evolution method: ex. tree metric.

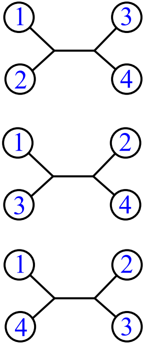


$$\begin{bmatrix} 0 & 6 & 8 & 9 \\ 6 & 0 & 12 & 7 \\ 8 & 12 & 0 & 15 \\ 9 & 7 & 15 & 0 \end{bmatrix}$$

$$\boldsymbol{d} = \langle 6, 8, 9, 12, 7, 15 \rangle$$

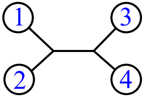
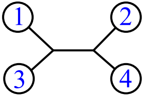
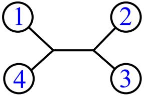
$$x(t)_{ij} = 2^{(n-2-l_{ij})}$$

t $\quad$ $x(t)$



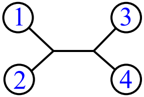
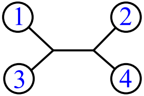
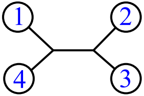
The Balanced minimal evolution method: ex. tree metric.

$$x(t)_{ij} = 2^{(n-2-l_{ij})}$$

t	$x(t)$	$d \cdot x(t)$
	$\langle 2, 1, 1, 1, 1, 2 \rangle$	
	$\langle 1, 2, 1, 1, 2, 1 \rangle$	
	$\langle 1, 1, 2, 2, 1, 1 \rangle$	

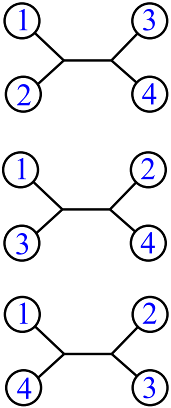
The Balanced minimal evolution method: ex. tree metric.

$$x(t)_{ij} = 2^{(n-2-l_{ij})}$$

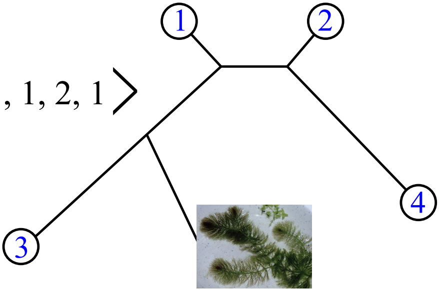
t	$x(t)$	$\boldsymbol{d}\cdot x(t)$
	$\langle 2, 1, 1, 1, 1, 2 \rangle$ $\langle 6, 8, 9, 12, 7, 15 \rangle$	78
	$\langle 1, 2, 1, 1, 2, 1 \rangle$	72
	$\langle 1, 1, 2, 2, 1, 1 \rangle$	78

The Balanced minimal evolution method: ex. tree metric.

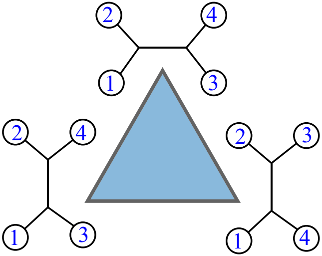
t $\quad$ $x(t)$

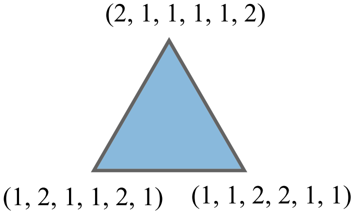


$\langle 1, 2, 1, 1, 2, 1 \rangle$

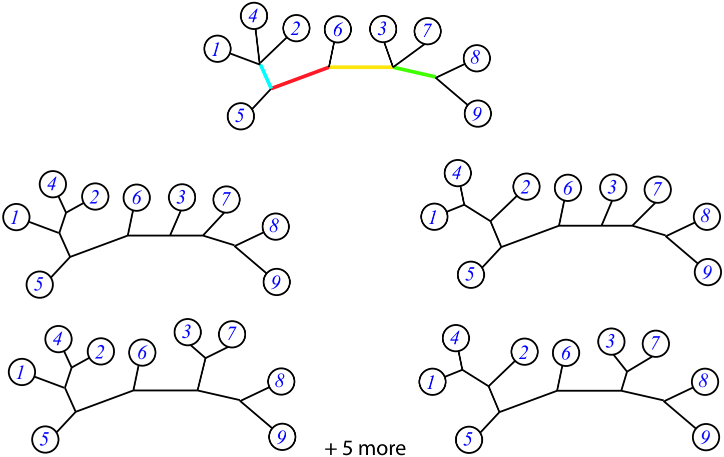


The Balanced minimal evolution polytope $\mathcal{P}_4$.

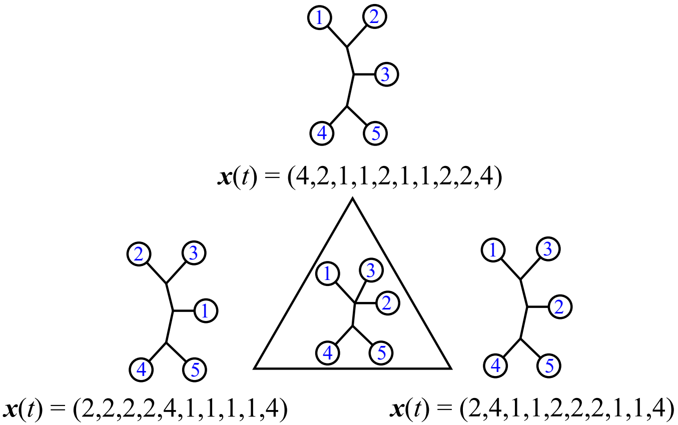




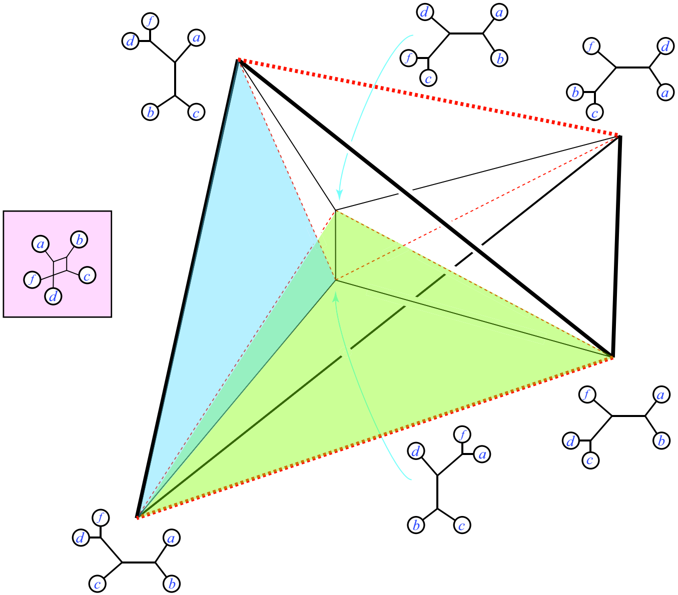
A1. any set of compatible splits.



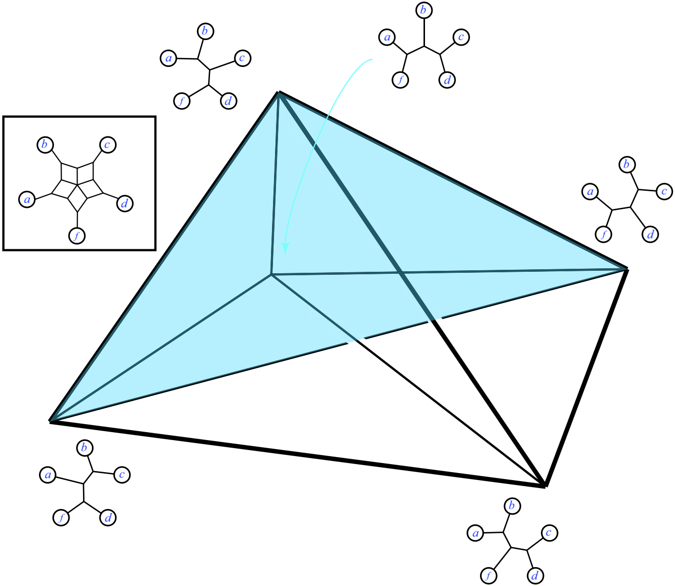
A1. any set of compatible splits.



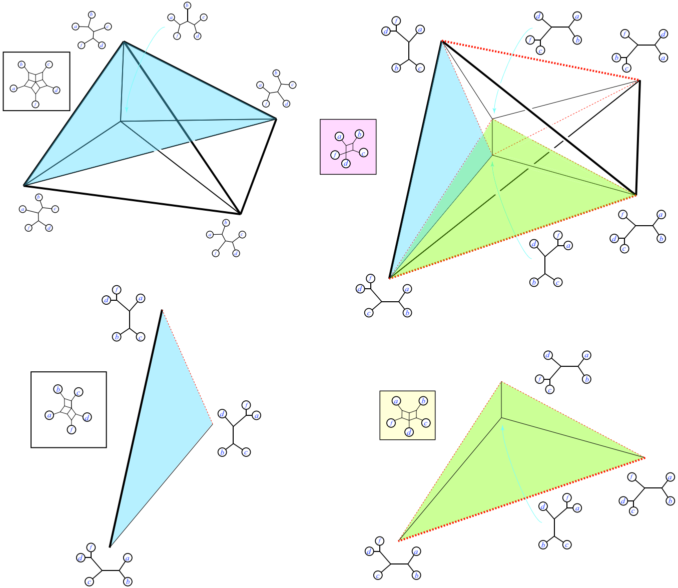
A1. Intersecting cherry splits



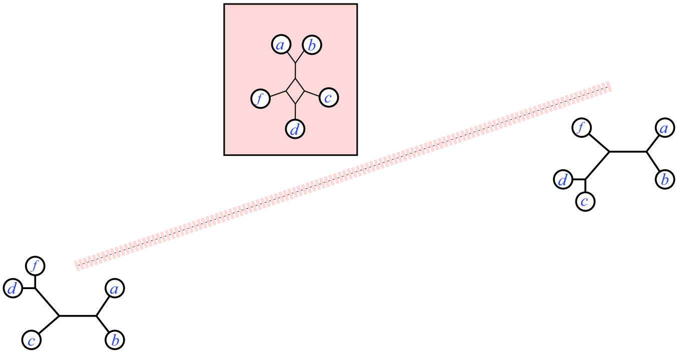
A1: Cyclic splits for $n = 5$



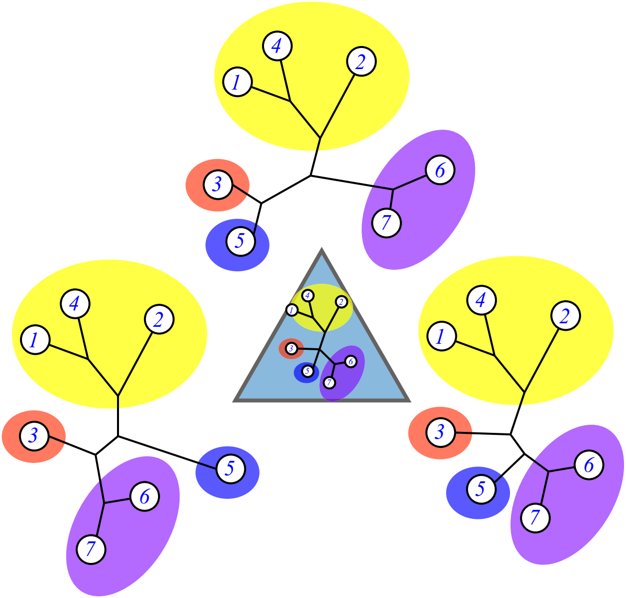
A1: Four split networks.



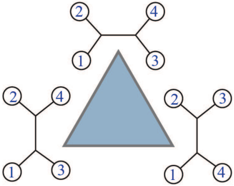
A1: Nearest Neighbor Interchange.

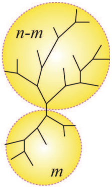


A1: Clade face

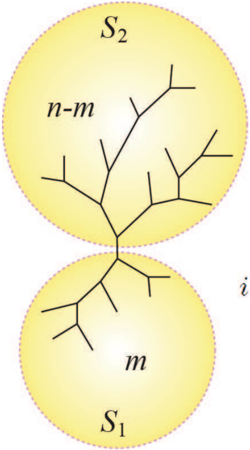


Question 2. If we use branch and bound to optimize on the region bounded by split faces of the BME polytope, are we guaranteed to get a valid tree?





Split faces; split facets.

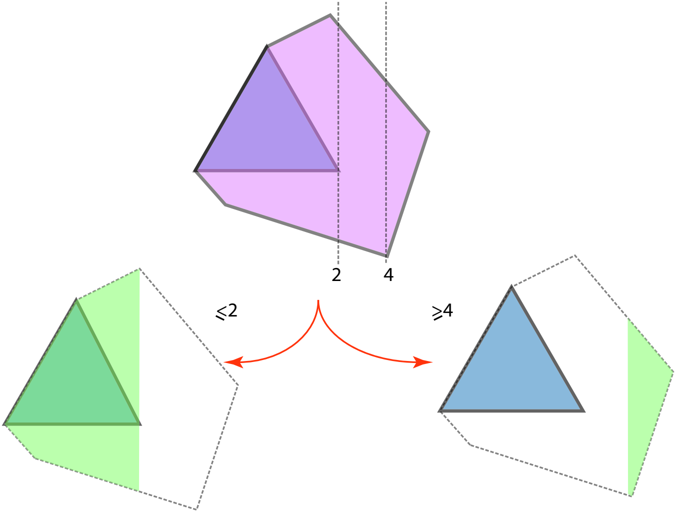


$$\sum_{i<j,\ \text{leaves}\ i,j \in S_1} x_{ij} \leq (m-1)2^{n-3}$$

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, $m > 2, n > 5$	$2^{n-1} - \binom{n}{2} - n - 1$	$(2(n-m)-3)!! \times (2m-3)!!$

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`

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

Thanks!

Questions and comments?

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