

Algebraic Statistics

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“Does Watching Football on TV Cause Hair Loss?”

- ▶ 296 British subjects were asked about their hair loss and how much football they watch on television, [MSS03].

Contingency Table

One can represent the responses in a 3×3 *contingency table*:

TV Hours	Hair Amount		
	lots	medium	balding
$\leq 2\text{h}$	51	45	33
$2 - 6\text{ h}$	28	30	29
$\geq 6\text{h}$	15	27	38

- ▶ Is there an association between the variables, or are they independent?

“Does Watching Football on TV Cause Hair Loss?”

$$M = \begin{bmatrix} 51 & 45 & 33 \\ 28 & 30 & 29 \\ 15 & 27 & 38 \end{bmatrix}$$

Null Hypothesis

$H_0 :$ *Football on TV and Hair Loss are Independent.*

- Independence \Rightarrow odds ratios all equal one:

$$\text{Odds Ratio} = \frac{m_{ij} \cdot m_{(i+1)(j+1)}}{m_{(i+1)j} \cdot m_{i(j+1)}} = 1, \quad (\text{for all } i, j).$$

- But (for example):

$$51 \cdot 30 - 45 \cdot 28 = 1530 - 1260 = 270 \neq 0 \dots ?$$

“Does Watching Football on TV Cause Hair Loss?”

- ▶ A better explanation is obtained by identifying a certain *hidden variable*, which is the *gender identification* of the respondents:

$$M = M_m + M_f = \underbrace{\begin{bmatrix} 3 & 9 & 15 \\ 4 & 12 & 20 \\ 7 & 21 & 35 \end{bmatrix}}_{126 \text{ male}} + \underbrace{\begin{bmatrix} 48 & 36 & 18 \\ 24 & 18 & 9 \\ 8 & 6 & 3 \end{bmatrix}}_{170 \text{ female}}.$$

Alternative Hypothesis

Instead, we include *conditional independence*:

H_1 : *Football on TV & Hair Loss are Independent given Gender.*

Definition

A *statistical model* \mathcal{P} is the collection of probability distributions, usually parameterised by a function called a *parametrisation*

$\Theta \rightarrow \mathcal{P}$, given by $\theta \mapsto P_\theta$, so that $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$,

where Θ is the *parameter space*. Θ is usually a subset of \mathbb{R}^n .

McCullagh, [McC02]

This should be defined using category theory.

Contingency Tables

- ▶ Classify using two criteria with r and c levels, yielding two random variables X and Y .
- ▶ Note outcomes as $[r] := \{1, \dots, r\}$, and $[c] := \{1, \dots, c\}$.

All information about X and Y is contained in the *joint probabilities*:

$$p_{ij} = P(X = i; Y = j), \quad i \in [r], j \in [c].$$

- ▶ These in turn determine the *marginal probabilities*:

$$p_{i+} := \sum_{j=1}^c p_{ij} = P(X = i), \quad i \in [r],$$
$$p_{+j} := \sum_{i=1}^r p_{ij} = P(Y = j), \quad j \in [c].$$

Definition

- ▶ Two random variables X and Y are *independent* if the joint probabilities factor as $p_{ij} = p_{i+} \cdot p_{+j}$, for all $i \in [r]$ and $j \in [c]$.
- ▶ Denote independence of X and Y by $X \perp\!\!\!\perp Y$.

Proposition, [DSS09]

Two random variables X and Y are independent if and only if the $(r \times c)$ -matrix, $p = (p_{ij})$, has rank one.

For a (2×2) -table, we thus have:

	$P(Y = 1)$	$P(Y = 2)$	
$P(X = 1)$	p_{11}	p_{12}	$\overset{X \perp\!\!\!\perp Y}{\rightsquigarrow} p_{11}p_{22} = p_{12}p_{21}.$
$P(X = 2)$	p_{21}	p_{22}	

Some Geometry

Suppose now we select n cases, giving rise to n independent pairs of discrete random variables:

$$\begin{pmatrix} X^{(1)} \\ Y^{(1)} \end{pmatrix}, \begin{pmatrix} X^{(2)} \\ Y^{(2)} \end{pmatrix}, \dots, \begin{pmatrix} X^{(n)} \\ Y^{(n)} \end{pmatrix},$$

all drawn from the same distribution, i.e.:

$$P(X^{(k)} = i; Y^{(k)} = j) = p_{ij}, \quad \text{for all } i \in [r], j \in [c], k \in [n].$$

Probability Simplices

Joint probability matrix $p = (p_{ij})$ is an *unknown* element of the $(rc - 1)$ -dimensional *probability simplex*:

$$\Delta_{rc-1} = \left\{ q \in \mathbb{R}^{r \times c} \mid q_{ij} \geq 0, \text{ for all } i, j, \text{ and } \sum_{i=1}^r \sum_{j=1}^c q_{ij} = 1 \right\}.$$

Definitions

- ▶ A *statistical model* \mathcal{M} is a subset of Δ_{rc-1} . It represents the set of all candidates for the unknown distribution p .
- ▶ The *independence model* for X and Y is the set

$$\mathcal{M}_{X \perp\!\!\!\perp Y} := \{ p \in \Delta_{rc-1} \mid \text{rank}(p) = 1 \}.$$

$\mathcal{M}_{X \perp\!\!\!\perp Y}$ is the intersection of Δ_{rc-1} and the set of all matrices $p = (p_{ij})$ such that

$$p_{ij}p_{kl} - p_{il}p_{jk} = 0, \quad (1 \leq i < k \leq r, \text{ and } 1 \leq j < l \leq c).$$

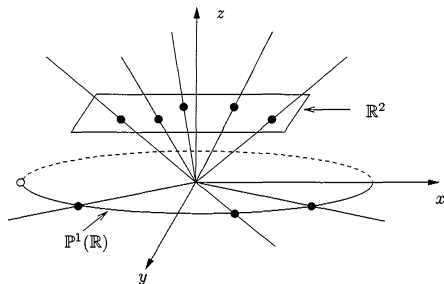
These are called *Segre varieties* in algebraic geometry.

Projective Space

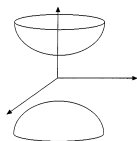
Playing field is n -dimensional projective space, \mathbb{P}^n :

$$\mathbb{P}^n := \{(z_0, \dots, z_n) \in \mathbb{C}^n\} / (\mathbf{x} \sim \lambda \cdot \mathbf{y}), \quad \lambda \neq 0,$$

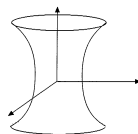
that is, its elements consists of *lines through the origin* in \mathbb{C}^n .



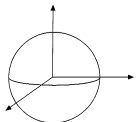
Varieties are the objects studied in algebraic geometry, determined by the *vanishing set*¹ $V(-)$, for a system of polynomials.



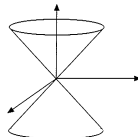
(a) $V(x^2 + y^2 - z^2 + 1)$



(b) $V(x^2 + y^2 - z^2 - 1)$



(c) $V(x^2 + y^2 + z^2 - 1)$



(d) $V(x^2 + y^2 - z^2)$

¹from 'Verschwindungsmenge'

Segre varieties come from $\sigma : \mathbb{P}^n \times \mathbb{P}^m \rightarrow \mathbb{P}^{(n+1)(m+1)-1}$, that sends $([X], [Y])$ to the pairwise products of their components:

$$\sigma : ([X_1, \dots, X_{n+1}], [Y_1, \dots, Y_{m+1}]) \mapsto [\dots, X_i Y_j, \dots].$$

Example (Segre quadric surface)

$$\sigma : \mathbb{P}^1 \times \mathbb{P}^1 \rightarrow \mathbb{P}^3, ([X_1, X_2], [Y_1, Y_2]) \mapsto [X_1 Y_1, X_1 Y_2, X_2 Y_1, X_2 Y_2].$$

Set $[X_1 Y_1, X_1 Y_2, X_2 Y_1, X_2 Y_2] =: [p_{11}, p_{12}, p_{21}, p_{22}]$, then:

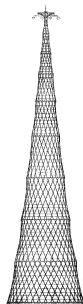
$$\rightsquigarrow \det \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix} = 0 \iff \text{rank} \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix} \leq 1.$$

Rulings

The Segre quadric surface has two families of lines in it, called *rulings*. These are the images of $\sigma(\mathbb{P}^1 \times \{\text{pt}\})$ and $\sigma(\{\text{pt}\} \times \mathbb{P}^1)$ in \mathbb{P}^3 .



Shukhov Tower,
Nizhny Novgorod



Shukhov Tower,
Moscow



Tractricious,
Fermilab

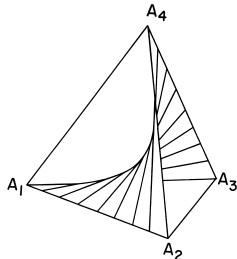
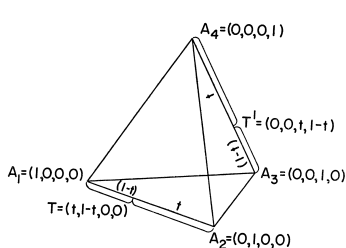
Manifold of Independence

- Let $\Delta_3 \subset \mathbb{R}^4$, with vertices $A_i = e_i$, and let $p = (p_{ij}) \in \Delta_3$ be

$$p_{ij} = (p_{11}, p_{12}, p_{21}, p_{22}) = \begin{array}{|c|c|} \hline p_{11} & p_{12} \\ \hline p_{21} & p_{22} \\ \hline \end{array}$$

- Has been shown that the two rulings are given by [FG70]:

$$p_{ij}(s, t) = \begin{array}{|c|c|} \hline st & s(1-t) \\ \hline t(1-s) & (1-s)(1-t) \\ \hline \end{array} \quad (0 \leq s, t \leq 1).$$



“Absence of evidence is not evidence of absence.”

- ▶ Suppose $\mathcal{P} \subset \Delta_{r-1}$ is a model for a random variable X with state space $[r]$.
- ▶ Assume Y is a *hidden* or *latent* random variable, with state space $[s]$; for each $j \in [s]$, the conditional distribution of X given $Y = j$ is $p^{(j)} \in \mathcal{P}$.
- ▶ Y also has some probability distribution $\pi \in \Delta_{s-1}$.

So the joint distribution of Y and X is given by the formula

$$P(Y = j; X = i) = \pi_j \cdot p_i^{(j)}.$$

Donald Rumsfeld, 21st US Secretary of Defense, [Rum02]

“[T]here are known knowns; there are things we know we know. We also know there are known unknowns; that is to say we know there are some things we do not know.”

Mixture Models

- ▶ But as Y is hidden, we can only observe the marginal distribution of X , that is

$$P(X = i) = \sum_{j=1}^s \pi_j \cdot p_i^{(j)}.$$

- ▶ In other words, the marginal distribution of X is the convex combination of the s distributions $p^{(1)}, \dots, p^{(s)}$, with weights given by π .

Definition [DSS09]

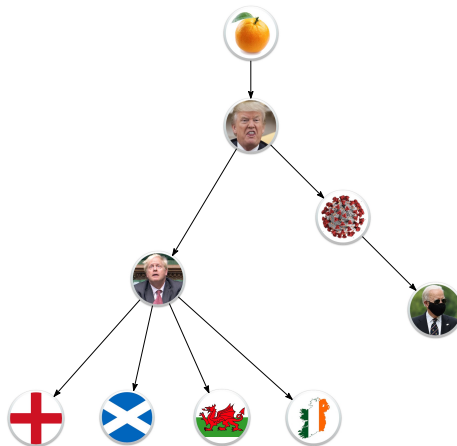
Let $\mathcal{P} \subset \Delta_{r-1}$ be a statistical model. The s -th mixture model is

$$\text{Mixt}^s(\mathcal{P}) := \left\{ \sum_{j=1}^s \pi_j \cdot p^{(j)} \mid \pi \in \Delta_{s-1}, p^{(j)} \in \mathcal{P}, \text{ for all } j \right\}.$$

- ▶ Mixture models provide ways to build complex models out of simpler ones.
- ▶ Basic assumption is that the underlying population to be modelled can be split into s disjoint sub-populations.
- ▶ Restricted to each sub-population, the observable X follows a probability distribution from the simple model \mathcal{P} .
- ▶ After marginalisation though, the structure becomes significantly more complex as it is now a convex combination of these simple distributions.

Phylogenetic Trees

- Introduce *phylogenetic trees*; describe the descent of species from a common ancestor:



- ▶ Sequence of DNA molecules in a genome is represented as a sequence of letters from the four letter alphabet $\Sigma = \{A, C, G, T\}$.
- ▶ *Fix for now* an ancestral nucleotide $Y \in \Sigma$; we assume that the following evolution events occur independently [All07]:

$$Y \xrightarrow{\pi_Y \cdot p_A^{(Y)}} A, \quad Y \xrightarrow{\pi_Y \cdot p_C^{(Y)}} C, \quad Y \xrightarrow{\pi_Y \cdot p_G^{(Y)}} G, \quad Y \xrightarrow{\pi_Y \cdot p_T^{(Y)}} T,$$

- ▶ So *given* Y , we have a joint distribution:

$$\pi_Y \cdot [p_A^{(Y)}, p_C^{(Y)}, p_G^{(Y)}, p_T^{(Y)}] \in \Delta_3 = \Delta_{4-1}.$$

Example

- ▶ Y is a hidden variable though; could have been anything from $\Sigma = \{A, C, G, T\}$.
- ▶ For *exactly one given choice* of Y , we had the distribution Δ_3 ; need to consider *all choices* of ancestral nucleotide Y .
- ▶ Hence, we get the mixture model [All07]:

$$\begin{aligned} & \text{Mixt}^4(\Delta_3) \\ &= \left\{ \sum_{Y \in \Sigma} \pi_Y \cdot p^{(Y)} \mid \pi \in \Delta_3, p^{(Y)} \in \mathcal{P} \subseteq \Delta_3, \text{ for each } Y \right\}. \end{aligned}$$

Question?

What is the analogue for mixture models in algebraic statistics?

Answer!

Secant² varieties [DSS09]!

Definitions

- ▶ Consider two varieties $V, W \subseteq \mathbb{R}^k$. The *join* of V and W is the variety

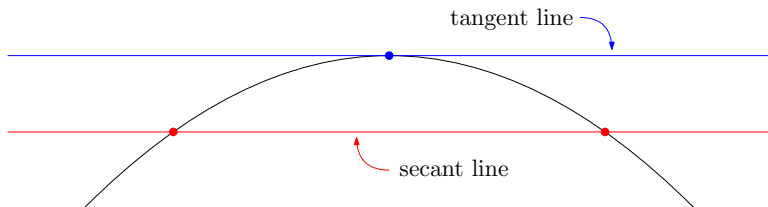
$$\mathcal{J}(V, W) := \{\lambda v + (1 - \lambda)w : v \in V, w \in W, \lambda \in [0, 1]\}.$$

- ▶ If $V = W$, then this is the *secant variety* of V , denoted $\text{Sec}^2(V) = \mathcal{J}(V, V)$. The *s-th higher secant variety* is:

$$\text{Sec}^1(V) := V, \quad \text{Sec}^s(V) := \mathcal{J}(\text{Sec}^{s-1}(V), V).$$

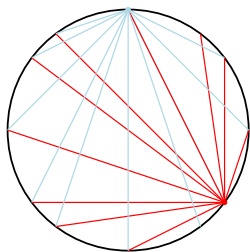
²from *secare*, “to cut” in Latin; *c.f.* *tangō*, “to touch”.

Secant Varieties

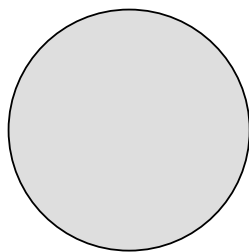


$$S^1 = V(x^2 + y^2 - 1)$$

$$\text{Sec}^2(S^1)$$

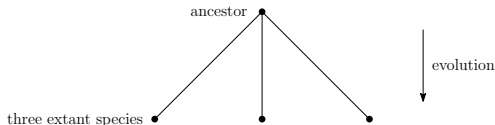


etc.
→



More Complicated Phylogenetic Trees

- ▶ Last example only had one extant species; what about if we had three extant species, all coming from the same ancestor?



- ▶ Now we have to consider: $\text{Sec}^4(\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3)$; or equivalently $\text{Mixt}^4(\Delta_3 \times \Delta_3 \times \Delta_3)$ [All07].
- ▶ Finding the minimal set of polynomials defining $\text{Sec}^4(\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3)$ once gave rise to a very important application of algebraic statistics...

*The Salmon Problem**Statement*

Determine the ideal³ defining $\text{Sec}^4(\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3)$, [All07].

Prize

- ▶ At an IMA workshop in 2007, Elizabeth Allman stated that she would personally catch and smoke copper river salmon from Alaska for whomever solved this problem.
- ▶ Solved in 2010 by Shmuel Friedland & Elizabeth Gross [FG12] (see [BO11] too for an in-depth discussion).

Solving this would then provide all polynomial invariants of the statistical model for any binary evolutionary tree, with any number of states [AR08]; [BO11].

³read this as “set of defining polynomials”.

Why $\text{Sec}^4(\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3)$ again?

- ▶ Three independent variables (nucleotides in extant species) \rightsquigarrow three factors in product;
- ▶ Each independently assumes one value from $\Sigma = \{\text{A, C, G, T}\} \rightsquigarrow$ distribution is a point in $\mathbb{P}^3 = \mathbb{P}^{4-1}$;
- ▶ The ancestral nucleotide is unknown, but could assume any of the four values in $\Sigma \rightsquigarrow$ mix four such independence models;
- ▶ The model for the three observed nucleotides is therefore

$$\text{Sec}^4(\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3), \quad \text{c.f.,} \quad \text{Mixt}^4(\Delta_3 \times \Delta_3 \times \Delta_3).$$

A Dank Meme

Henri Poincaré

“[L]a mathématique est l’art de donner le même nom à des choses différentes,” [Poi96].



H. Poincaré, 1887.



H. Poincaré, colourised.

The solution to the salmon conjecture is equivalent to [Stu09]:

- ▶ the mixture of four models for three independent variables;
- ▶ the fourth secant variety of the Segre variety $\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3$;
- ▶ the set of $(4 \times 4 \times 4)$ -tables of tensor rank ≤ 4 ;
- ▶ the naive Bayes model with four classes and three features;
- ▶ the conditional independence model $[X_1 \perp\!\!\!\perp X_2 \perp\!\!\!\perp X_3 | Y]$;
- ▶ the general Markov model for the phylogenetic tree, $K_{1,3}$;
- ▶ the superposition of four pure states in a quantum system, [BH01]; [Hey06].

A 'Statistics to Algebraic Geometry' Lexicon, [PS05]

Statistics		Algebra/Geometry
independence	~	Segre variety
exponential family (log-linear models)	~	toric variety
curved exponential family	~	manifold
mixture model	~	secant variety
inference	~	tropicalisation
	⋮	

Applications

We finish by mentioning that algebraic statistics thus has at least a few important & interesting applications:

- ▶ It can win you salmon;
- ▶ It can win you 100 Swiss francs⁴ (CHF 100 \sim £85);
- ▶ One gets to learn lots of big words;
- ▶ It can provide one with a topic for an (excellent) colloquium talk;
- ▶ Algebraists & statisticians may try to talk to one other (this may be a con rather than a pro).

⁴The *100 Swiss Francs Conjecture* was on maximising the likelihood function over the space of 4×4 stochastic matrices, of rank ≤ 2 [Stu09], and was solved in [ZJG11].

Questions?

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