Algebraic Statistics

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A *statistical model* is 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, 2002 [McC02]

This should be defined using category theory.

Note on References

General theory without particular references comes from either [PS05] or [DSS09].

A contingency table contains counts obtained by cross-classifying observed cases according to two or more discrete criteria.

Example

TODO: Figure (Florida death sentences)

We ask whether the sentences were made independently of the defendant's race.

- Classify using two criteria with r and c levels, yields two random variables X and Y.
- Code 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}

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

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.:

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

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

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

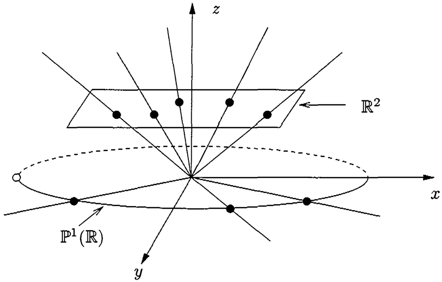
These are called *Segre varieties* in algebraic geometry.

Projective Space

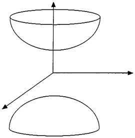
Playing field is *n-dimensional projective space*, $\mathbb{P}^n$:

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

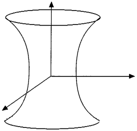
that is, its elements consists of *lines through the origin* in $\mathbb{C}^n$.



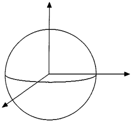
Varieties are the objects studied in algebraic geometry, determined by the *vanishing set*[1] $V(-)$, for a system of polynomials.



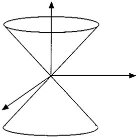
(a) $V(x^2 + y^2 - z^2 + 1)$



(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 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)

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

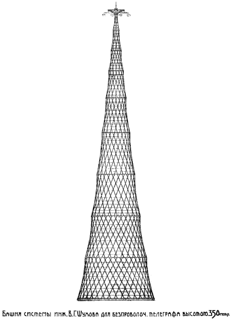
Set $[X_1 Y_1, X_1 Y_2, X_2 Y_1, X_2 Y_2] =: [p_{11}, p_{12}, p_{21}, p_{22}]$, then:

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

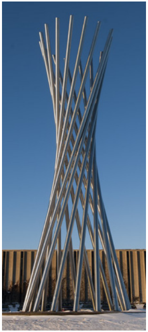
Rulings

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

Shukhov Tower, Nizhny Novgorod



Shukhov Tower, Moscow



Tractricious, Fermilab

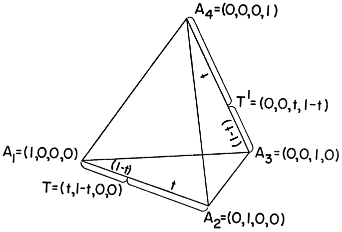
- Let $\Delta_3 \subset \mathbb{R}^4$, with vertices $A_i = e_i$, and let $p = (p_{ij}) \in \Delta_3$ be

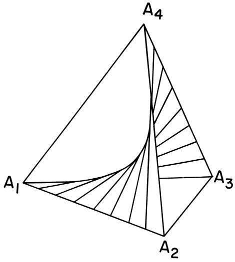
$$p_{ij} = (p_{11}, p_{12}, p_{21}, p_{22}) = \begin{array}{|c|c|} \hline p_{11} & p_{12} \\ \hline p_{21} & p_{22} \\ \hline \end{array}$$

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

st	$s(1-t)$
$t(1-s)$	$(1-s)(1-t)$

$$(0 \le s, t \le 1).$$





Hidden Variables

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

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

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

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

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

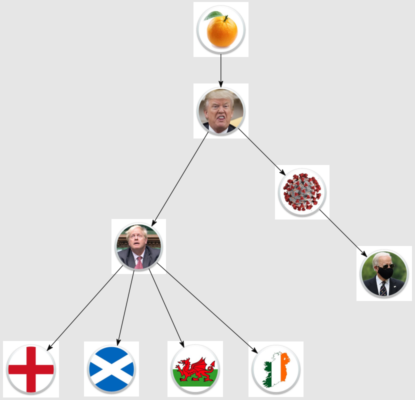
$$\mathrm{Mixt}^s(\mathcal{P}) := \left\{ \sum_{j=1}^{s} \pi_j \cdot p^{(j)} \;\middle|\; \pi \in \Delta_{s-1},\ p^{(j)} \in \mathcal{P},\ \text{for all } j \right\}.$$

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.

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

Example Cartoon



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

$$\mathsf{Y} \xmapsto{\pi_{\mathsf{Y}} \cdot p_{\mathsf{A}}^{(\mathsf{Y})}} \mathsf{A}, \quad \mathsf{Y} \xmapsto{\pi_{\mathsf{Y}} \cdot p_{\mathsf{C}}^{(\mathsf{Y})}} \mathsf{C}, \quad \mathsf{Y} \xmapsto{\pi_{\mathsf{Y}} \cdot p_{\mathsf{G}}^{(\mathsf{Y})}} \mathsf{G}, \quad \mathsf{Y} \xmapsto{\pi_{\mathsf{Y}} \cdot p_{\mathsf{T}}^{(\mathsf{Y})}} \mathsf{T},$$

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

$$\pi_{\mathsf{Y}} \cdot [p_{\mathsf{A}}^{(\mathsf{Y})}, p_{\mathsf{C}}^{(\mathsf{Y})}, p_{\mathsf{G}}^{(\mathsf{Y})}, p_{\mathsf{T}}^{(\mathsf{Y})}] \in \Delta_3 = \Delta_{4-1}.$$

Example

- Y is a hidden variable though; could have been any one of A, C, G, or 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:

$$\mathrm{Mixt}^4(\Delta_3)$$
$$= \left\{ \sum_{\mathsf{Y}\in\{\mathsf{A},\mathsf{C},\mathsf{G},\mathsf{T}\}} \pi_{\mathsf{Y}} \cdot p^{(\mathsf{Y})} \;\middle|\; \pi \in \Delta_3,\ p^{(\mathsf{Y})} \in \mathcal{P} \subseteq \Delta_3,\ \text{for each } \mathsf{Y} \right\}.$$

Question?

What is the analogue for mixture models in algebraic statistics?

Answer!

Secant[2] varieties [DSS09]!

Definitions

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

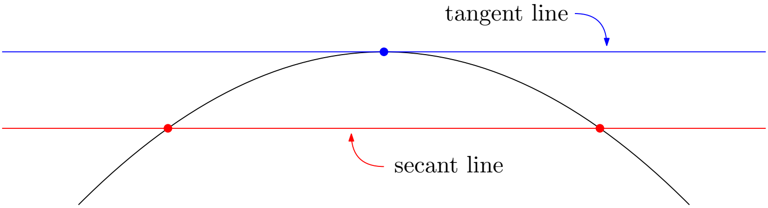
$$\mathcal{J}(V, W) := \{\lambda v + (1-\lambda) w : v \in v, w \in W, \lambda \in [0,1]\}.$$

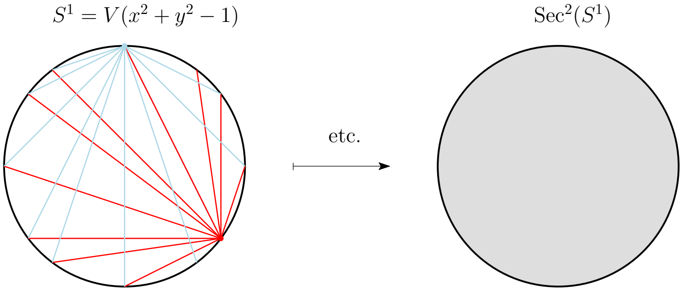
- If $V = W$, then this is the *secant variety* of V, denoted $\mathrm{Sec}^2(V) = \mathcal{J}(V, V)$. The *s-th higher secant variety* is:

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

[2]from *secare*, "to cut" in Latin; *c.f. tangō*, "to touch".

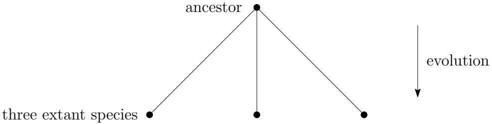
Secant Varieties





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 $\mathrm{Mixt}^4(\Delta_3 \times \Delta_3 \times \Delta_3)$.
- 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* $\mathrm{Sec}^4(\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3)$.

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).

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

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 $\Sigma = \{\mathtt{A}, \mathtt{C}, \mathtt{G}, \mathtt{T}\}$ $\rightsquigarrow$ 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 Σ $\rightsquigarrow$ mix four such independence models;
- The model for the three observed nucleotides is therefore

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

An Opportunity for a Stupid Joke

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, $K_{1,3}$;
- superposition of four pure states in a quantum system.

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 has at least a few important applications:

- It can win you salmon;
- It can win you 100 Swiss francs[4] (CHF $100 \sim £85$);
- One gets to learn lots of polysyllabic words;
- It can provide an individual with a topic for an (excellent) colloquium talk;
- Algebraists & statisticians *could* talk to one other (not that they *would* want to).

[4]Not mentioned in this talk.

Questions?

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