Counting Points in Polytopes and Models of Phylogenetic Trees

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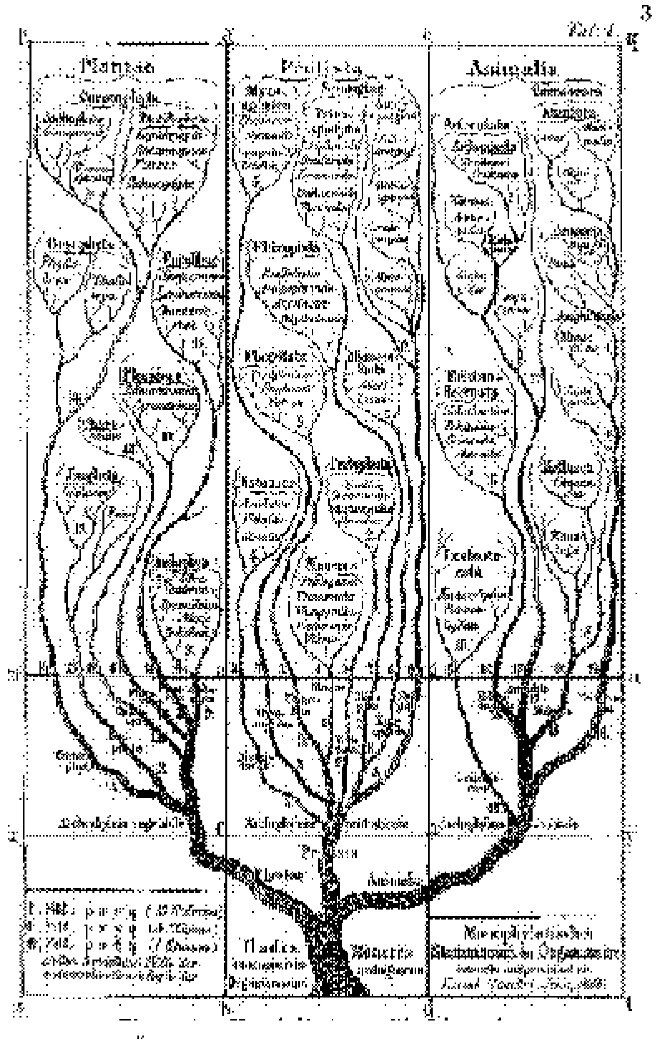
- Banach/Tarski: mathematicians look for analogies between theorems, theories . . . and analogies
- Poincaré: poets use different words for the same thing, mathematicians use the same words for different things

phylogenetics

Phylogenetics: re-constructing historical relation between species by analyzing their *present* features and putting their common ancestors in a diagram which forms a tree. [e.g. Häckel, 1866]



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- counting lattice points in polytopes and their fiber products
- networks of paths in a tree
- Markov processes on a tree (phylogenetics)
- group actions and quotients

⋆ product of functions

For a positive integer n let $[n] = \{0, \dots n\}$.
Function $f : [n] \to \mathbb{Z}$ is symmetric if for every $k \in [n]$ it holds $f(k) = f(n-k)$.
By $\mathbf{1} : [n] \to \mathbb{Z}$ denote the unit function.

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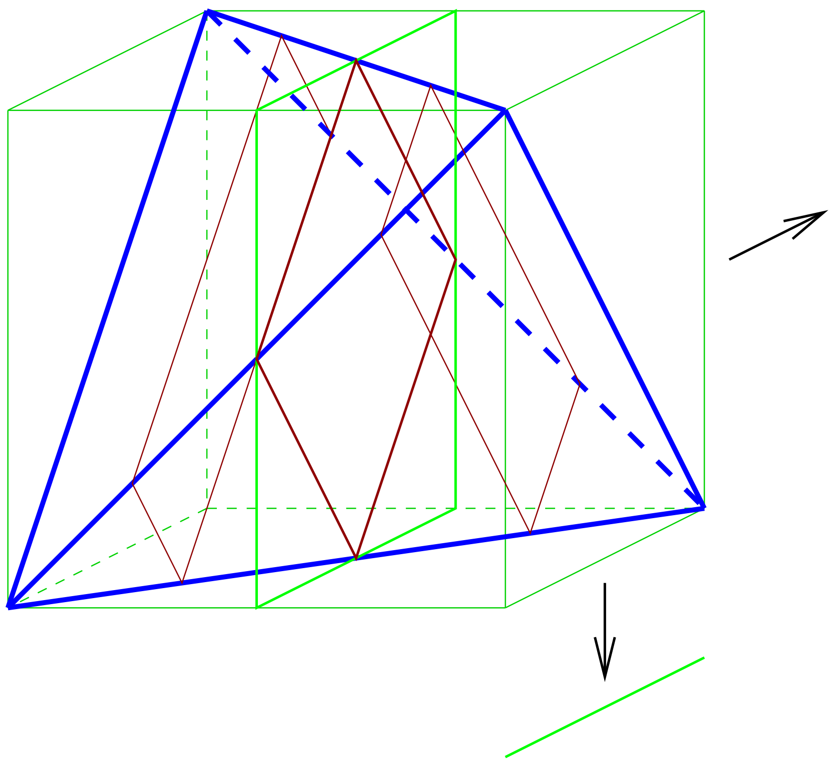
By $\mathbf{1} : [n] \to \mathbb{Z}$ denote the unit function.
If $f_1\ f_2 : [n] \to \mathbb{Z}$ are symmetric functions then we define their symmetric product $f_1 \star f_2 : [n] \to \mathbb{Z}$ such that for $k \le n/2$:

$$(f_1 \star f_2)(k) = 2 \cdot \left(\sum_{i=0}^{k-1} \sum_{j=0}^{i} f_1(i) f_2(k+i-2j) \right) + \left(\sum_{i=k}^{n-k} \sum_{j=0}^{k} f_1(i) f_2(k+i-2j) \right)$$

geometric interpretation of $\star$



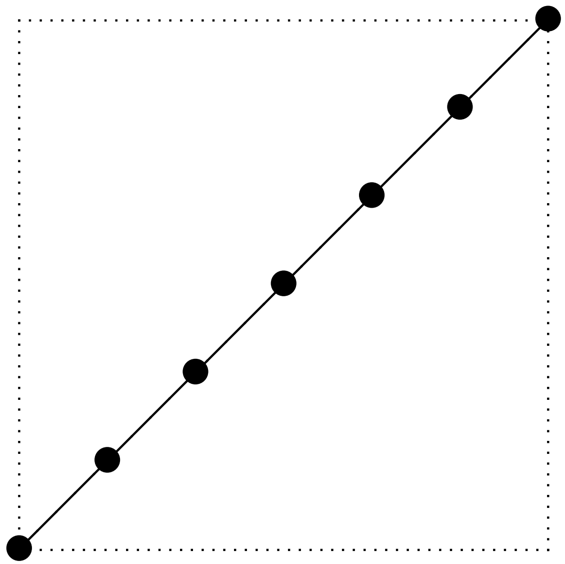
Consider the simplex Δ as in the picture

$(f_1 \star f_2)(k)$ is equal to the sum of products of f_1 and f_2 counted over points of lattice spanned by Δ in k-th slice of $n \cdot \Delta$

$(\mathbf{1} \star \mathbf{1})(k) = (k+1)(n-k+1)$ is the number of lattice points in k-th slice of $n \cdot \Delta$

travel trough $6 \cdot \Delta$

$k = 0$



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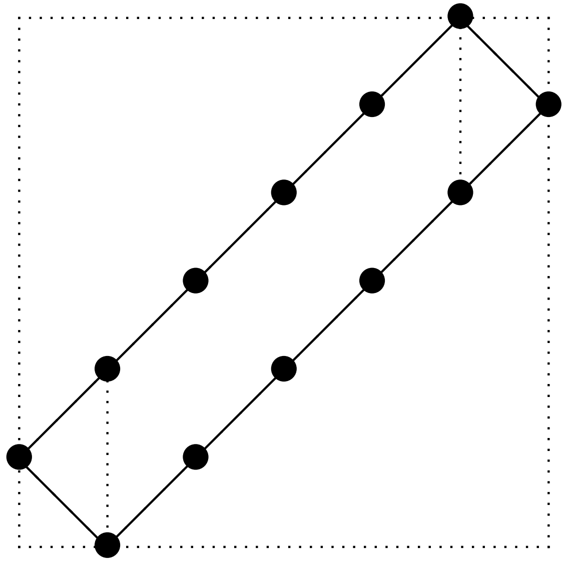
$k = 1$



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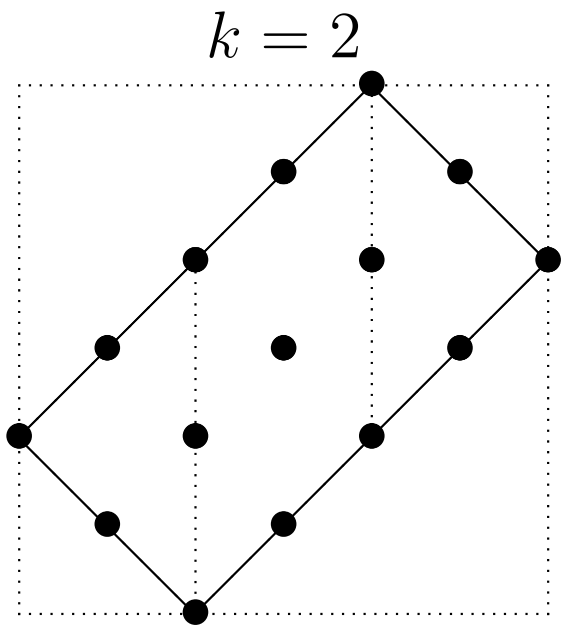

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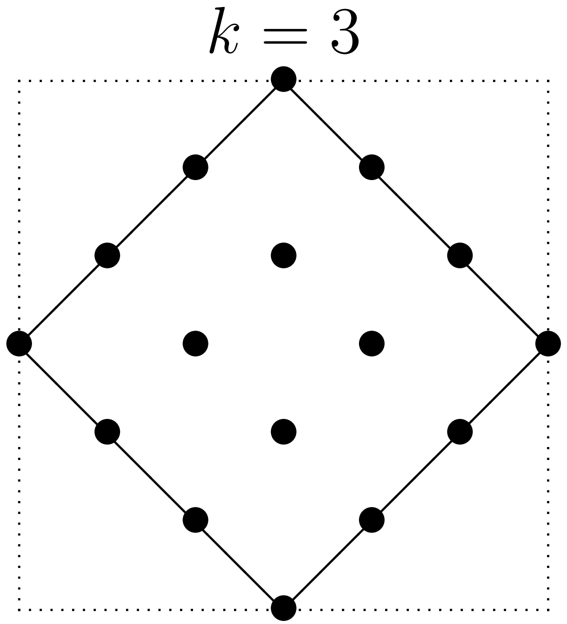

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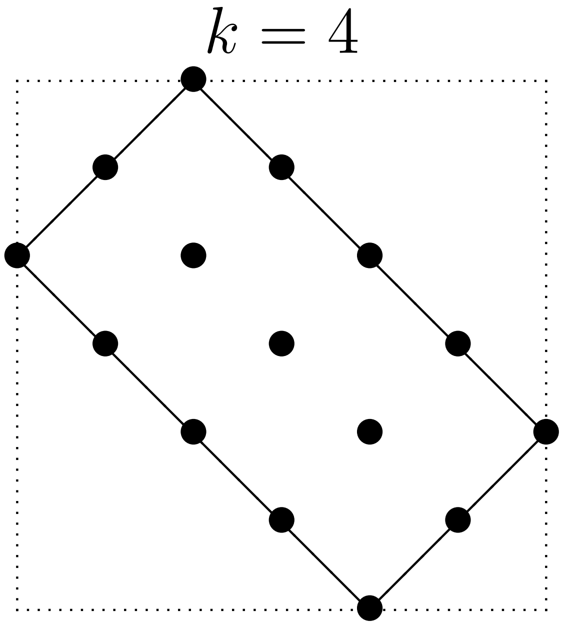

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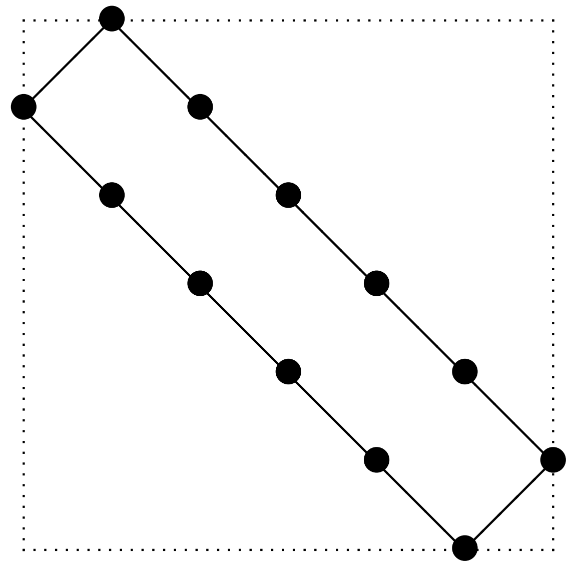

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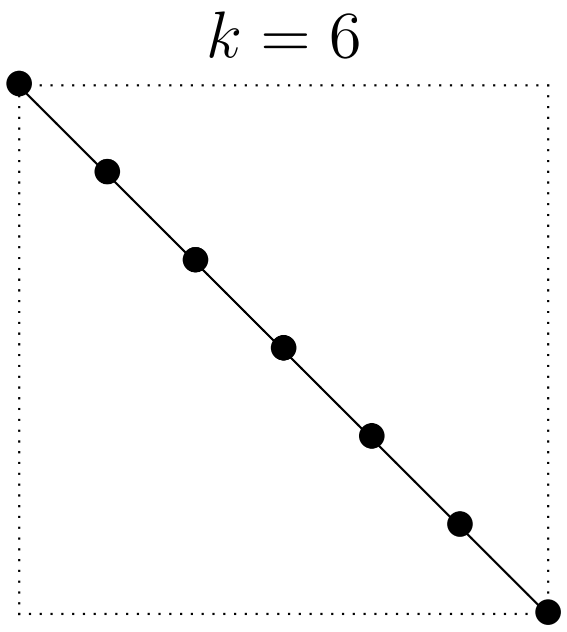

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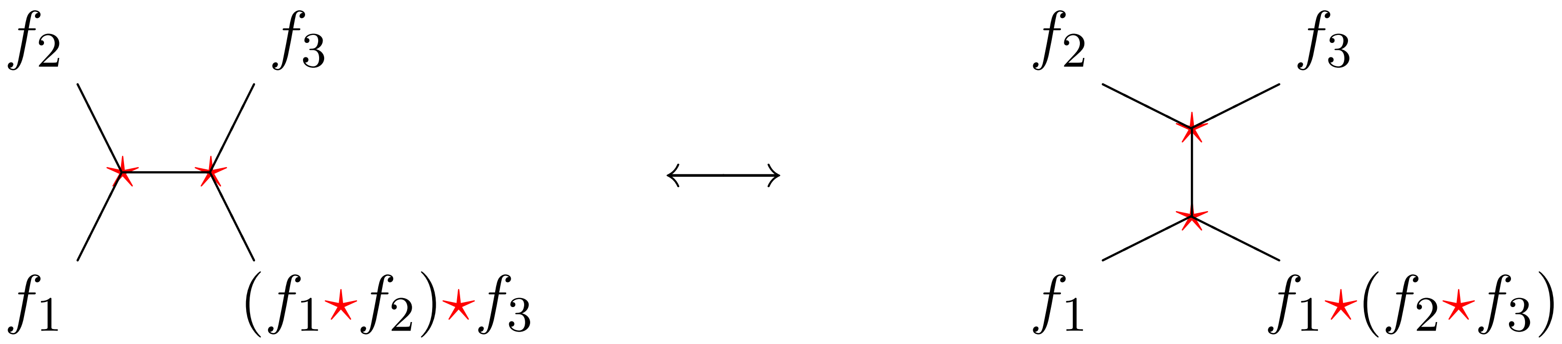
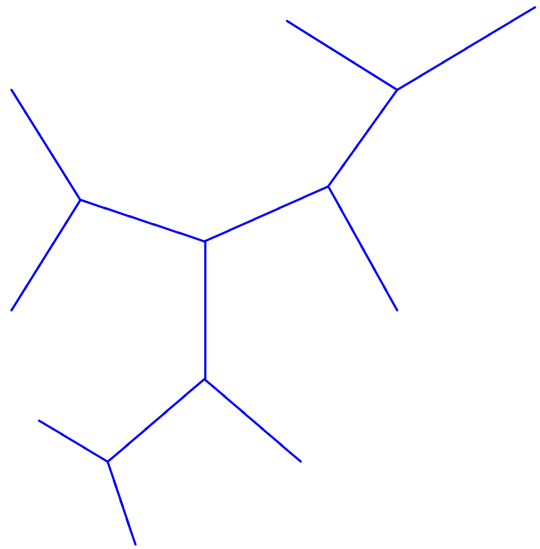
- 

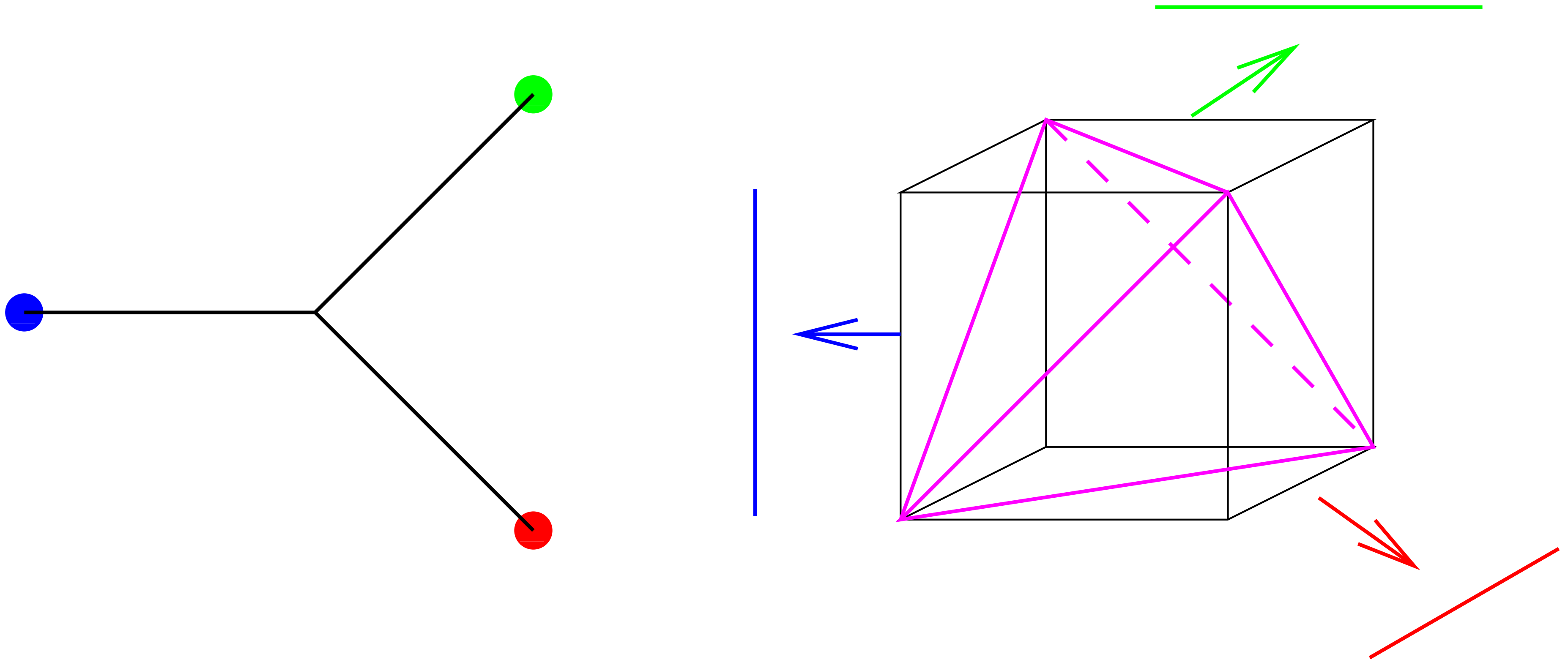
tree→polytope

Consider a tree $\mathcal{T}$ which has $2d-3$ edges in set $\mathcal{E}$, and $2d-2$ vertices in $\mathcal{V}$ including d leaves in $\mathcal{L}$ and $d-2$ inner trivalent nodes in $\mathcal{N}$.



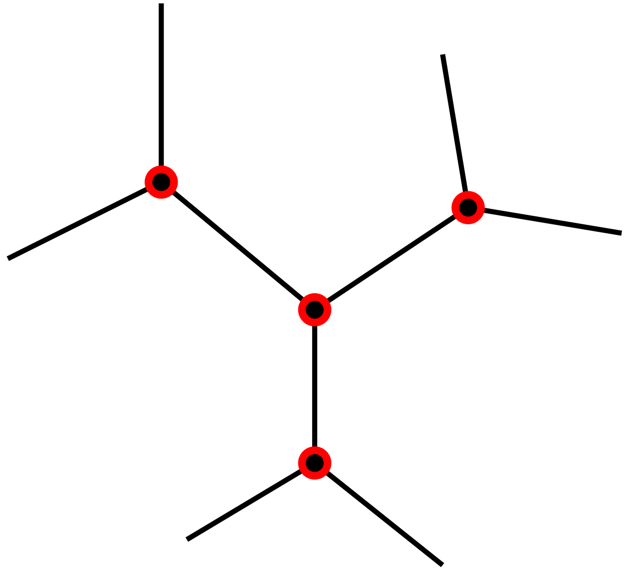
tree→polytope

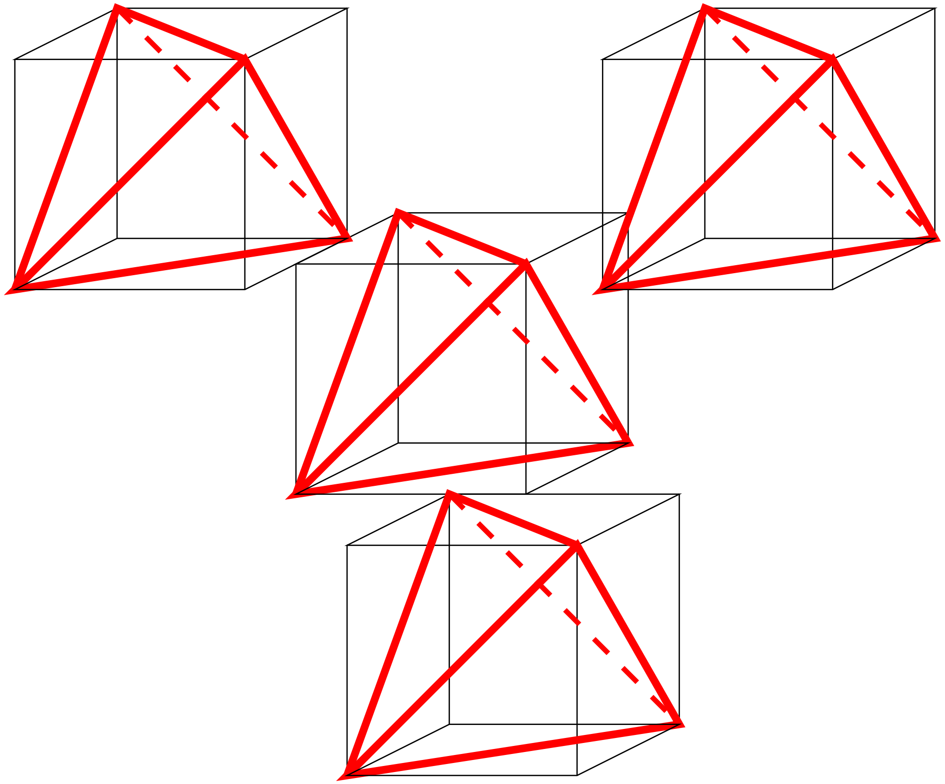
Basic example: tripod tree which we associate with a tetrahedron with three projections, each one for one leaf.



tree→polytope

Constructing a polytope $\Delta(\mathcal{T}) \subset [0,1]^{|\mathcal{E}|}$ via fibered products of tetrahedra according to relations coming from inner edges of the tree.





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If Δ is a polytope with vertices in a lattice M then define function counting lattice points

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The lattice M for $\Delta(\mathcal{T})$ is generated by its vertices.

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(!!) Observation: the polynomial

$$\eta_{\Delta(\mathcal{T}),M}(t)$$

does not depend on the shape of $\mathcal{T}$ but only on the number $|\mathcal{L}|$.

tree$\rightarrow$variety (1)

Given a lattice polytope Δ in $M_{\mathbb{R}}$ we consider a cone $\Sigma(\Delta)$ in $(M \times \mathbb{Z})_{\mathbb{R}}$ which is spanned by the set $\Delta \times \{1\}$.

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Given a lattice polytope Δ in $M_{\mathbb{R}}$ we consider a cone $\Sigma(\Delta)$ in $(M \times \mathbb{Z})_{\mathbb{R}}$ which is spanned by the set $\Delta \times \{1\}$. Next define a graded algebra $A(\Delta) = \bigoplus_{t \geq 0} A^t$ where A^t is a $\mathbb{C}$-vector space with basis

$$\left\{ \chi^{(u,t)} : (u,t) \in \Sigma(\Delta) \cap M \times \mathbb{Z} \right\}$$

and multiplication is defined as follows:

$$\chi^{(u_1,t_1)} \cdot \chi^{(u_2,t_2)} = \chi^{(u_1+u_2,t_1+t_2)}$$

tree→variety (1)

The algebra $X(\Delta(\mathcal{T}))$ is generated by its first gradation (!!) and we define a projective variety

$$X(\mathcal{T}) = Proj(A(\Delta(\mathcal{T})))$$

which we call a model of the tree $\mathcal{T}$.

sockets and networks

Given a trivalent tree $\mathcal{T}$ a *socket* of $\mathcal{T}$ is a subset of $\mathcal{L}$ which has even number of elements; a *path* in $\mathcal{T}$ is a connected union of edges with ends in $\mathcal{L}$; a *network* is a set of non-meeting paths in $\mathcal{T}$.

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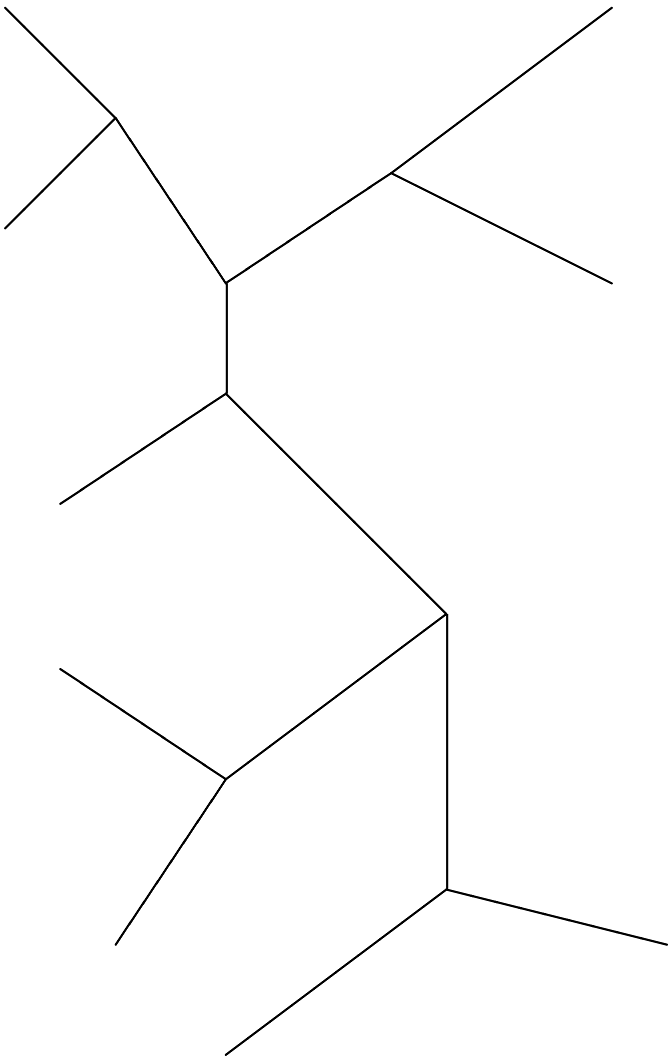

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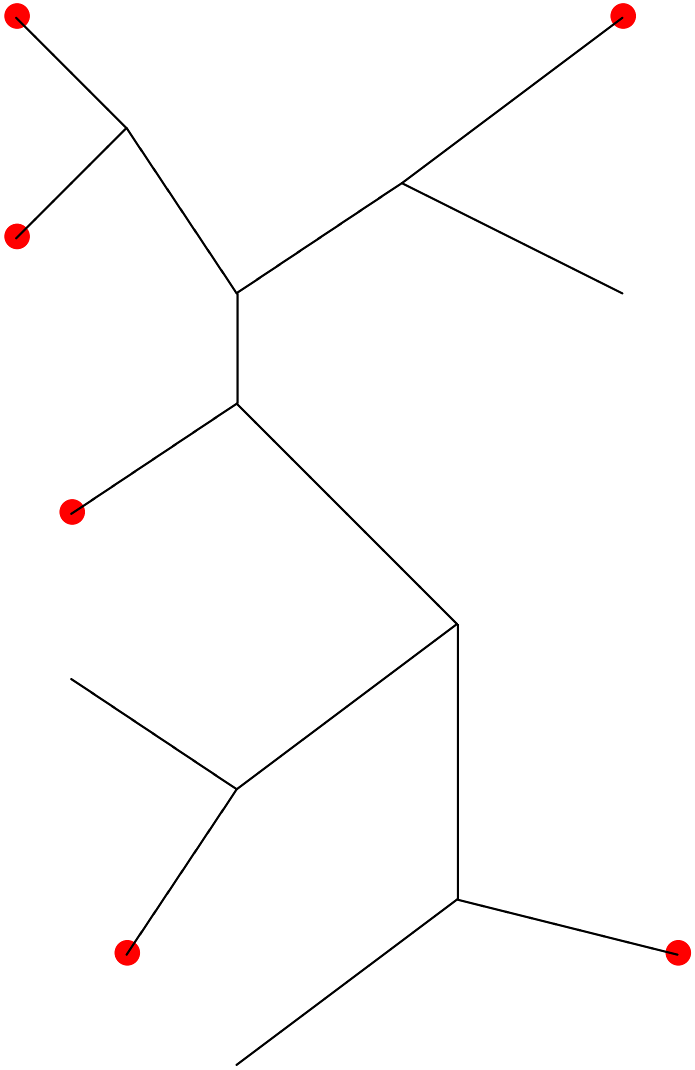

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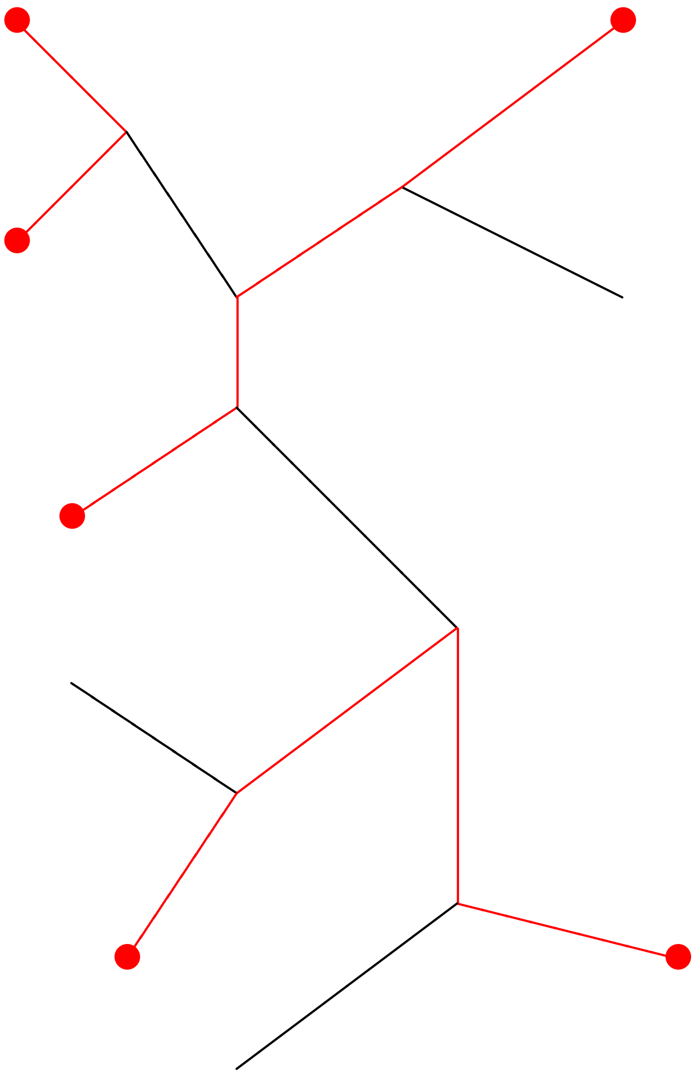

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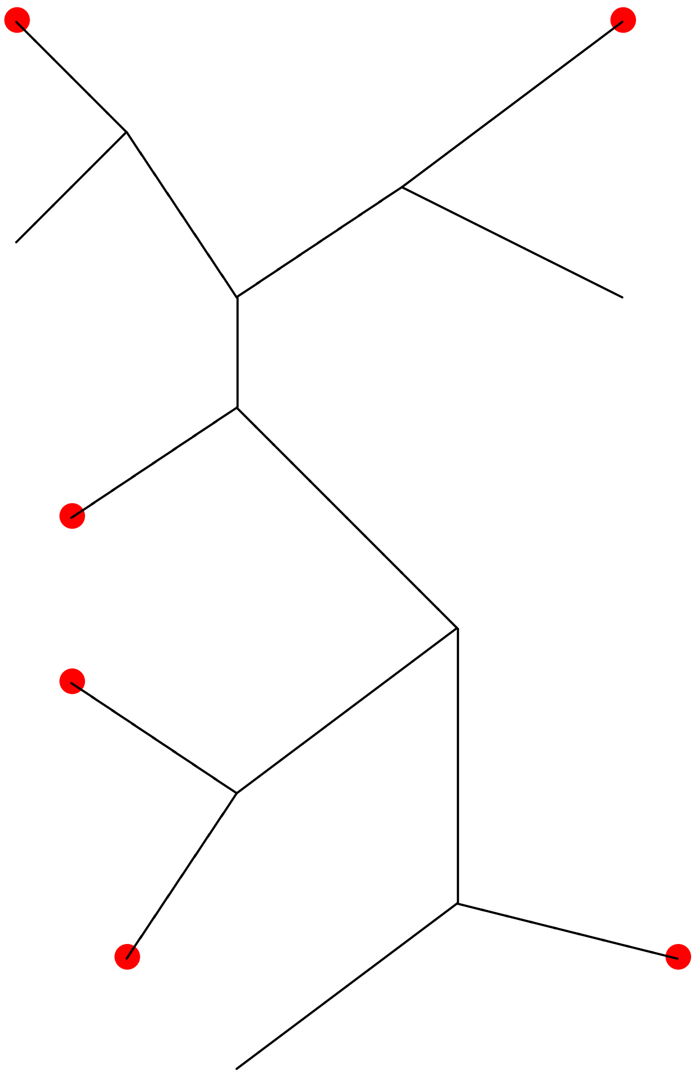

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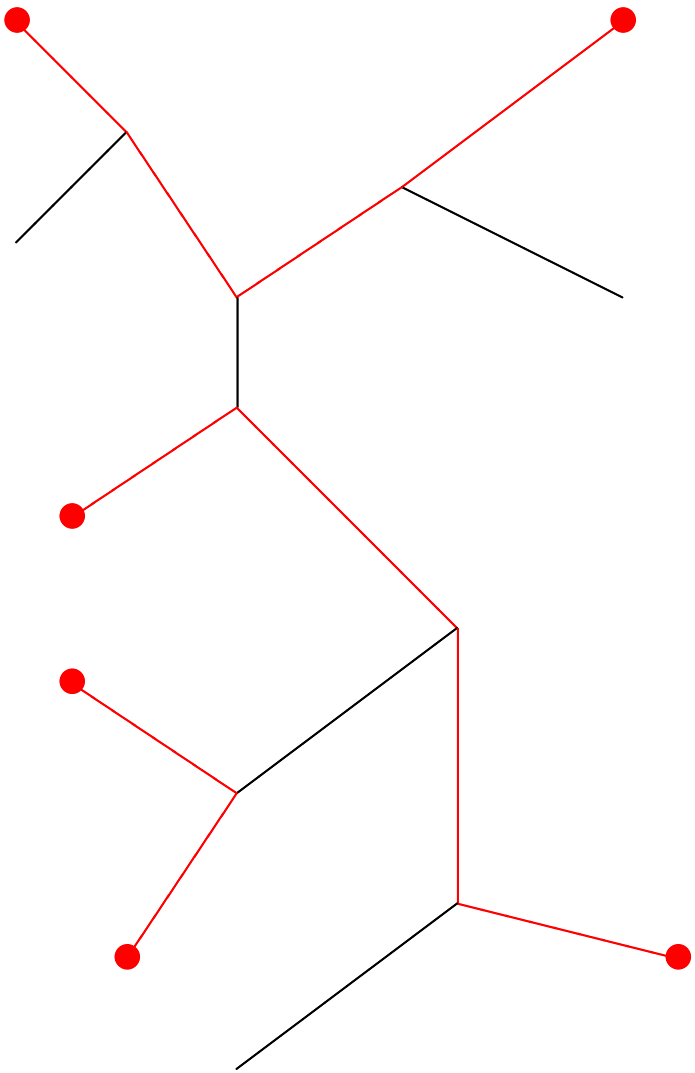

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For every edge $e \in \mathcal{E}$ we consider a $\mathbb{P}^1_e$ with homogeneous coordinates $[y_0^e, y_1^e]$.

Moreover consider a projective space $\mathbb{P}_\Sigma$ of dimension $2^{d-1} - 1$ with homogeneous coordinates $[z_\sigma]$ indexed by sockets of $\mathcal{T}$.

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Define rational map $\prod_{e\in\mathcal{E}} \mathbb{P}^1_e \rightarrow \mathbb{P}_\Sigma$ such that

$$z_\sigma = \prod_{e\in\mu(\sigma)} y_1^e \cdot \prod_{e\notin\mu(\sigma)} y_0^e$$

The closure of the image of this map is the model of the tree, $X(\mathcal{T}) \subset \mathbb{P}_\Sigma$ and $\dim X(\mathcal{T}) = 2d-3$.

deforming $X(\mathcal{T})$ within $\mathbb{P}_\Sigma$

Leaves of $\mathcal{T}$ can be labeled by numbers $1, \ldots, d$ or, equivalently, given d points we can make them leaves of a (non-unique) tree $\mathcal{T}$.

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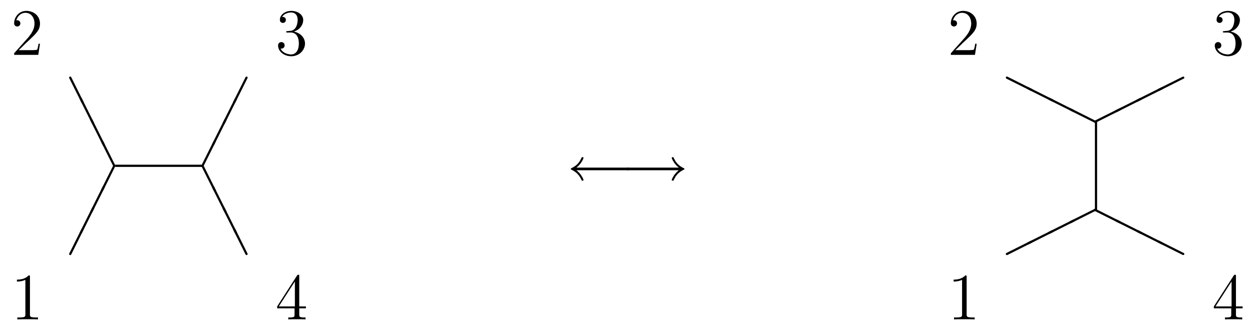

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These varieties can be non-isomorphic (check it), however (!!) they are in the same connected component of the Hilbert scheme of $\mathbb{P}_\Sigma$, that is $X(\mathcal{T}_1)$ can be deformed to $X(\mathcal{T}_2)$ if only $\mathcal{T}_1$ and $\mathcal{T}_2$ have the same number of leaves.

binary Markov process on tree

Fix a root r in tree $\mathcal{T}$ - this implies an order $<$ on the set of vertexes $\mathcal{V} = \mathcal{L} \cup \mathcal{N}$. To each vertex $v \in \mathcal{V}$ assign a random variable ξ_v which takes value in $\{\alpha_1, \alpha_2\}$.

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For each edge $e = \langle u, v \rangle$ bounded by vertexes $u < v$ define the transition matrix A^e:

$$A^e_{ij} = P(\xi_v = \alpha_j | \xi_u = \alpha_i)$$

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and set the probability of the variable ξ_r at the root:
$P^r_i = P(\xi_r = \alpha_i)$

from Markov to phylogenetics

For a Markov process on a rooted tree $\mathcal{T}$ as above

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For a Markov process on a rooted tree $\mathcal{T}$ as above and any function $\mathcal{V} \ni v \rightarrow \rho(v) \in \{1,2\}$

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where the sum is taken over all $\widehat{\rho} : \mathcal{V} \to \{1, 2\}$ which extend ρ.

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Phylogenetics: understand the shape of $\mathcal{T}$ by looking at the distribution of $P(\bigwedge_{v \in \mathcal{L}} \xi_v = \alpha_{\rho(v)})$.

tree→variety (3)

Consider the locus of possible probability values of a Markov process on a fixed tree $\mathcal{T}$

$$\mathcal{X}(\mathcal{T}) :=$$
$$\{\zeta_\rho = P(\bigwedge_{v\in\mathcal{L}} \xi_v = \alpha_{\rho(v)}) : A^e_{ij}, P^r_i \text{ are arbitrary}\}$$

in the simplex with coordinates ζ_ρ where $\zeta_\rho \geq 0$, $\sum_\rho \zeta_\rho = 1$.

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then [theorem, Sturmfels, Sullivant] after suitable change of coordinates and replacing the simplex with the projective space varieties $\mathcal{X}(\mathcal{T})$ and $X(\mathcal{T})$ coincide.

examples

Leaves of $\mathcal{T}$ are labeled by numbers $1, \ldots, d$ and sockets are denoted by $0/1$ sequence of length d. Edges are labeled by letters.

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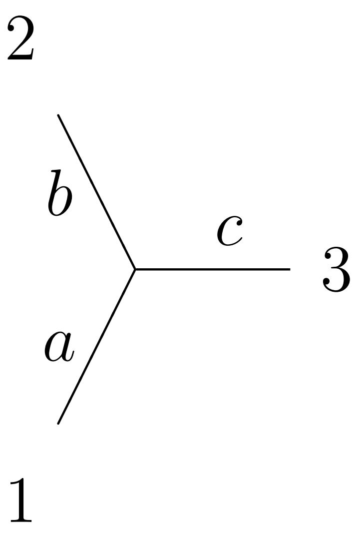
Tripod tree model:

$$\mathbb{P}^1_a \times \mathbb{P}^1_b \times \mathbb{P}^1_c \to \mathbb{P}^3$$

$$z_{000} = y^a_0 y^b_0 y^c_0 \quad z_{110} = y^a_1 y^b_1 y^c_0$$
$$z_{101} = y^a_1 y^b_0 y^c_1 \quad z_{011} = y^a_0 y^b_1 y^c_1$$



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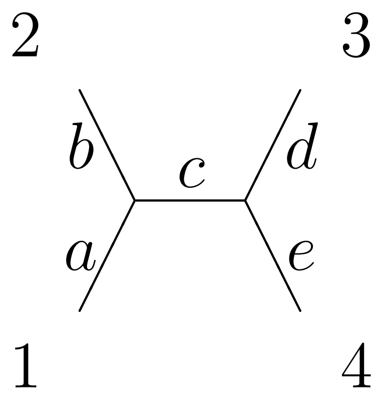
Four leaf tree model in $\mathbb{P}^7$

$$
\begin{array}{ll}
z_{0000} = y_0^a y_0^b y_0^c y_0^d y_0^e & z_{1111} = y_1^a y_1^b y_0^c y_1^d y_1^e \\
z_{1100} = y_1^a y_1^b y_0^c y_0^d y_0^e & z_{0011} = y_0^a y_0^b y_0^c y_1^d y_1^e \\
z_{1010} = y_1^a y_0^b y_1^c y_1^d y_0^e & z_{1001} = y_1^a y_0^b y_1^c y_0^d y_1^e \\
z_{0110} = y_0^a y_1^b y_1^c y_1^d y_0^e & z_{0101} = y_0^a y_1^b y_1^c y_0^d y_1^e
\end{array}
$$



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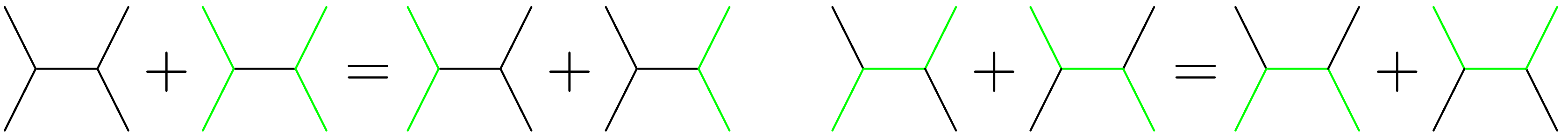
Leaves of $\mathcal{T}$ are labeled by numbers $1, \ldots, d$ and sockets are denoted by $0/1$ sequence of length d. Edges are labeled by letters.
Therefore $X(\rangle\!-) \simeq \mathbb{P}^3$ and $X(\rangle\!-\!\langle)$ is a complete intersection in $\mathbb{P}^7$:

$$z_{0000}z_{1111} = z_{1100}z_{0011} \qquad z_{1010}z_{0101} = z_{1001}z_{0110}$$



tree→variety (4)

On $\mathbb{P}^3$ with homogeneous coordinates $[z_{000}, z_{110}, z_{101}, z_{011}]$ we distinguish three actions of $\mathbb{C}^*$ whose weights are determined by socket $0/1$ sequences, for example:

$$\lambda_1(t)[z_{000}, z_{110}, z_{101}, z_{011}] = [z_{000}, tz_{110}, tz_{101}, z_{011}]$$

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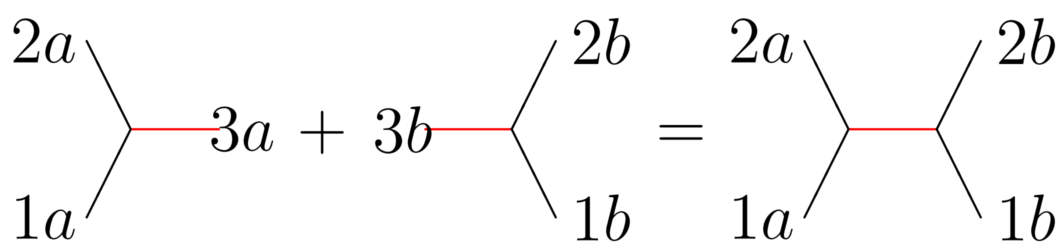
$$\lambda_1(t)[z_{000}, z_{110}, z_{101}, z_{011}] = [z_{000}, tz_{110}, tz_{101}, z_{011}]$$

Trivalent trees can be built from tripods (here denoted by letters) by identifying edges of leaves:



tree→variety (4)

On $\mathbb{P}^3$ with homogeneous coordinates $[z_{000}, z_{110}, z_{101}, z_{011}]$ we distinguish three actions of $\mathbb{C}^*$ whose weights are determined by socket $0/1$ sequences, for example:

$$\lambda_1(t)[z_{000}, z_{110}, z_{101}, z_{011}] = [z_{000}, tz_{110}, tz_{101}, z_{011}]$$

Respectively, take quotient $\mathbb{P}^3_a \times \mathbb{P}^3_b // (\lambda_{3a} \cdot \lambda_{3b}^{-1})$

$$([z^a_{000}, z^a_{110}, z^a_{101}, z^a_{011}], [z^b_{000}, z^b_{110}, z^b_{101}, z^b_{011}]) \to$$
$$[z^a_{000}z^b_{000}, z^a_{000}z^b_{110}, z^a_{110}z^b_{000}, z^a_{110}z^b_{110}, z^a_{101}z^b_{101},$$
$$z^a_{101}z^b_{011}, z^a_{011}z^b_{101}, z^a_{011}z^b_{011}]$$

equivariant subvarieties

There is a $\mathbb{C}^*$ action associated to leaf l on $\mathbb{P}_\Sigma$: its weight on the coordinate z_σ is $1/0$ depending on whether l is in the socket σ or not.

This defines an action of torus $T_\mathcal{L}$ whose coordinates are leaves of $\mathcal{T}$.

The variety $X(\mathcal{T}) \subset \mathbb{P}_\Sigma$ is $T_\mathcal{L}$ equivariant.

equivariant subvarieties

As argued before, $X(\rangle\!\!-\!\!\langle)$ is a complete intersection of quadrics in $\mathbb{P}^7$:

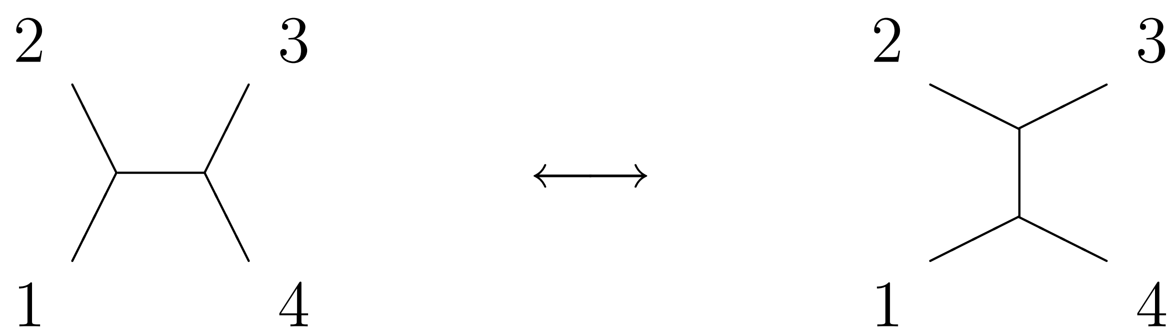
$$z_{0000}z_{1111} \quad = \quad z_{1100}z_{0011} \qquad z_{1010}z_{0101} \quad = \quad z_{1001}z_{0110}$$

thus it is defined by pencil in a linear system of $T_{\mathcal{L}}$ equvariant quadrics spanned by

$$z_{0000}z_{1111} \quad z_{1100}z_{0011} \quad z_{1010}z_{0101} \quad z_{1001}z_{0110}$$

equivariant subvarieties

Hence we get a $T_{\mathcal{L}}$ equivariant deformation

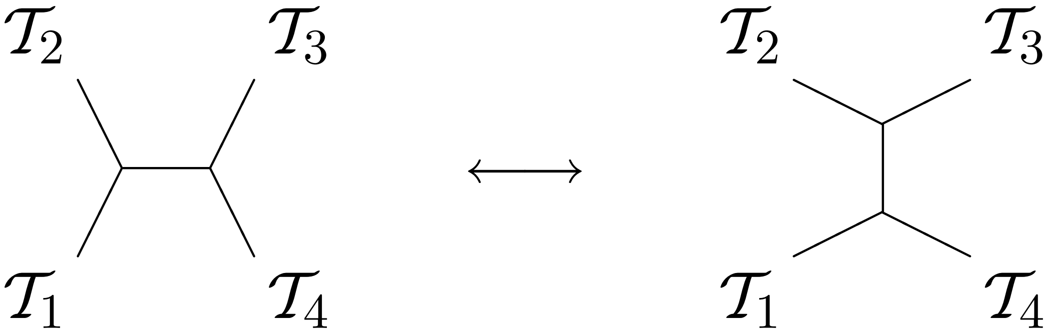


$$z_{0000}z_{1111} = z_{1100}z_{0011} \qquad z_{0000}z_{1111} = z_{1001}z_{0110}$$

$$z_{1010}z_{0101} = z_{1001}z_{0110} \qquad z_{1100}z_{0011} = z_{1010}z_{0101}$$

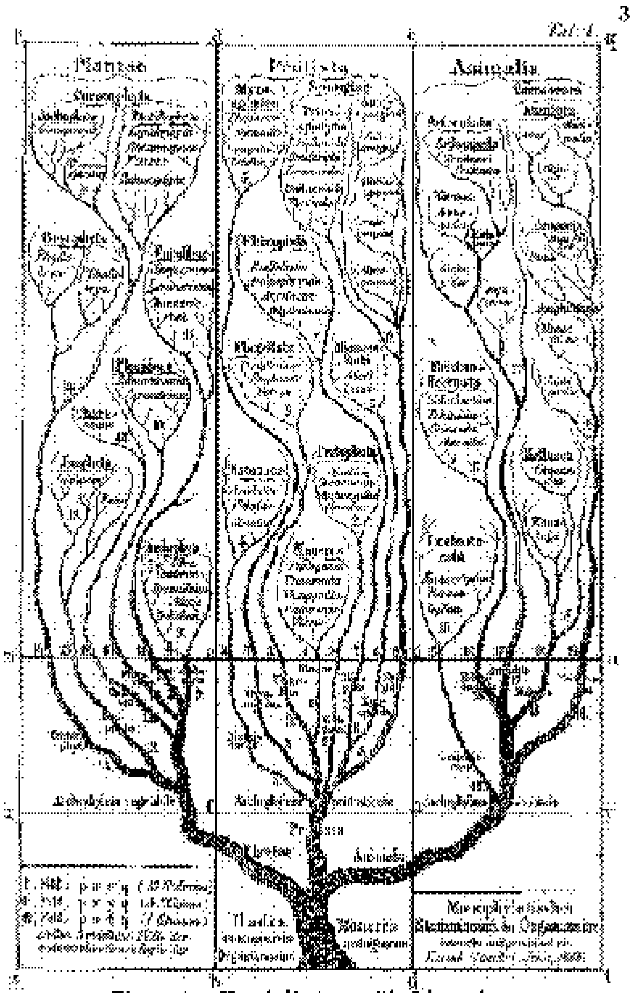
equivariant subvarieties

Because of the quotient construction this can be applied to produce deformation of respective models of trees who differ by "elementary transformation" along an inner edge.



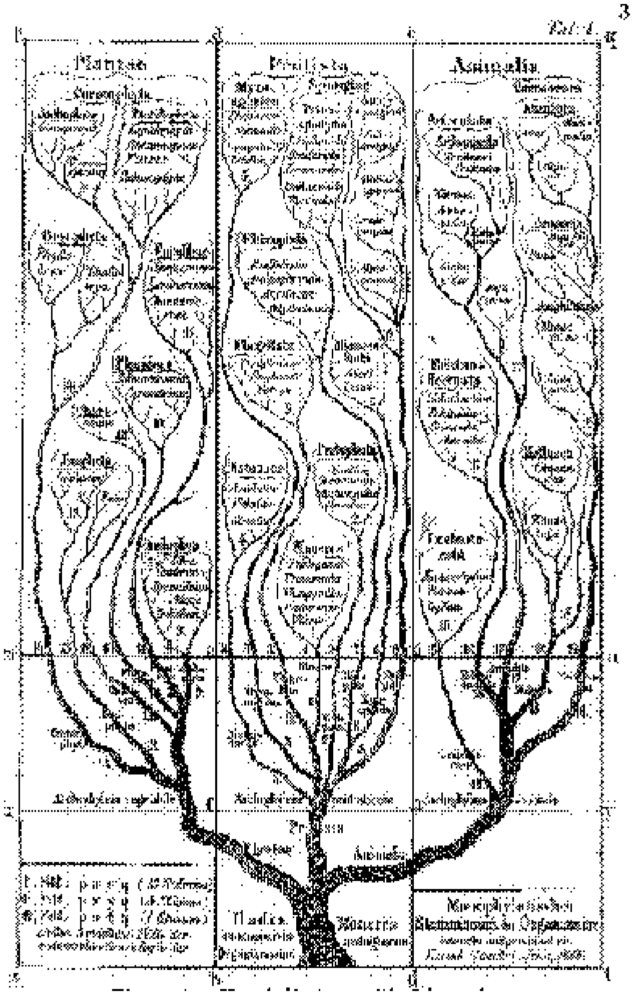
epilogue: an analogy

Biology: XIX century

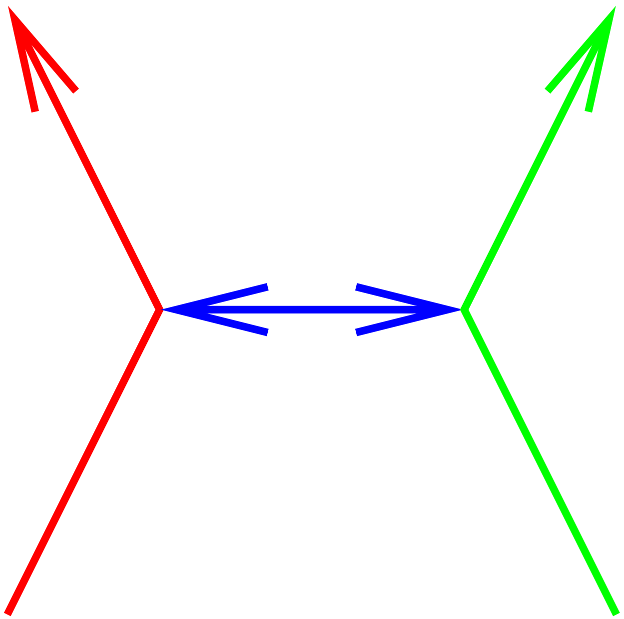


epilogue: an analogy

Biology: XIX century

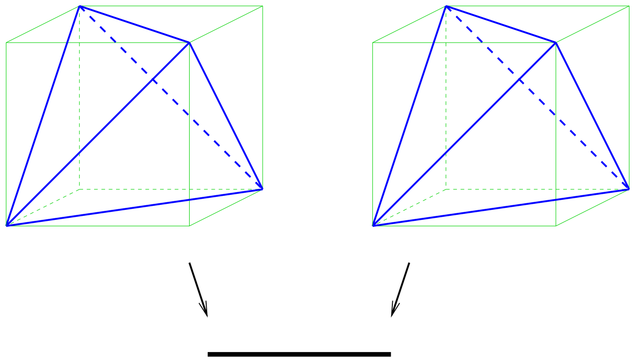


Physics: XX century



epilogue: an analogy

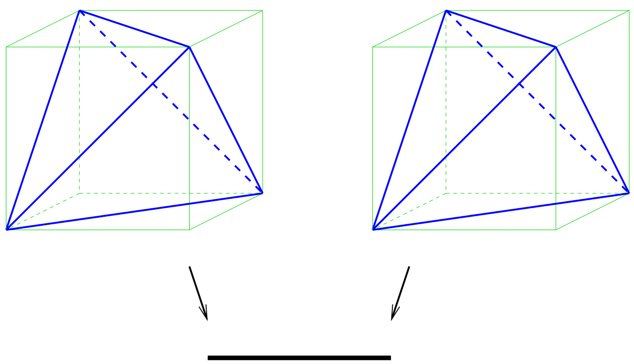
Algebraic models of phylogenetic trees.



Deformations, moduli?

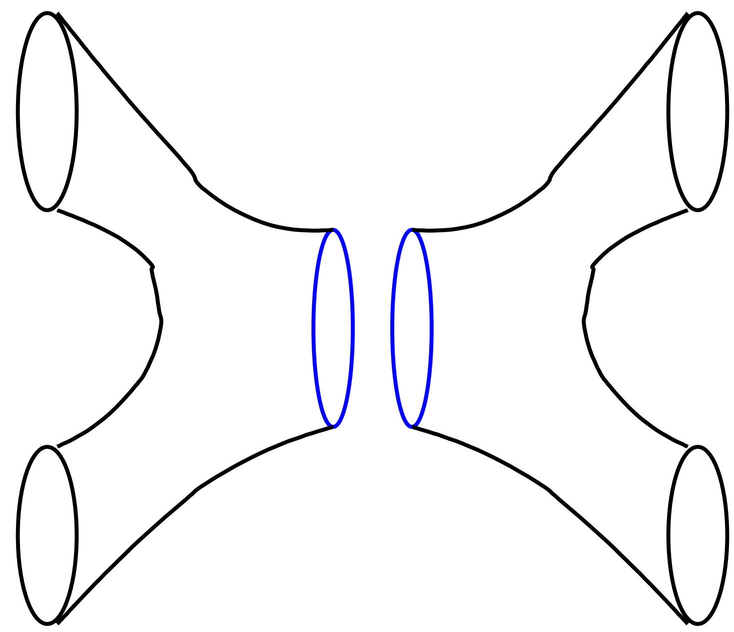
epilogue: an analogy

Algebraic models of phylogenetic trees.



Deformations, moduli?

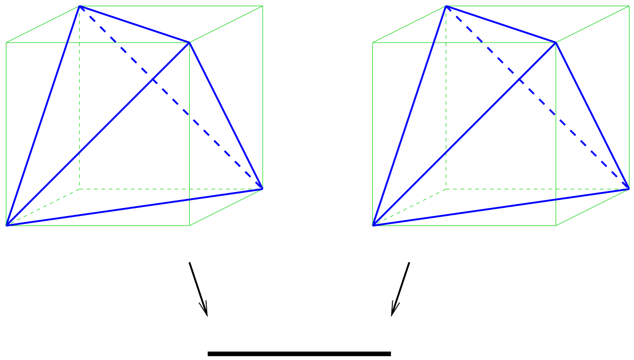
Riemann surfaces, algebraic (pointed) curves.



Moduli of stable pointed curves $\overline{\mathcal{M}}_{0,n}$

epilogue: an analogy

Algebraic models of phylogenetic trees.

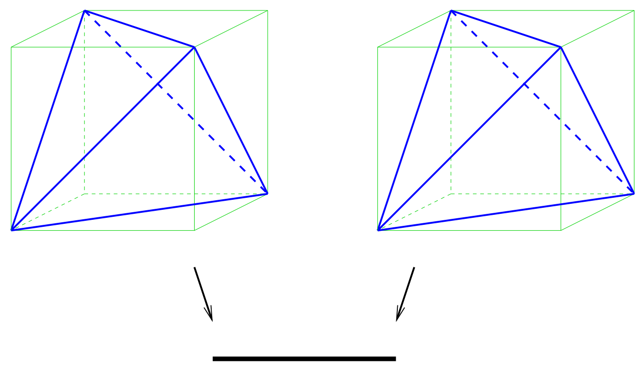


Deformations, moduli?

Sturmfels-Xu: models of trees deform to proj. of Cox rings on moduli of parabolic bundles on pointed curves (Nagata, Mukai, Castravet, Tevelev).

epilogue: an analogy

Algebraic models of phylogenetic trees.



Deformations, moduli?

Sturmfels-Xu: models of trees deform to proj. of Cox rings on moduli of parabolic bundles on pointed curves (Nagata, Mukai, Castravet, Tevelev).

Proof depends on Verlinde formula (physics !).