The EM Fixed Point Ideal and the Nonnegative Tensor Rank

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Nonnegative tensor rank

Rank-one tensor: an outer product of vectors

$$\left(\begin{array}{cc|cc} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}\right) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\left(\begin{array}{cc|cc} 0 & 1 & 0 & 1 \\ 0 & 2 & 0 & 2 \end{array}\right) = \begin{pmatrix} 1 \\ 2 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

A tensor has nonnegative rank (rank_+) at most r if it can be written as a sum of r nonnegative tensors of rank one:

$$P = P_1 + P_2 + \ldots + P_r,$$

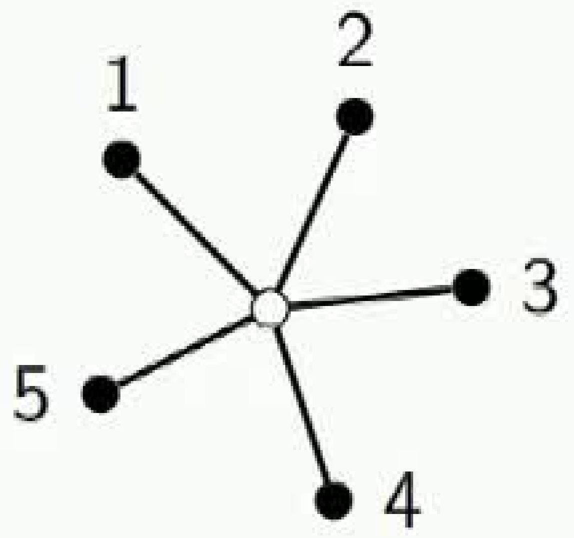
where $P_1, P_2, \ldots, P_r$ are nonnegative tensors of rank 1.

A tensor of nonnegative rank 2:

$$\left(\begin{array}{cc|cc} 1 & 1 & 0 & 1 \\ 0 & 2 & 0 & 2 \end{array}\right) = \left(\begin{array}{cc|cc} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}\right) + \left(\begin{array}{cc|cc} 0 & 1 & 0 & 1 \\ 0 & 2 & 0 & 2 \end{array}\right)$$

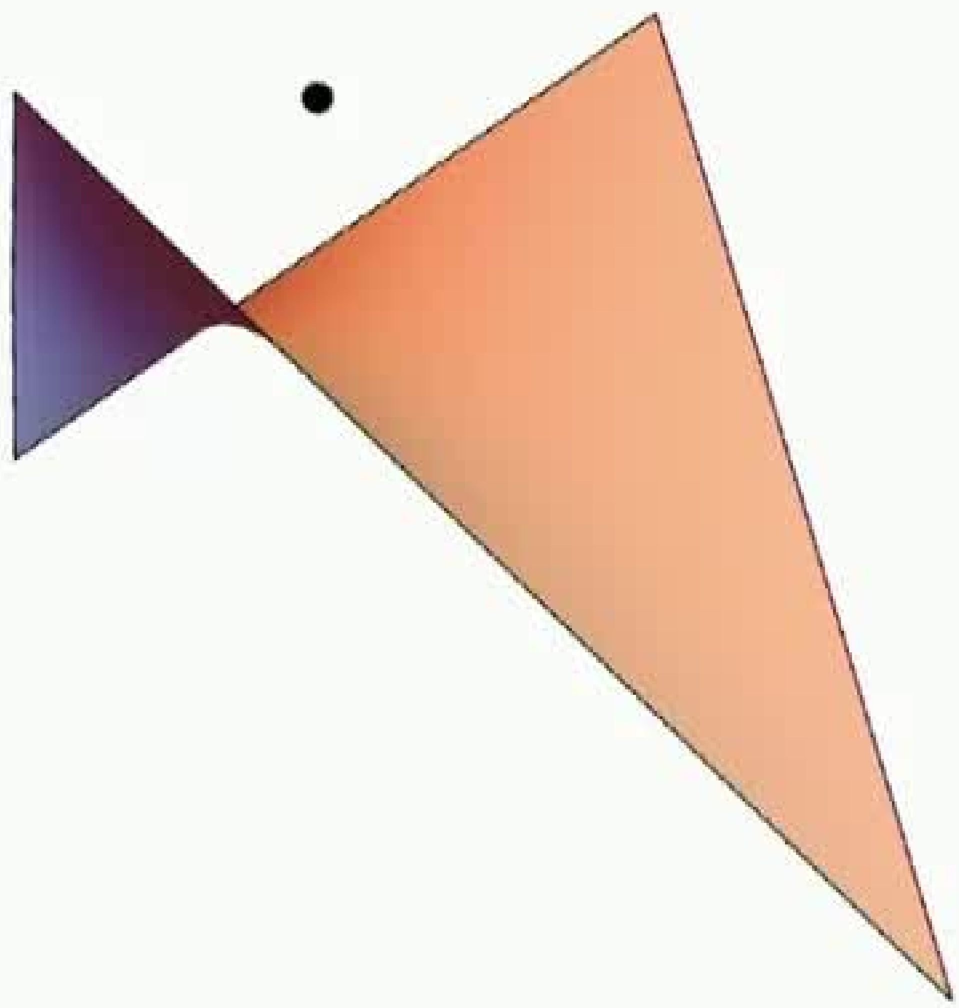
Latent class models

In statistics, the model of normalized tensors of nonnegative rank at most r is the latent class model.



Binary latent class model $\mathcal{M}_n$: $2 \times 2 \times 2 \cdots \times 2$ tensors of nonnegative rank at most two and entries summing to one (of order n)

Maximum likelihood estimation



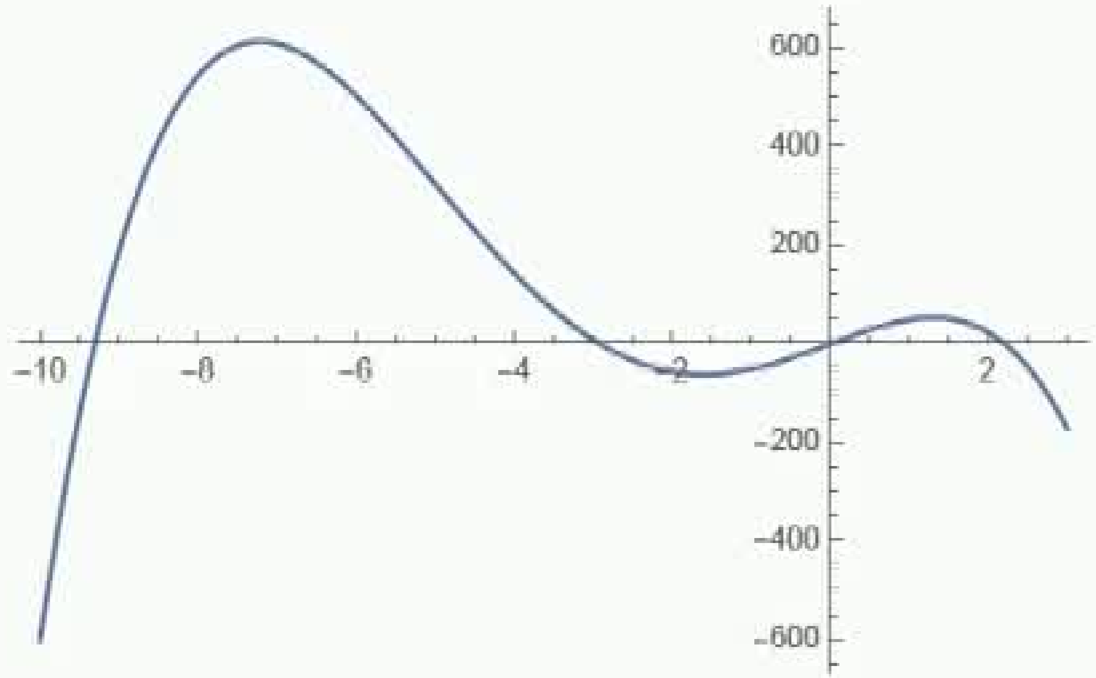
statistical model + data

$\Downarrow$

find the point of the statistical model that best explains the data

Challenges of MLE

- In general, MLE is a non-convex optimization problem.



- The MLE can lie in the interior or on the boundary
- Sometimes: MLE is an explicit function of the observed data
- Often: MLE is found numerically using optimization methods
- Standard numerical methods find a local maximum

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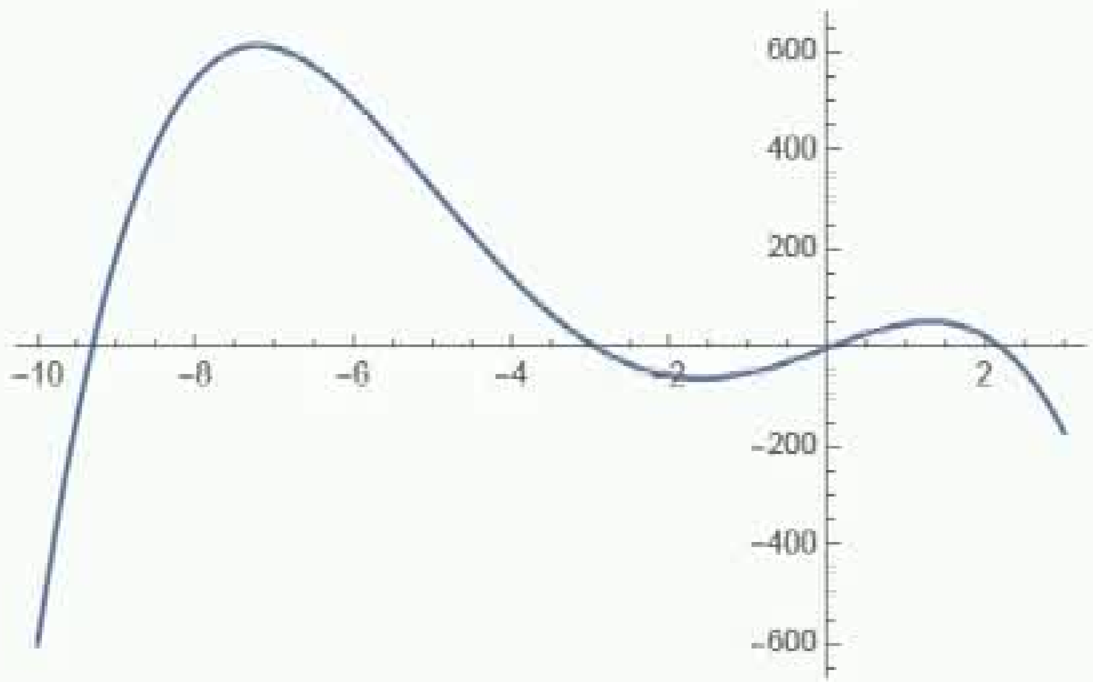

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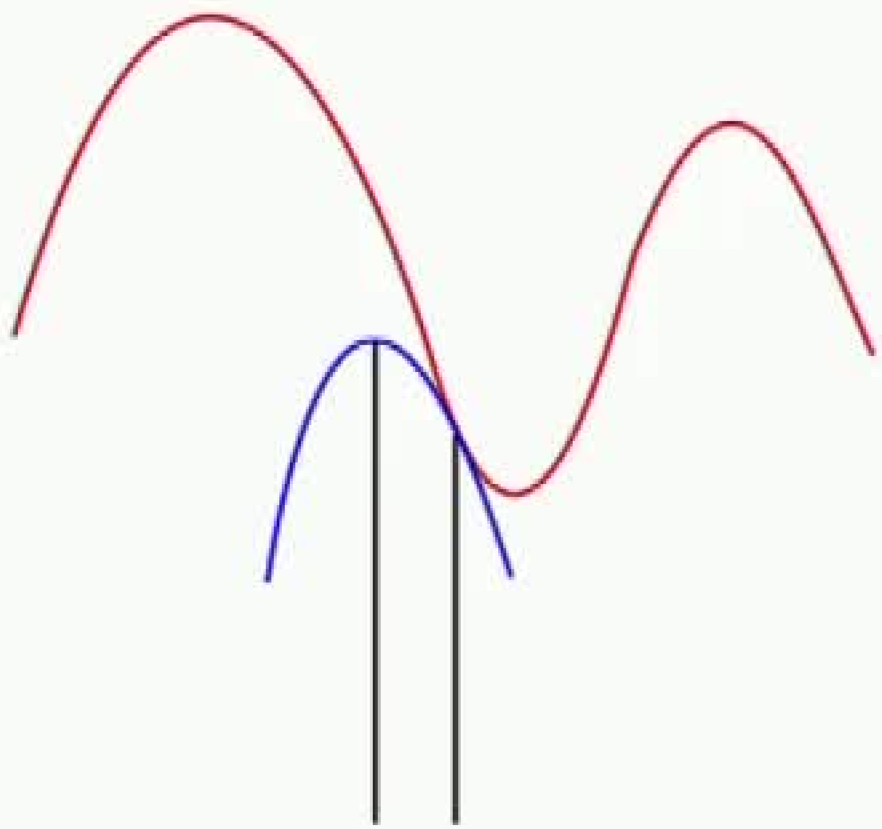
EM algorithm



Initialize parameters.
Run until parameters converge.
E-step: Bound the log-likelihood function below by a simple concave function.
M-step: Maximize the concave function.

Parametrization of the binary latent class model

Let $P = (p_{ijk})$ be a $2 \times 2 \times 2$ tensor. It has nonnegative rank at most 2 if there exist three nonnegative matrices

$$A = \begin{pmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{pmatrix}, B = \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix}, C = \begin{pmatrix} c_{00} & c_{01} \\ c_{10} & c_{11} \end{pmatrix}$$

such that

$$p_{ijk} = a_{0i} b_{0j} c_{0k} + a_{1i} b_{1j} c_{1k}.$$

The parameter space of the $2 \times 2 \times 2$ tensors of nonnegative rank at most two is $\Theta := \mathbb{R}^{12}_{\geq 0}$ with elements

$$(a_{00}, \ldots, a_{11}, b_{00}, \ldots, b_{11}, c_{00}, \ldots, c_{11}).$$

EM algorithm

Input: Observed data tensor $U \in \mathbb{Z}^{d_1 \times d_2 \times d_3}$.
Output: A proposed maximum $\hat{P} \in \Delta_{d_1 d_2 d_3 - 1}$ of the log-likelihood function ℓ on the model $\mathcal{M}_{d_1 \times d_2 \times d_3, r}$.

Step 0: Select random $(\lambda_1, \ldots, \lambda_r) \in \Delta_{r-1}$, $(a_{i1}, \ldots, a_{id_1}) \in \Delta_{d_1 - 1}$, $(b_{i1}, \ldots, b_{id_2}) \in \Delta_{d_2 - 1}$, and $(c_{i1}, \ldots, c_{id_3}) \in \Delta_{d_3 - 1}$ for $i = 1, \ldots, r$.
Run the following steps until the entries of the $d_1 \times d_2 \times d_3$-tensor $P = (p_{ijk})$ converge.
E-Step: *Estimate the $r \times d_1 \times d_2 \times d_3$-table that represents the expected hidden data:*
Set $v_{lijk} := \frac{\lambda_l a_{li} b_{lj} c_{lk}}{\sum_{l=1}^{r} \lambda_l a_{li} b_{lj} c_{lk}} u_{ijk}$ for $l = 1, \ldots, r$, $i = 1, \ldots, d_1$, $j = 1, \ldots, d_2$, and $k = 1, \ldots, d_3$.
M-Step: *Maximize the likelihood function of the model for the hidden data:*
Set $\lambda_l := \sum_{i=1}^{d_1} \sum_{i=1}^{d_2} \sum_{i=1}^{d_3} v_{ijkl}/u_{+++}$ for $l = 1, ..., r$.
Set $a_{li} := \sum_{j=1}^{d_2} \sum_{k=1}^{d_3} v_{ijkl}/(u_{+++}\lambda_l)$ for $l = 1, \ldots, r$, $i = 1, \ldots, d_1$.
Set $b_{lj} := \sum_{i=1}^{d_1} \sum_{k=1}^{d_3} v_{ijkl}/(u_{+++}\lambda_l)$ for $l = 1, \ldots, r$, $j = 1, \ldots, d_2$.
Set $c_{lk} := \sum_{i=1}^{d_1} \sum_{j=1}^{d_2} v_{ijkl}/(u_{+++}\lambda_l)$ for $l = 1, \ldots, r$, $k = 1, \ldots, d_3$.
Update *the estimate of the joint distribution for our mixture model:*
Set $p_{ijk} := \sum_{l=1}^{r} \lambda_l a_{li} b_{lj} c_{lk}$ for $i = 1, \ldots, d_1$, $j = 1, \ldots, d_2$, $k = 1, \ldots, d_3$.
Return P.

EM fixed point ideal

- An EM fixed point for an observed data tensor U is a parameter vector in Θ which stays fixed after one iteration of the EM algorithm.
- An element of Θ to which the EM-algorithm can converge to for some random starting point is an EM fixed point.
- The minimal set of polynomial equations that all EM fixed points satisfy are called the EM fixed point equations.
- They define the EM fixed point ideal.

EM fixed point ideal

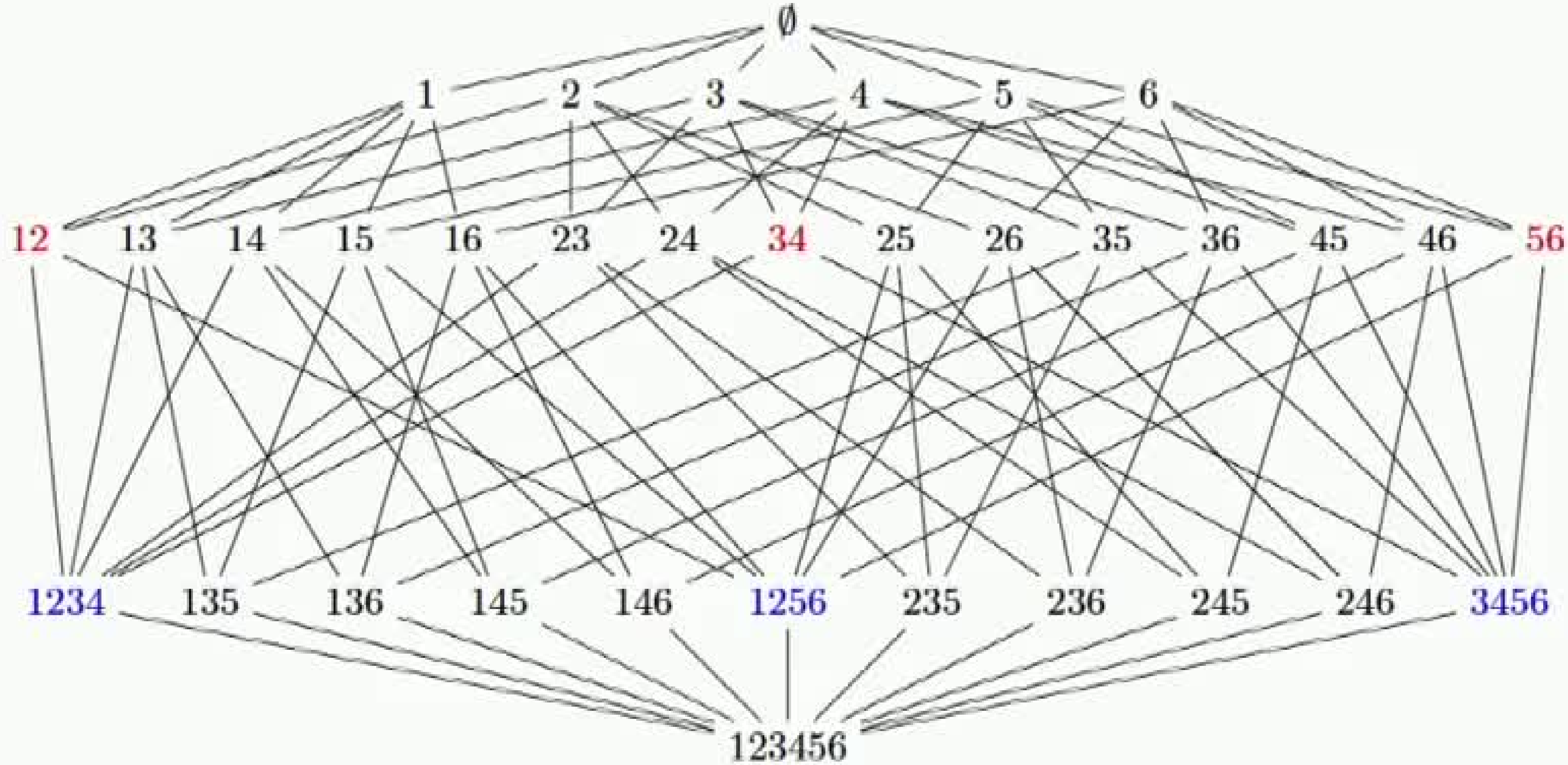
Theorem

The radical of the EM fixed point ideal $\mathcal{F}$ for $\mathcal{M}_3$ has precisely 63 relevant primes consisting of 9 orbital classes.

Table: Minimal primes of EM fixed point ideal for $2 \times 2 \times 2$ tensors of $\text{rank}_+ \leq 2$.

Class S	|S|	a's	b's	c's	deg	codim	rA	rB	rC	orbit
$\{\emptyset\}$	0	0	0	0	60	7	1	1	1	1
	0	0	0	0	48	7	2	2	1	1
	0	0	0	0	48	7	2	1	2	1
	0	0	0	0	48	7	1	2	2	1
	0	0	0	0	1	8	2	2	2	1
$\{a_{00}\}$	1	1	0	0	5	8	2	2	2	12
$\{a_{00}, a_{11}\}$	2	2	0	0	25	8	2	2	2	6
$\{a_{00}, b_{00}\}$	2	1	1	0	11	8	2	2	2	24
$\{a_{00}, b_{00}, c_{00}\}$	3	1	1	1	23	8	2	2	2	16

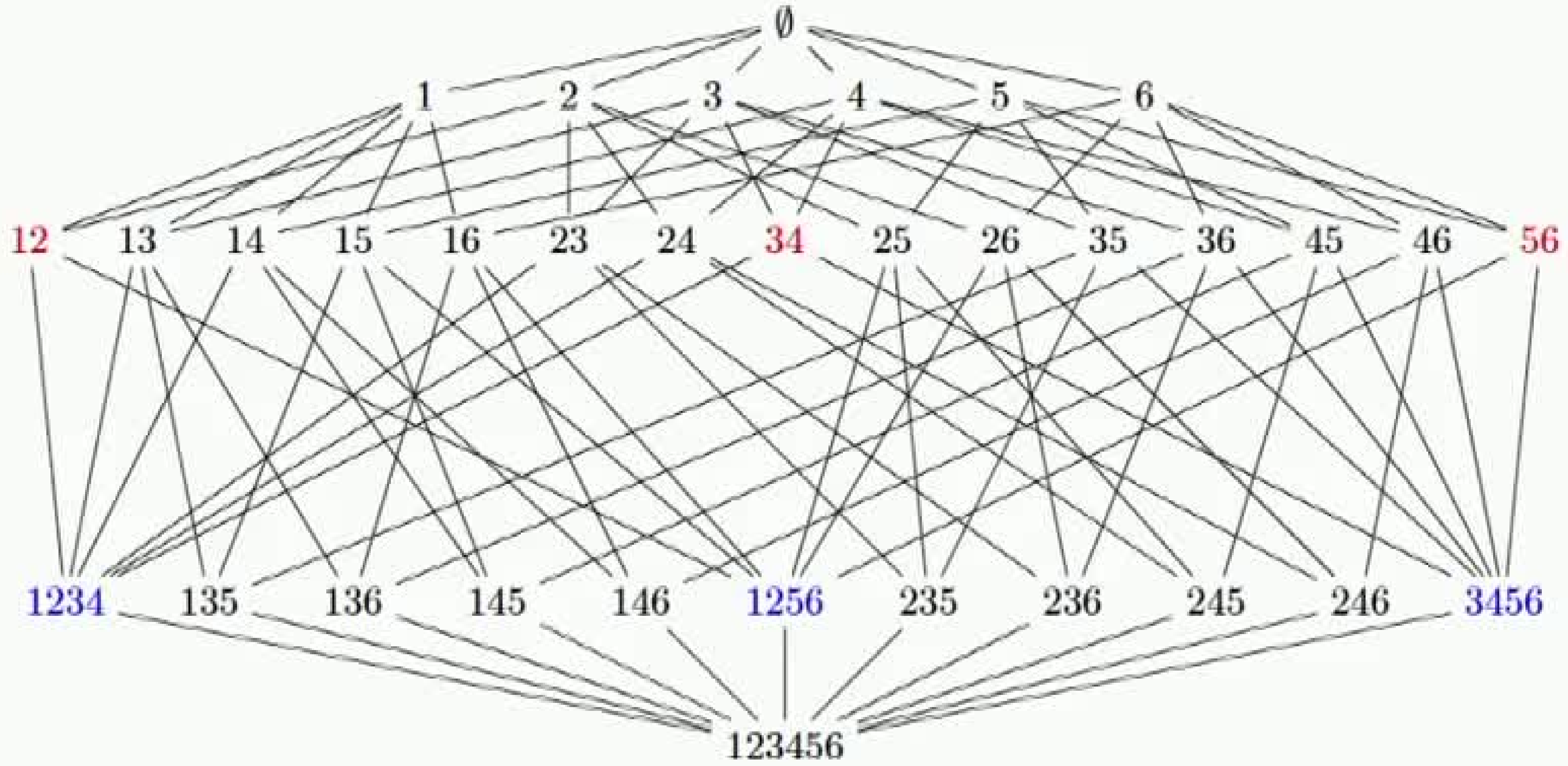
Boundary stratification



Proposition

The dimension of the model $\mathcal{M}_n$ is $2n+1$. The boundary of this semi-algebraic set is defined by $2n$ irreducible components.

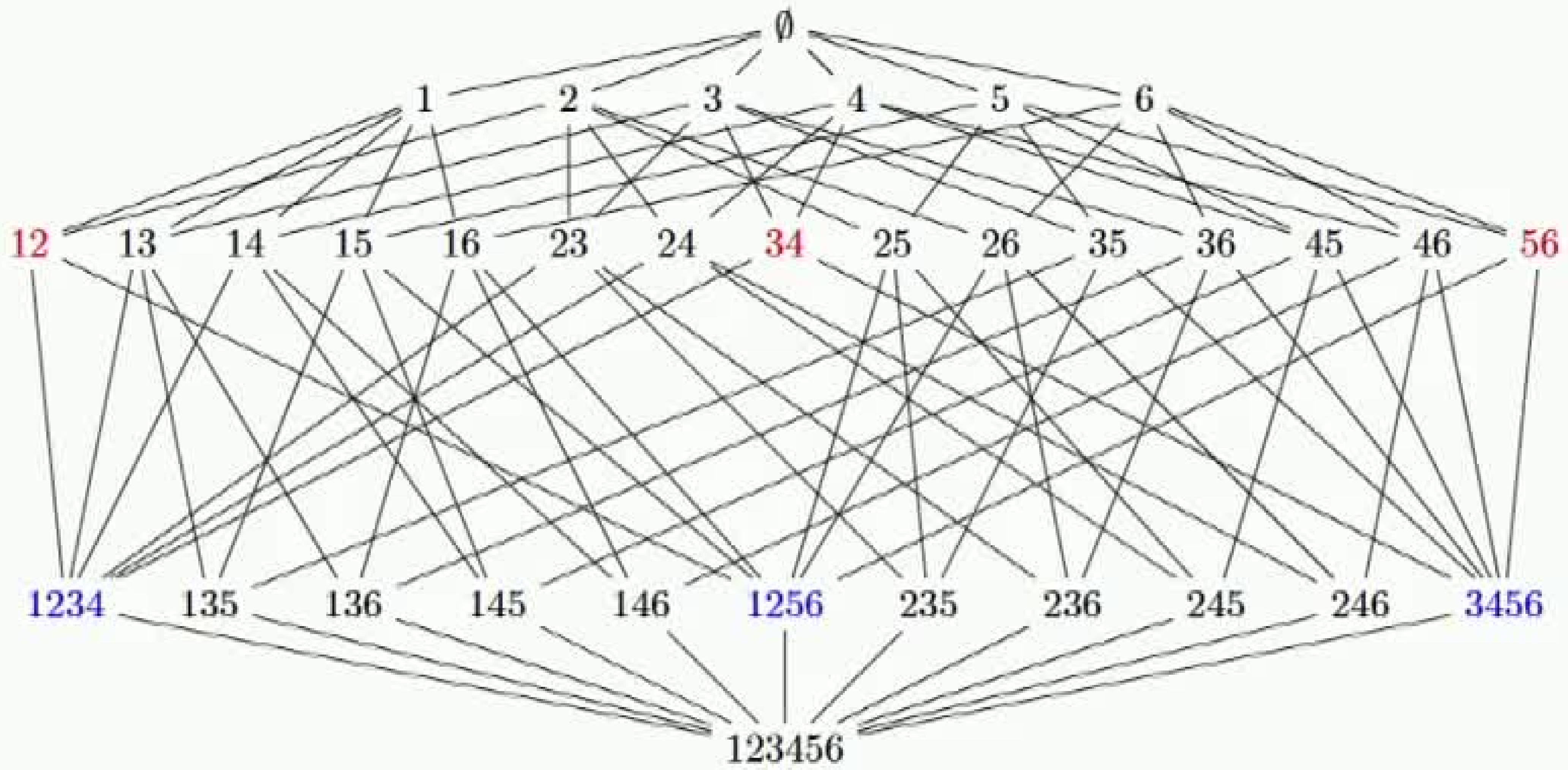
Boundary stratification



Theorem

For $n \leq k \leq 2n+1$, the k-dimensional strata of the nondegenerate part of $\mathcal{M}_n$ are in bijection with the $k-(n+1)$-dimensional faces of the cube C_n, except for $k = 2n-1$ when n additional strata are present, and for $k = n+1$ when $\binom{n}{2}$ additional strata are present.

Class S	|S|	a's	b's	c's	deg	codim	rA	rB	rC	orbit	type
$\{\emptyset\}$	0	0	0	0	60	7	1	1	1	1	3-dimensional
	0	0	0	0	48	7	2	2	1	1	4-dimensional
	0	0	0	0	48	7	2	1	2	1	4-dimensional
	0	0	0	0	48	7	1	2	2	1	4-dimensional
	0	0	0	0	1	8	2	2	2	1	7-dimensional
$\{a_{11}\}$	1	1	0	0	5	8	2	2	2	12	6-dimensional
$\{a_{11}, a_{22}\}$	2	2	0	0	25	8	2	2	2	6	5-dimensional
$\{a_{11}, b_{11}\}$	2	1	1	0	11	8	2	2	2	24	5-dimensional
$\{a_{11}, b_{11}, c_{11}\}$	3	1	1	1	23	8	2	2	2	16	4-dimensional



Example

Consider the minimal prime of the EM fixed point ideal corresponding to $a_{11} = a_{22} = 0$:

$$\begin{aligned} I_1 = \langle & a_{22}, a_{11}, r_{212}r_{221} - r_{211}r_{222}, c_{11}r_{221} + c_{12}r_{222}, b_{11}r_{212} + b_{12}r_{222}, c_{11}r_{211} + c_{12}r_{212}, \\ & b_{11}r_{211} + b_{12}r_{221}, r_{112}r_{121} - r_{111}r_{122}, c_{21}r_{121} + c_{22}r_{122}, b_{21}r_{112} + b_{22}r_{122}, \\ & c_{21}r_{111} + c_{22}r_{112}, b_{21}r_{111} + b_{22}r_{121}\rangle. \end{aligned}$$

We add to the ideal I_1 the ideal of the parametrization map

$$\begin{aligned} I_2 = \langle & -a_{21}b_{21}c_{21} + p_{111}, -a_{21}b_{21}c_{22} + p_{112}, -a_{21}b_{22}c_{21} + p_{121}, -a_{21}b_{22}c_{22} + p_{122}, \\ & -a_{12}b_{11}c_{11} + p_{211}, -a_{12}b_{11}c_{12} + p_{212}, -a_{12}b_{12}c_{11} + p_{221}, -a_{12}b_{12}c_{12} + p_{222}\rangle. \end{aligned}$$

Eliminating parameters $a_{11}, \ldots, c_{22}$ from $I_1 + I_2$, gives the ideal

$$\begin{aligned} J = \langle & p_{212}p_{221} - p_{211}p_{222}, r_{221}p_{221} + r_{222}p_{222}, r_{211}p_{221} + r_{212}p_{222}, r_{212}p_{212} + r_{222}p_{222}, \\ & r_{211}p_{212} + r_{221}p_{222}, r_{221}p_{211} + r_{222}p_{212}, r_{212}p_{211} + r_{222}p_{221}, r_{211}p_{211} - r_{222}p_{222}, \\ & p_{112}p_{121} - p_{111}p_{122}, r_{121}p_{121} + r_{122}p_{122}, r_{111}p_{121} + r_{112}p_{122}, r_{112}p_{112} + r_{122}p_{122}, \\ & r_{111}p_{112} + r_{121}p_{122}, r_{121}p_{111} + r_{122}p_{112}, r_{112}p_{111} + r_{122}p_{121}, r_{111}p_{111} - r_{122}p_{122}, \\ & r_{212}r_{221} - r_{211}r_{222}, r_{112}r_{121} - r_{111}r_{122}\rangle \end{aligned}$$

Finally, we substitute to the ideal J the expressions

$$r_{ijk} = u_{+++} - \frac{u_{ijk}}{p_{ijk}}$$

and clear the denominators. To obtain an estimate for p_{111}, we eliminate all other p_{ijk}. This gives the ideal generated by $p_{111}u_{1++}u_{+++} - u_{11+}u_{1+1}$. Hence

$$p_{111} = \frac{u_{11+}u_{1+1}}{u_{1++}u_{+++}}.$$

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	0	0	0	0	1	8	2	2	2	1	7-dimensional
$\{a_{11}\}$	1	1	0	0	5	8	2	2	2	12	6-dimensional
$\{a_{11}, a_{22}\}$	2	2	0	0	25	8	2	2	2	6	5-dimensional
$\{a_{11}, b_{11}\}$	2	1	1	0	11	8	2	2	2	24	5-dimensional
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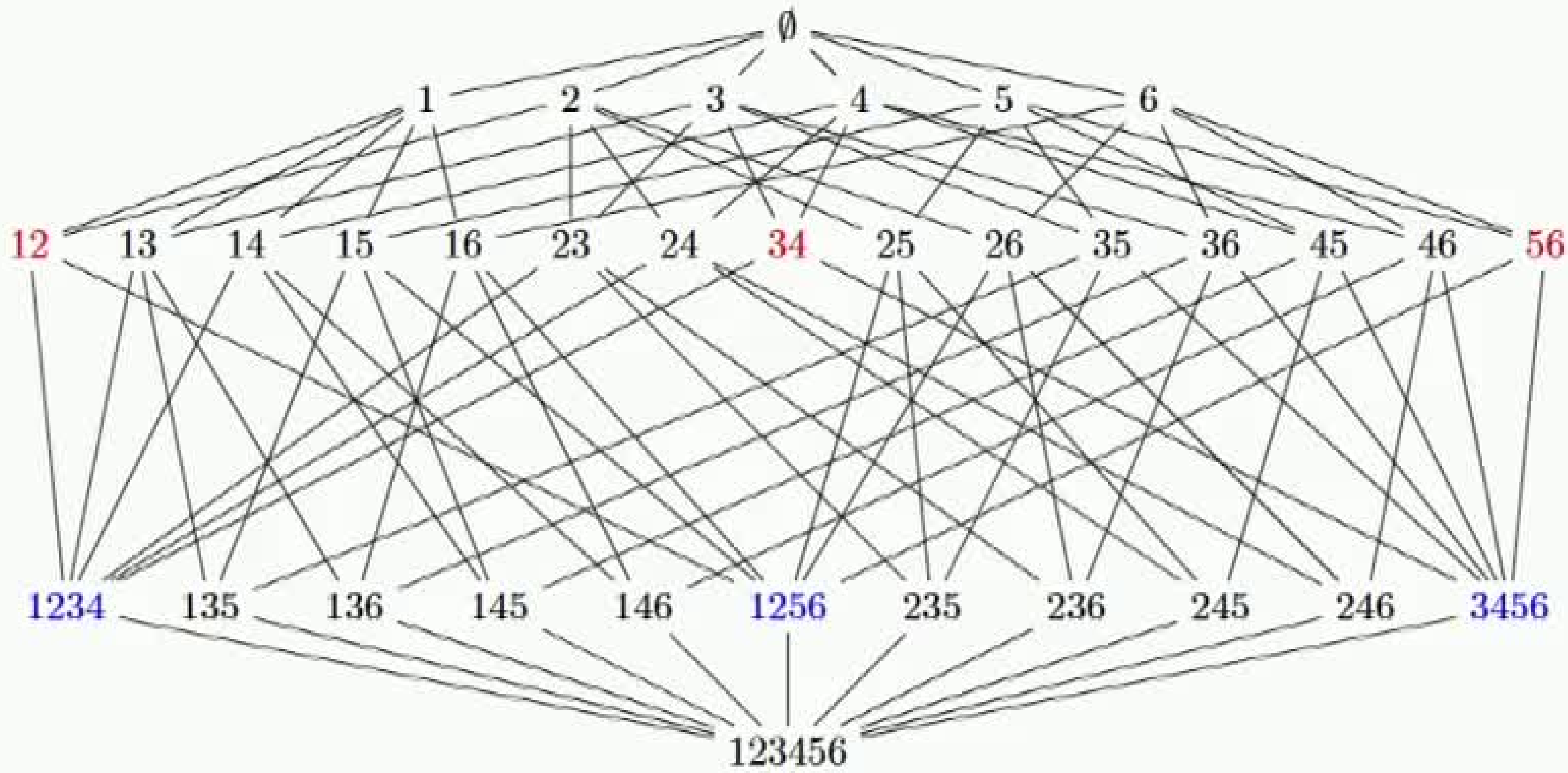

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& b_{11}r_{211} + b_{12}r_{221}, r_{112}r_{121} - r_{111}r_{122}, c_{21}r_{121} + c_{22}r_{122}, b_{21}r_{112} + b_{22}r_{122}, \\
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& -a_{12}b_{11}c_{11} + p_{211}, -a_{12}b_{11}c_{12} + p_{212}, -a_{12}b_{12}c_{11} + p_{221}, -a_{12}b_{12}c_{12} + p_{222}\rangle.
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Eliminating parameters $a_{11}, \ldots, c_{22}$ from $I_1 + I_2$, gives the ideal

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J = \langle & p_{212}p_{221} - p_{211}p_{222}, r_{221}p_{221} + r_{222}p_{222}, r_{211}p_{221} + r_{212}p_{222}, r_{212}p_{212} + r_{222}p_{222}, \\
& r_{211}p_{212} + r_{221}p_{222}, r_{221}p_{211} + r_{222}p_{212}, r_{212}p_{211} + r_{222}p_{221}, r_{211}p_{211} - r_{222}p_{222}, \\
& p_{112}p_{121} - p_{111}p_{122}, r_{121}p_{121} + r_{122}p_{122}, r_{111}p_{121} + r_{112}p_{122}, r_{112}p_{112} + r_{122}p_{122}, \\
& r_{111}p_{112} + r_{121}p_{122}, r_{121}p_{111} + r_{122}p_{112}, r_{112}p_{111} + r_{122}p_{121}, r_{111}p_{111} - r_{122}p_{122}, \\
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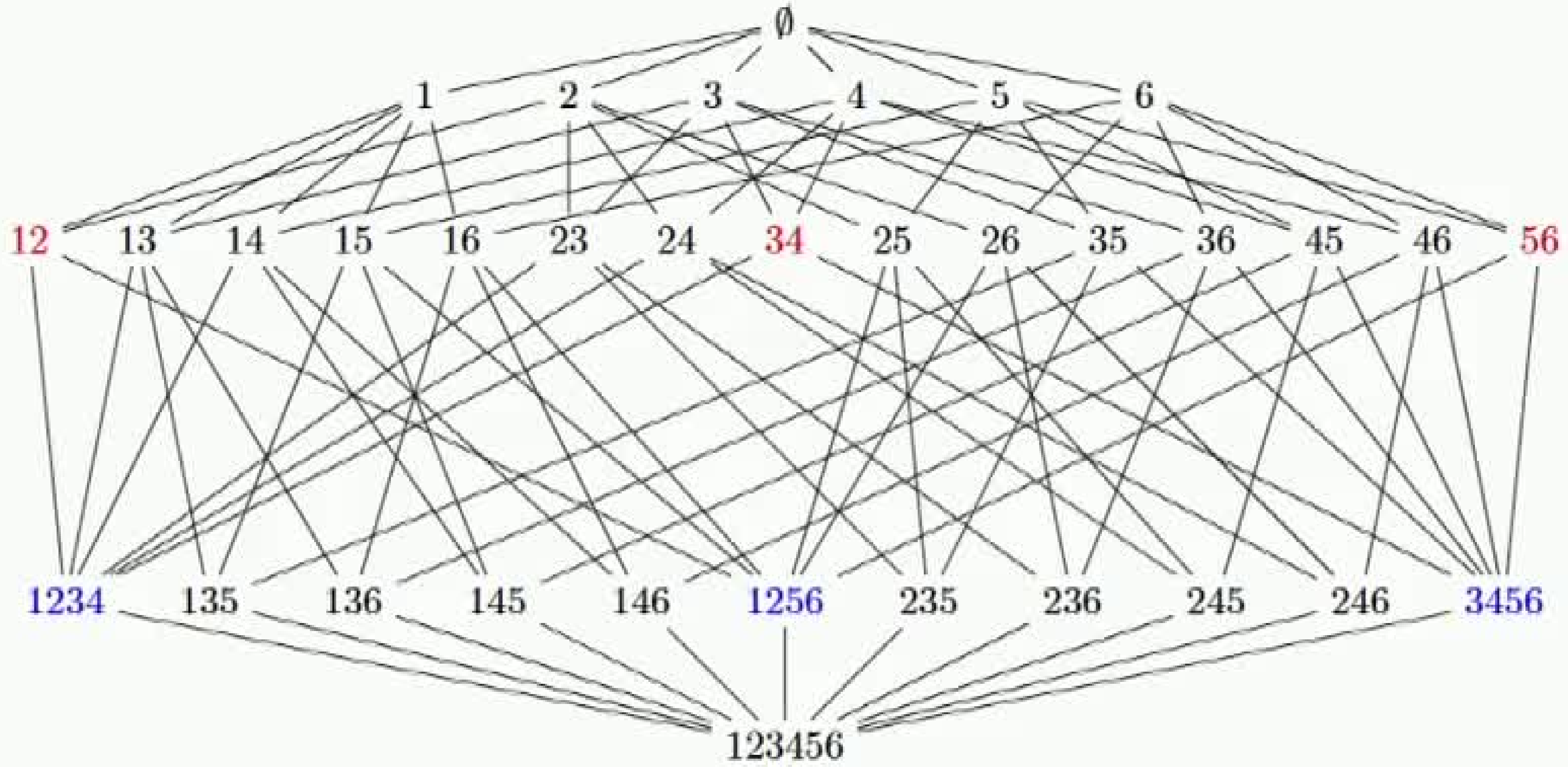

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Eliminating parameters $a_{11}, \ldots, c_{22}$ from $I_1 + I_2$, gives the ideal

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$$p_{111} = \frac{u_{11+}u_{1+1}}{u_{1++}u_{+++}}.$$

EM fixed point ideal

Theorem

The radical of the EM fixed point ideal $\mathcal{F}$ for $\mathcal{M}_{3,3}$ has precisely 317 *relevant primes consisting of* 21 *orbital classes.*

Table: Minimal primes of EM fixed point ideal for $2 \times 2 \times 2$ tensors of $\text{rank}_+ \leq 3$.

Class S	|S|	a's	b's	c's	deg	codim	rA	rB	rC	orbit
$\{\emptyset\}$	0	0	0	0	121	10	1	1	1	1
	0	0	0	0	162	9	1	2	2	1
	0	0	0	0	162	9	2	1	2	1
	0	0	0	0	162	9	2	2	1	1
*	0	0	0	0	38	10	2	2	2	6×1
	0	0	0	0	1	8	2	2	2	1
$\{a_{00}\}$	1	1	0	0	10	10	2	2	2	18
$\{a_{00}, a_{10}\}$	2	2	0	0	5	9	2	2	2	18
$\{a_{00}, b_{00}\}$	2	1	1	0	39	10	2	2	2	36
$\{a_{00}, a_{10}, a_{21}\}$	3	3	0	0	50	11	2	2	2	18
$\{a_{00}, b_{00}, c_{00}\}$	3	1	1	1	60	11	2	2	2	24
$\{a_{00}, a_{10}, b_{00}, b_{10}\}$	4	2	2	0	11	10	2	2	2	36
$\{a_{00}, a_{11}, b_{00}, b_{11}\}$	4	2	2	0	8	11	2	2	2	36
$\{a_{00}, a_{10}, b_{00}, b_{10}, c_{00}, c_{10}\}$	6	2	2	2	23	11	2	2	2	24
$\{a_{00}, a_{10}, b_{00}, b_{11}, c_{00}, c_{11}\}$	6	2	2	2	20	12	2	2	2	72
$\{a_{00}, a_{11}, b_{00}, b_{11}, c_{00}, c_{11}\}$	6	2	2	2	23	12	2	2	2	24

This table contains all the boundary strata of $\mathcal{M}_{3,3}$ from (Seigal,