One-dimensional Models of ML Degree One: Algebraic Statistics Meets Cauchy-Riemann Geometry

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New Directions in Algebraic Statistics, IMSI

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Dèja Vu: Introductory Example

Example (Flipping a coin)

Probability of Tails: $t \in [0,1]$ Probability of Heads: $1 - t \in [0,1]$

For each t we have a *Bernoulli* probability distribution represented by $p_t = (\mathbb{P}(X = H), \mathbb{P}(X = T)) = (1 - t, t)$; we have the *statistical model*

$$\mathcal{M} = \{(1 - t, t) | t \in [0,1]\} = \Delta_1$$

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- A *discrete* probability distribution on $[n] = \{0, 1, \ldots, n\}$ is determined by the probability p_i that the ith state occurs, $i = 0, \ldots, n$.
  This is a point in

$$\Delta_n = \left\{ p \in \mathbb{R}^{n+1} \mid p_i \geq 0 \text{ for all } i \text{ and } p_+ = \sum_{i=0}^{n} p_i = 1 \right\}.$$

$\rightarrow$ statistical model $\mathcal{M}$ is a subset of the *probability simplex* Δ_n.

Mantra: "Statistical models are algebraic varieties"

Example (Flipping a coin twice)

Binomial$(2, t)$ distribution with $n = 2$ (# tails observed).

$$\mathcal{M} = \left\{ \left((1-t)^2, 2t(1-t), t^2 \right) | t \in [0,1] \right\} \subset \Delta_2$$

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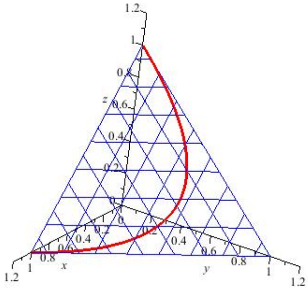
distributions $p_t = (p_0, p_1, p_2)$ defined by the *Hardy-Weinberg* equation:

$$4 p_0 p_2 = p_1^2 \, .$$



Maximum Likelihood Estimation

- Data from a sample can be summarized in a *vector of counts* $u \in \mathbb{N}^{n+1}$, where $u_i = \#$ times state i occurs.
- The empirical distribution is given by $\bar{u} = \frac{1}{N} u \in \Delta_n$ where $u_+ = N$.
- The *likelihood function* given u is

$$L_u(p) = p_0^{u_0} p_1^{u_1} \cdots p_n^{u_n}.$$

- The *MLE* given u is the maximizer $\hat{p}$ of $L_u(p)$ over $\mathcal{M} \subseteq \Delta_n$.

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Example (MLE for Binomial$(2,t)$)

Suppose we repeat the 'flipping a coin twice' experiment $N = 50$ times, observing the count vector $u = (u_0, u_1, u_2) = (10, 20, 20)$.
$\mathcal{M} = \left\{ \left((1-t)^2, 2t(1-t), t^2 \right) \mid t \in [0,1] \right\}$. What would be an *estimate* $\hat{t}$?

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The MLE for the model is $\hat{p}$, given by $\hat{t} = \frac{u_1 + 2u_2}{2(u_0 + u_1 + u_2)}$.

The ML Degree

- In many models used in practice (such as parametric discrete exponential models), computing the MLEs is equivalent to solving an *algebraic optimization* problem.

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- ML degree $= 1 \iff$ MLE is a *rational function* of u

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Characterizing ML degree one Models

Great result by Huh [3] and refinement by Duarte-Marigliano-Sturmfels [4].

Theorem (Huh, Duarte-Marigliano-Sturmfels)

The following are equivalent:

1. *The model $\mathcal{M} \subset \Delta_n$ has ML degree one.*

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3. *There exists a discriminantal triple $(A, \Delta, \mathbf{m})$ such that $\mathcal{M}$ is the image under the monomial map $\phi_{(\Delta,\mathbf{m})}$ of precisely one orthant of the dual toric variety Y_A^*.*

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Question: Can such models be classified?

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Curves of ML degree one

Bik and Marigliano [5] study the classification when $\dim(\mathcal{M}) = 1$.

Proposition

Let $\mathcal{M} \subset \Delta_n$ *with* $\dim(\mathcal{M}) = 1$ *and ML degree one. Then*

$$\mathcal{M} = \{(c_0 t^{\nu_0}(1-t)^{\mu_0}, c_1 t^{\nu_1}(1-t)^{\mu_1}, \ldots, c_n t^{\nu_n}(1-t)^{\mu_n}) | t \in [0,1]\},$$

for some $c_i > 0$ *and* $\nu_i, \mu_i \in \mathbb{N}$, $\forall i \in [n]$.

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for some $c_i > 0$ *and* $\nu_i, \mu_i \in \mathbb{N}$, $\forall i \in [n]$.

Moreover, the identity

$$c_0 t^{\nu_0}(1-t)^{\mu_0} + c_1 t^{\nu_1}(1-t)^{\mu_1} + \cdots + c_n t^{\nu_n}(1-t)^{\mu_n} = 1$$

must hold in the *polynomial ring* $\mathbb{R}[t]$.

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Reduced Models

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We say $\mathcal{M}$ is *reduced* iff all exponent pairs (ν_i, μ_i) are pairwise distinct and different from $(0,0)$. We also have

$$\deg(\mathcal{M}) = \max\{\nu_i + \mu_i \mid i \in [n]\}.$$

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Every one-dimensional model of ML degree one is the image of a reduced model under a chain of linear embeddings of the form

$$\Delta_{n-1} \to \Delta_n, \quad (p_0, \ldots, p_j, \ldots, p_n) \mapsto (\lambda p_0, \ldots, 1-\lambda, \ldots, \lambda p_n), \quad \lambda \in [0,1]$$

or of the form

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Hence, it suffices to study *reduced models*.

Composite Models

- If $\mathcal{M}$ is a reduced model represented by $(c_i, \nu_i, \mu_i)_{i=0}^n$, the *support* of $\mathcal{M}$ is the set of all pairs (ν_i, μ_i).
- We can encode reduced models as functions

$$h : \mathbb{Z}^2 \to \mathbb{R}_{\geq 0}, \quad (\nu_i, \mu_i) \mapsto c_i$$

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- Let $\mathcal{M}_1$ and $\mathcal{M}_2$ be reduced models represented by h_1, h_2 and $0 < \lambda < 1$. Then the *composite* model $\mathcal{M}_1 *_\lambda \mathcal{M}_2$ is the reduced model represented by $h = (1 - \lambda) h_1 + \lambda h_2 : \mathbb{Z}^2 \to \mathbb{R}_{\geq 0}$.

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Example (Composite of $\mathrm{Ber}(t)$ and $\mathrm{Bin}(2,t)$)

Let $\mathcal{M}_1 : t \mapsto (1-t, t) \subseteq \Delta_1$ and $\mathcal{M}_2 : t \mapsto \left((1-t)^2, 2t(1-t), t^2\right) \subset \Delta_2$.

$$\mathcal{M}_1 *_\lambda \mathcal{M}_2 : t \mapsto \left((1-\lambda)(1-t), (1-\lambda)t, \lambda(1-t)^2, 2\lambda t(1-t), \lambda t^2\right) \subset \Delta_4$$

Fundamental Models

Definition

A reduced model represented by $(c_i, \nu_i, \mu_i)_{i=0}^n$ is *fundamental* if, given (ν_i, μ_i), the scalings c_i are uniquely determined by the constraint $p_0 + p_1 + \ldots + p_n = 1$.

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Consider the support $\{(2,0), (1,1), (0,2)\}$. The polynomial constraint

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Fundamental Theorem of Reduced Models

Every reduced model can be constructed from finitely many fundamental models in a finite number of steps.

Theorem (Bik-Marigliano)

Every reduced model in Δ_n is a composite of at most n fundamental models, each one in a Δ_m with $m < n$.

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- Given n, is there an *upper bound* on $\deg(\mathcal{M})$?
- If this were the case, there would be only finitely many fundamental models in Δ_n for any $n \in \mathbb{N}$!

Fundamental models in Δ_2

- Let $\mathcal{M} \subset \Delta_2$ fundamental of $\deg(\mathcal{M}) = d$.
- Possible supports are subsets of size 3 of

$$\{(i,j) \mid 0 < i + j \leq d\} \subset \mathbb{Z}^2$$

- $d = 1$: no reduced models, $\mathcal{M} : t \mapsto (1 - t, t, 0)$
- $d = 2$: there are *three* fundamental models

$$\begin{aligned} \mathcal{M}_1 : &\quad t \mapsto \left((1-t)^2, 2t(1-t), t^2\right) \\ \mathcal{M}_2 : &\quad t \mapsto \left(1-t, t(1-t), t^2\right) \\ \mathcal{M}_3 : &\quad t \mapsto \left((1-t)^2, t(1-t), t\right) \end{aligned}$$

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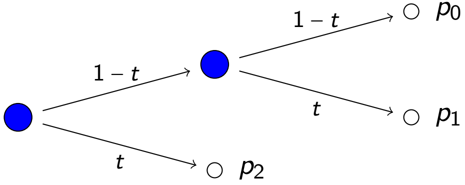

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- $d = 3$: there is a *unique* fundamental model:

$$\mathcal{M}: \quad t \mapsto \left((1-t)^3, 3t(1-t), t^3\right).$$

This model is obtained by *merging* states $1, 2$ from a $\mathrm{Bin}(3, t)$:

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This model is obtained by *merging* states $1, 2$ from a $\mathrm{Bin}(3, t)$:

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- $d > 3$: *no* fundamental models!

In order to conclude the last statement, Bik and Marigliano develop a range of combinatorial criteria to rule out supports for fundamental models, and keep track of possible supports through *Chipsplitting games*.

·	·	·	·	1	1	1
· ·	· ·	· ·	1 ·	· 1	· 1	· ·
· · ·	1 · ·	1 1 ·	· 2 ·	· 2 ·	· 2 1	· 3 ·
0 · · ·	−1 1 · ·	−1 · 1 ·	−1 · 1 ·	−1 · 1 ·	−1 · · 1	−1 · · 1

State-of-the-Art (Bik-Marigliano)

$n \setminus d$	1	2	3	4	5	6	7	8	9
1	1								
2		3	1						
3			12	4	2				
4				82	38	10	4		
5					602	254	88	24	2

Number of fundamental models in Δ_n of degree d.

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Conjecture

Let $\mathcal{M} \subseteq \Delta_n$ be a one-dimensional model with ML degree one. Then

$$\deg(\mathcal{M}) \leq 2n - 1.$$

Resolving the Conjecture

Theorem (Am., Nguyen, Oldekop)

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Corollary

For any $n \in \mathbb{N}$, the number of fundamental models in Δ_n is finite.

Crucial fundamental model:

Proposition

The binomial model $\mathrm{Bin}(n,t) \subset \Delta_n$ parametrized by

$$p : [0,1] \to \Delta_n, \quad t \mapsto \left(\binom{n}{i} t^i (1-t)^{n-i} \right)_{i=0}^{n}$$

is fundamental. Moreover, it is the unique reduced model that is homogeneous of degree d.

CR Geometry

- Branch of mathematics which arose from the theory of functions of *several complex variables* [6]
- CR stands for *Cauchy-Riemann* → Cauchy-Riemann equations
- CR also for *complex-real* → real submanifolds of complex spaces
- Relate the geometry of the boundary of a domain in complex Euclidean space to the function theory on the domain

[6] G. Zampieri (2008). *Complex Analysis and CR Geometry*. University Lecture Series, American Mathematical Society

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- Relate the geometry of the boundary of a domain in complex Euclidean space to the function theory on the domain
- *Classical problem*: study of proper holomorphic mappings between complex unit balls:

$$F : \mathbb{B}_N \to \mathbb{B}_{n+1}$$

- If F extends continuously to the boundaries, F is proper if it maps the unit sphere in $\mathbb{C}^N$ to the unit sphere in $\mathbb{C}^{n+1}$

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CR Geometry: Faran's Classification

Invent. math. 68, 441–475 (1982)

Inventiones mathematicae

Maps from the Two-Ball to the Three-Ball

James J. Faran*

Department of Mathematics, Princeton University, Princeton, NJ 08544, USA

Given such a map $F : \mathbb{B}_2 \to \mathbb{B}_3$, we can get another such by composing with an automorphism of $\mathbb{B}_2$ and an automorphism of $\mathbb{B}_3$:

spherical equivalence

Faran's Classification (1982)

Theorem. *Let* $f\colon \mathbf{B}_2 \to \mathbf{B}_3$ *be a proper holomorphic map that is* C^3 *up to the boundary. Then* f *is spherically equivalent to one of the following maps:*

(1) $(z, w) \to (z^3, w^3, \sqrt{3}\, z w)$,

(2) $(z, w) \to (z, z w, w^2)$,

(3) $(z, w) \to (z^2, \sqrt{2}\, z w, w^2)$,

(4) $(z, w) \to (z, w, 0)$.

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Note that indeed for (3):

$$z^2 + w^2 = 1 \quad \Longrightarrow \quad z^4 + 2z^2w^2 + w^4 = 1$$

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These are the *fundamental models* in Δ_2!

Some CR Geometry Literature

Non-exhaustive list of relevant references:

- John D'Angelo. *Polynomial proper maps between balls*. Duke Mathematical Journal, 57(1):211 219, 1988.
- John D'Angelo, Simon Kos, and Emily Riehl. *A sharp bound for the degree of proper monomial mappings between balls*. The Journal of Geometric Analysis, 13(4):581593, 2003.
- John D'Angelo, Jirí Lebl, and Han Peters. *Degree estimates for polynomials constant on a hyperplane*. Michigan Mathematical Journal, 55(3):693-713, 2007.
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- John D'Angelo. *Rational Sphere Maps*. Progress in Mathematics. Birkhäuser Cham, 2021.

Proving the Upper Bound $2n - 1$

- For a reduced model $\mathcal{M} \subseteq \Delta_n$ represented by $(c_i, \nu_i, \mu_i)_{i=0}^n$, define

$$f_{\mathcal{M}} = c_0 x^{\mu_0} y^{\nu_0} + c_1 x^{\mu_1} y^{\nu_1} + \ldots + c_n x^{\mu_n} y^{\nu_n} \in \mathbb{R}[x, y].$$

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- Define the *Newton diagram* $G_{\mathcal{M}}$ of $g_{\mathcal{M}}$ as

$$G_{\mathcal{M}} : \mathbb{Z}^2 \to \{\mathtt{0}, \mathtt{P}, \mathtt{N}\}, \qquad (a,b) \mapsto \begin{cases} \mathtt{P}, & \text{if } g_{ab} > 0, \\ \mathtt{0}, & \text{if } g_{ab} = 0, \\ \mathtt{N}, & \text{if } g_{ab} < 0. \end{cases}$$

Example

Consider the fundamental model $\mathcal{M} \subset \Delta_4$ parametrized by

$$t \mapsto \left(t^7, \frac{7}{2} t^5(1-t), \frac{7}{2} t(1-t), \frac{7}{2} t(1-t)^5, (1-t)^7 \right).$$

Then we have

$$\begin{aligned} g_{\mathcal{M}} = 1 &+ x + y + x^2 - \frac{3}{2}xy + y^2 + x^3 - \frac{1}{2}x^2y - \frac{1}{2}xy^2 + y^3 + x^4 + \frac{1}{2}x^3y \\ &- x^2y^2 + \frac{1}{2}xy^3 + y^4 + x^5 + \frac{3}{2}x^4y - \frac{1}{2}x^3y^2 - \frac{1}{2}x^2y^3 \\ &+ \frac{3}{2}xy^4 + y^5 + x^6 - x^5y + x^4y^2 - x^3y^3 + x^2y^4 - xy^5 + y^6 \end{aligned}$$

```
0
P 0
P N 0
P P P 0
P P N N 0
P N N N P 0
P N N P P N 0
P P P P P P P 0
```

Proving the Upper Bound $2n - 1$

Proof technique largely inspired by *d'Angelo-Kos-Riehl (2003)*.

- (a, b) in $G_{\mathcal{M}}$ is a *sink* if the subdiagram of the entry itself, the entry just below and the entry to the left is one of

P	N	P	N	0	N	0	N	P	0	0	0	P	0
	P		0		P		0		P		P		0

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	P		0		P		0		P		P		0

- *Key* observation: if $G_{\mathcal{M}}$ has a sink at (a,b) then the coefficient of $x^a y^b$ in $f_{\mathcal{M}}$ is positive:

$$(x+y-1)(g_{(a-1)b}x^{a-1}y^b + g_{a(b-1)}x^a y^{b-1} + g_{ab}x^a y^b)$$

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```
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  P      0      P      0      P      P      0
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- Hence, the support size of $\mathcal{M}$ is at least the number of sinks in $G_{\mathcal{M}}$.

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P	0	P	0	P	P	0

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- Hence, the support size of $\mathcal{M}$ is at least the number of sinks in $G_{\mathcal{M}}$.
- (DKR03, Prop 3.11) For any $\mathcal{M}$ of degree d, $G_{\mathcal{M}}$ has at least $2+\lceil \frac{d-1}{2} \rceil$ sinks.

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```
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- (DKR03, Prop 3.11) For any $\mathcal{M}$ of degree d, $G_{\mathcal{M}}$ has at least $2+\lceil \frac{d-1}{2} \rceil$ sinks.
- Finally, from $2+\lceil \frac{d-1}{2} \rceil \leq n+1$, we obtain $d \leq 2n-1$.

Sharp Models

Definition

A reduced model $\mathcal{M} \subset \Delta_n$ is *sharp* if $\deg(\mathcal{M}) = 2n - 1$

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Sharp models always exist for every $n \in \mathbb{N}^+$. A well-known family (also found by Bik-Marigliano) is

$$t \mapsto \left(t^{2n-1}, \left(\frac{2n-1}{2i+1} \binom{n+i-1}{2i} t^{n-i-1} (1-t)^{2i+1} \right)_{i=0}^{n-1} \right)$$

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Lebl and Lichtblau (2010) prove the following about the support of a sharp model $\mathcal{M}$ of degree d:

- The support of $\mathcal{M}$ contains $(d, 0)$ and $(0, d)$
- It does not contain any other elements (a, b) with $a + b = d$
- It does not contain $(k, 0)$ nor $(0, k)$ for all $k < d$
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- It contains at least one element (a, b) with $a + b = d - 1$.
- No two sharp models have the same support $\implies$

they are always fundamental!

Counting polynomials

Table 2 from *Lebl and Lichtblau (2010)*:

Table 2
Number of polynomials in the top 3 degrees for each N.

Degree	N								
	2	3	4	5	6	7	8	9	10
$d = 2N - 3$	1	1	2	4	2	4	8	4	2
$d = 2N - 4$	0	3	4	10	24	32	56	?	?
$d = 2N - 5$	0	0	11	38	88	198	?	?	?

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Compare with *Bik-Marigliano*:

$n \setminus d$	1	2	3	4	5	6	7	8	9
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3			12	4	2				
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Key message: *We can learn from each other!*

State-of-the-Art (Am., Nguyen, Oldekop)

n \ d	1	2	3	4	5	6	7	8	9	10	11	12	13
1	1												
2		3	1										
3			12	4	2								
4				82	38	10	4						
5					602	254	88	24	2				
6						6710	2421	643	198	32	4		
7							83906	23285	6445	1442	332	56	8

Number of fundamental models of degree d in the simplex Δ_n.

State-of-the-Art (Am., Nguyen, Oldekop)

n \ d	1	2	3	4	5	6	7	8	9	10	11	12	13
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7							83906	23285	6445	1442	332	56	8

Number of fundamental models of degree d in the simplex Δ_n.

We can now know that all blank entries are indeed zero.

Proposition

There exist fundamental models of degree d in Δ_n if and only if

$$n \leq d \leq 2n - 1.$$

Fundamental Models Triangle (Am., Nguyen, Oldekop)

1

1 3

2 4 12

4 10 38 82

2 24 88 254 602

4 32 198 643 2421 6710

8 56 332 1442 6445 23285 83906

4 96 ? ? ? ? 285601 1279349

[7] J. Lebl (2013). *Addendum to uniqueness of certain polynomials constant on a line*. arXiv: 1302.1441

Fundamental Models Triangle (Am., Nguyen, Oldekop)

1							
1	3						
2	4	12					
4	10	38	82				
2	24	88	254	602			
4	32	198	643	2421	6710		
8	56	332	1442	6445	23285	83906	
4	96	?	?	?	?	285601	1279349

Conjecture

Let a_n be the number of fundamental models in Δ_n of degree $2n-1$. Then the number of fundamental models in Δ_n of degree $2n-2$ is given by

$$2(a_1 a_{n-1} + a_2 a_{n-2} + \ldots + a_{n-1} a_1).$$

Example: for $n = 4 : 2(a_1 a_3 + a_2^2 + a_3 a_1) = 2(1 \cdot 2 + 2^2 + 2 \cdot 1) = 10$

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Example: for $n = 4: 2(a_1 a_3 + a_2^2 + a_3 a_1) = 2(1 \cdot 2 + 2^2 + 2 \cdot 1) = 10$

Lebl [7] reports $a_9 = 2, a_{10} = 24$ and $a_{11} = 2$ *(> 8 months computation time!)*

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Conclusion

- *Fundamental models* as building blocks for all one-dimensional discrete models of ML degree one.
- We show there exist (finitely many) fundamental models of degree d in Δ_n if and only if $n \leq d \leq 2n - 1$.
- *Sharp* models have nice combinatorial properties and correspond to well-studied special holomorphic maps between complex spheres.

Conclusion

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- Exciting link between *Algebraic Statistics* and *CR Geometry* !

THANK YOU!