Algebraic Statistics

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"Does Watching Football on TV Cause Hair Loss?"

In a fictional study, 296 British subjects between the ages of 40 – 50 were asked about their hair loss and how much football they watch on television.

3×3 *Contingency Table*

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

TV Time	Hair Amount		
	lots	medium	balding
≥ 2h	51	45	33
$2 - 6$ h	28	30	29
≥ 6h	15	27	38

Based on the data, are these two random variables independent, or is there a correlation?

"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 means that the (2×2)-minors of the data matrix M should vanish, but in fact they are all strictly quite positive, suggesting a positive correlation!

► For example, the top left (2×2)-minor equals:
$51 \cdot 30 - 45 \cdot 28 = 1530 - 1260 = 270 \neq 0$.

"Does Watching Football on TV Cause Hair Loss?"

▶ A better explanation for our data 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 have *conditional independence*:

H_0 : *Football on TV & Hair Loss are Independent* given *Gender*.

Statistical Models

Definition

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

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

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 $[r] := \{1, \ldots, r\}$, and $[c] := \{1, \ldots, c\}$.

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

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}
$P(X = 2)$	p_{21}	p_{22}

$\overset{X \perp\!\!\!\perp Y}{\rightsquigarrow} p_{11}p_{22} = p_{12}p_{21}.$

Finally Some Geometry

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

$$\binom{X^{(1)}}{Y^{(1)}}, \binom{X^{(2)}}{Y^{(2)}}, \ldots, \binom{X^{(n)}}{Y^{(n)}},$$

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*:

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

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

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

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

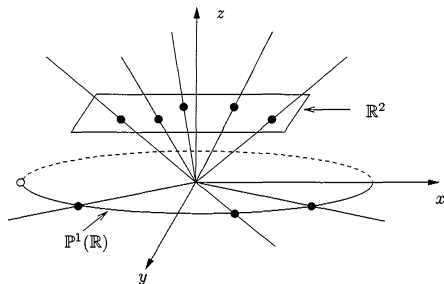$$p_{ij}p_{kl} - p_{il}p_{jk} = 0, \quad (1 \le i < k \le r, \text{ and } 1 \le j < l \le c).$$

These are called *Segre varieties* in algebraic geometry.

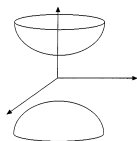Foray Into Algebraic Geometry

Projective Space

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

$$\mathbb{P}^n := \{(z_0, \ldots, z_n) \in \mathbb{C}^n\}/(\mathbf{x} \sim \lambda \cdot \mathbf{y}), \quad \lambda \neq 0,$$
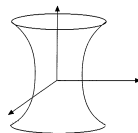
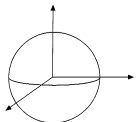that is, its elements consists of *lines through the origin* in $\mathbb{C}^n$.

Varieties

Varieties are the objects studied in algebraic geometry, determined by the *vanishing set*[1] $V(-)$, for a system of polynomials.
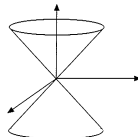
(a) $V(x^2 + y^2 - z^2 + 1)$

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

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

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

---

[1] from '*Verschwindungsmenge*'

Segre Varieties

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

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

Example (Segre quadric surface)

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

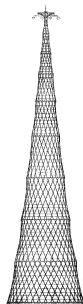Set $[X_1 Y_1, X_1 Y_2, X_2 Y_1, X_2 Y_2] =: [p_{11}, p_{12}, p_{21}, p_{22}]$, then:

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

Rulings

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

Shukhov Tower,
Nizhny Novgorod

Shukhov Tower,
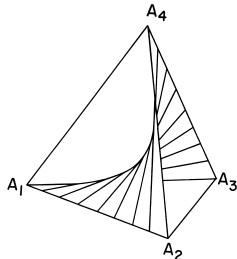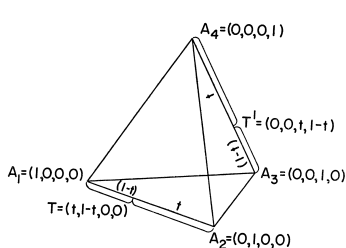Moscow

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]:

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

Hidden Variables Omake r: Known Unknowns

- ► 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 $p^{(1)}, \ldots, p^{(s)}$, with weights given by π.

Definition [DSS09]

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

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

Mixture Models

- ▶ 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:

Molecular Phylogenetics
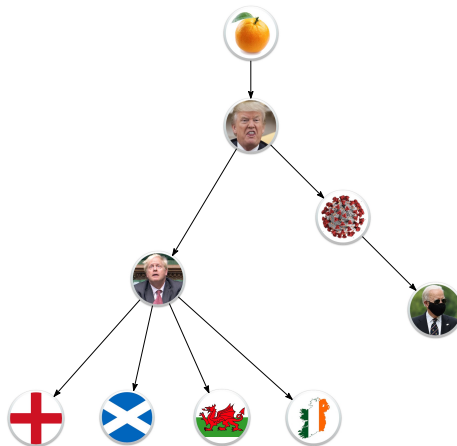
▶ Sequence of DNA molecules in a genome is represented as a sequence of letters from the four letter alphabet $\Sigma = \{A, C, G, T\}$.

▶ *Fix for now* an ancestral nucleotide $Y \in \Sigma$; we assume that the following evolution events occur independently [All07]:

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

▶ 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]:

$$\mathrm{Mixt}^4(\Delta_3)$$

$$= \left\{ \sum_{Y \in \Sigma} \pi_Y \cdot p^{(Y)} \ \middle| \ \pi \in \Delta_3, \ p^{(Y)} \in \mathcal{P} \subseteq \Delta_3, \ \text{for each } Y \right\}.$$

Question?

What is the analogue for mixture models in algebraic statistics?

Secant Varieties

Answer!

Secant² varieties [DSS09]!

Definitions

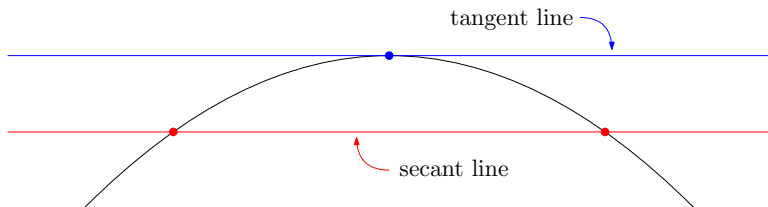▶ Consider two varieties $V, W \subseteq \mathbb{R}^k$. The *join* of V and W is the variety

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

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

$$\mathrm{Sec}^1(V) := V, \qquad \mathrm{Sec}^s(V) := \mathcal{J}(\mathrm{Sec}^{s-1}(V), V).$$
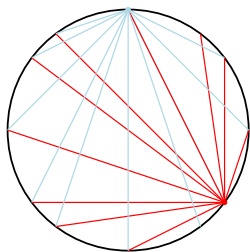
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²from *secare*, "to cut" in Latin; *c.f. tangō*, "to touch".
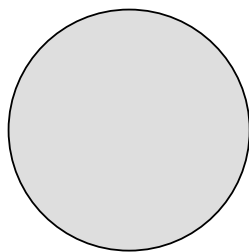
Secant Varieties

tangent line

secant line

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

$\mathrm{Sec}^2(S^1)$
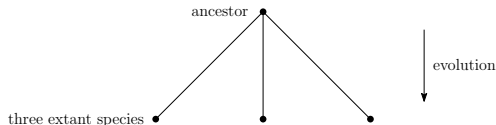
etc.

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: $\mathrm{Sec}^4(\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3)$; or
equivalently $\mathrm{Mixt}^4(\Delta_3 \times \Delta_3 \times \Delta_3)$ [All07].

▶ Finding the minimal set of polynomials defining
$\mathrm{Sec}^4(\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3)$ once gave rise to a very important
application of algebraic statistics...

The *Salmon Problem*

Statement

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

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[3]read this as "set of defining polynomials".

Revision

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

▶ Three independent variables (nucleotides in extant species) $\rightsquigarrow$ three factors in product;

▶ Each independently assumes one value from $\Sigma = \{A, C, G, T\} \rightsquigarrow$ 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

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

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	$\sim$	Segre variety
exponential family	$\sim$	toric variety
(log-linear models)		
curved exponential family	$\sim$	manifold
mixture model	$\sim$	secant variety
inference	$\sim$	tropicalisation
	$\vdots$	

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 francs[4] (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).

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[4]The 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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