

Algebraic Statistics

Benjamin C. W. Brown

B.Brown@ed.ac.uk

~

30th October 2020

1. INDEPENDENCE MODELS

2. CLASSICAL ALGEBRAIC GEOMETRY

3. MIXTURE MODELS & SECANT VARIETIES

4. SUMMARY

planetmath.org

A *statistical model* is 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, 2002

This should be defined using category theory.

Two-by-Two Contingency Tables

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.

Two-by-Two Contingency Tables

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

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}	$\xrightarrow{\text{~~~~~} X \perp\!\!\!\perp Y \text{~~~~~}}$
$P(X = 2)$	p_{21}	p_{22}	

$$p_{11}p_{22} = p_{12}p_{21}.$$

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*,

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

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

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

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

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

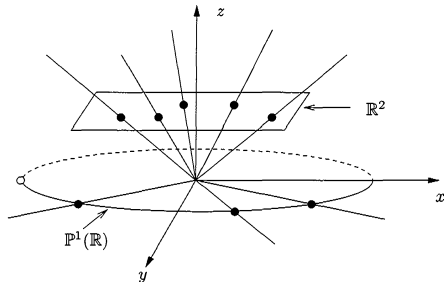
These are examples of *Segre varieties* in algebraic geometry.

Projective Space

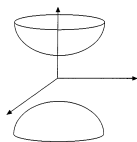
Playing field is n -dimensional projective space, \mathbb{P}^n :

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

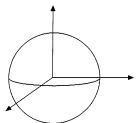
that is, its elements consists of *lines through the origin* in \mathbb{C}^n .



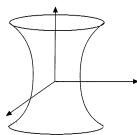
Varieties are the objects studied in algebraic geometry, determined by the *vanishing set*¹ $V(-)$, for a system of polynomials.



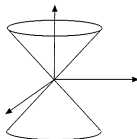
(a) $V(x^2 + y^2 - z^2 + 1)$



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



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



(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 - the Segre quadric surface

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

If we 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*. They are the images of $\sigma(\mathbb{P}^1 \times \{\text{pt}\})$ and $\sigma(\{\text{pt}\} \times \mathbb{P}^1)$.



Manifold of Independence

- Let $\Delta_3 \subset \mathbb{R}^4$, with vertices $A_i = e_i$. Denote a general point $p = (p_{ij}) \in \Delta_3$ by

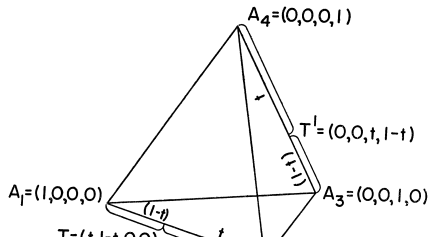
$$p_{ij} = (p_{11}, p_{12}, p_{21}, p_{22}) = \begin{array}{|c|c|} \hline p_{11} & p_{12} \\ \hline p_{21} & p_{22} \\ \hline \end{array}$$

- CITE!!!! have shown that the two rulings are given by

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

 $(0 \leq s, t \leq 1);$

a *hyperbolic paraboloid* inside of Δ_3 , called the *manifold of independence*.



TODO: FIGURE.

- ▶ 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

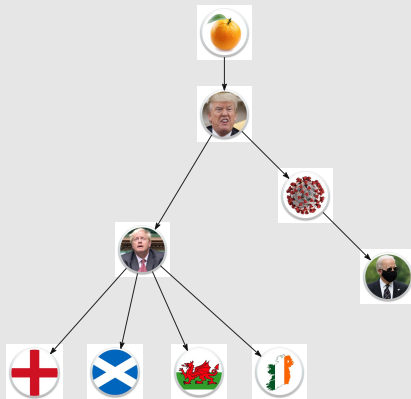
Let $\mathcal{P} \subset \Delta_{r-1}$ be a statistical model. The s -th mixture model is

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

- ▶ 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:

Example Cartoon

- ▶ Sequence of DNA molecules in a genome is represented as a sequence of letters from the four letter alphabet $\Sigma = \{A, C, G, T\}$.
- ▶ At a particular site of the genome, any of the four nucleotides $X \in \Sigma$, say, might be observed.
- ▶ Based on a particular ancestral nucleotide of X , might expect evolution to occur in a way that the state of the current nucleotide is independent of one another:

$$A \mapsto X, C \mapsto X, G \mapsto X, \text{ or } T \mapsto X.$$

- ▶ So for each ancestral nucleotide, we have an independence model; its distribution is determined by a point of $\Delta_3 = \Delta_{4-1}$.

Example

- ▶ X is a hidden variable though; could have been any one of A, C, G, or T.
- ▶ For *exactly one choice* of X , we had the distribution Δ_3 ; need to consider *all choices* of ancestral nucleotide.
- ▶ Hence we get the mixture model: $\text{Mixt}^4(\Delta_3) =$

$$\left\{ \sum_{i=1}^4 \text{Prob}(X = i) \cdot \lambda_i : i \in \Sigma, \lambda_i \in [0, 1], \lambda_1 + \dots + \lambda_4 = 1 \right\}.$$

- ▶ **Q?:** What is the analogue for mixture models in algebraic statistics?

- ▶ **A!:** Secant² varieties!

Definitions

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

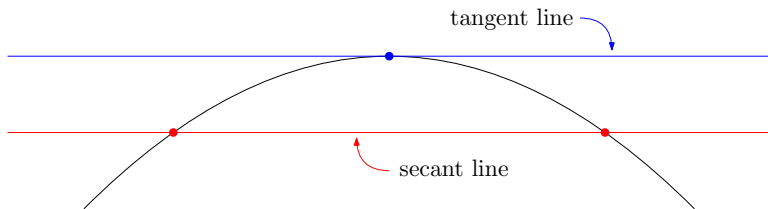
$$\mathcal{J}(V, W) := \{\lambda v + (1 - \lambda)w : v \in V, w \in W, \lambda \in [0, 1]\}.$$

- ▶ 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:

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

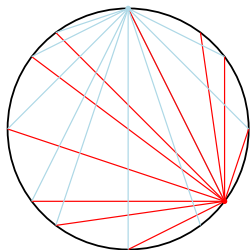
²from *secare*, “to cut” in Latin; c.f. *tangō*, “to touch”.

Secant Varieties

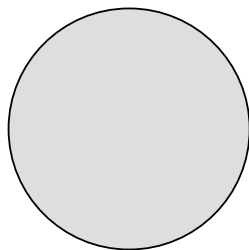


$$S^1 = V(x^2 + y^2 - 1)$$

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

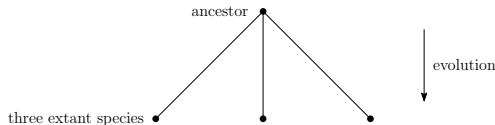


etc.
→



More Complicated Phylogenetic Trees

- ▶ Last example only had one extant species; $X \xrightarrow{?} A, C, G, T$.
- ▶ What if we had three extant species, coming from one ancestor?



- ▶ Now we have to consider: $\text{Sec}^4(\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3)$; or equivalently $\text{Mixt}^4(\Delta_3 \times \Delta_3 \times \Delta_3)$.
- ▶ 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 $\text{Sec}^4(\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3)$.

Prize

Personally caught, and smoked just for you, copper river salmon from Alaska.

Current Status

Solved.

- ▶ At an IMA workshop in 2007, Elizabeth Allman offered this prize to whomever solved the above problem.
- ▶ It was solved in 2010 by Shmuel Friedland.

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

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

An Opportunity for a Stupid Joke

Henri Poincaré

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



Figure: Henri Poincaré, 1887.



Figure: Poincaré, colourised.

The solution to the salmon conjecture is equivalent to:

Some familiar:

- ▶ the mixture of four models for three independent variables;
- ▶ the fourth secant variety of the Segre variety $\mathbb{P}^3 \times \mathbb{P}^3 \times \mathbb{P}^3$.

And some less familiar:

- ▶ the set of $(4 \times 4 \times 4)$ -tables of tensor rank ≤ 4 ;
- ▶ the naive Bayes model with four classes;
- ▶ 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.

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 francs⁴ (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).

⁴Not mentioned in this talk.

Questions?