

## week 5 day 2

“Likelihood Geometry & Intro to exact testing for log-linear models”  
“Algebraic & Geometric Methods in Statistics”

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Created for Math/Stat 561

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## Related readings

Chapter 7 from our textbook.

### Goals

- Understand examples
- Understand counting the number of solutions
- See how it all plays out in the discrete exponentail family case.

# Likelihood geometry

- Recap: Likelihood inference

$$\mathcal{M}_{X||Y} = \{p = \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix} \in \Delta_3 : p_{ij} = \alpha_i \beta_j, (\alpha, \beta) \in \Delta_1 \times \Delta_1\} \text{ and } u = \begin{pmatrix} 19 & 141 \\ 17 & 149 \end{pmatrix}$$

Log-likelihood function:  $l(\alpha, \beta | u) = 160 \log \alpha_1 + 166 \log \alpha_2 + 36 \log \beta_1 + 290 \log \beta_2$

$$= 160 \log \alpha_1 + 166 \log(1 - \alpha_1) + 36 \log \beta_1 + 290 \log(1 - \beta_1)$$

Score equations:

$$\frac{\partial l(\alpha, \beta | u)}{\partial \alpha_1} = \frac{160}{\alpha_1} - \frac{166}{1 - \alpha_1} = 0$$

$$\frac{\partial l(\alpha, \beta | u)}{\partial \beta_1} = \frac{36}{\beta_1} - \frac{290}{1 - \beta_1} = 0$$

Figure 1: Example of score equations

## Discrete setup

- Parametric model given by a *rational map*  $p : \Theta \rightarrow \Delta_{r-1}$
- *iid* samples  $X^{(1)}, X^{(2)}, \dots, X^{(n)}$  such that  $X^{(i)} \sim p$  for some **unknown**  $p$
- The vector of **counts**  $u \in \mathbb{N}^r$ , with  $u_j = |\{i : X^{(i)} = j\}|$
- *Log-likelihood function*  $\ell(\theta|u) = \sum_{j=1}^r u_j \log p_j$
- **Score equations**  $\sum_{j=1}^r \frac{u_j}{p_j} \frac{dp_j}{d\theta_i}$ . One equation for each  $\theta_i$ .

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## Theorem & Definition

Let  $\mathcal{M} \subseteq \Delta_{r-1}$  be a statistical model. For *generic*<sup>a</sup> data, the number of solutions to the score equations is independent of  $u$ .

The number of solutions to the score equations for generic  $u$  is called the **maximum likelihood degree** (ML degree) of the parametric discrete statistical model  $\mathcal{M}$ .

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<sup>a</sup>'sufficiently random', outside a variety

Computational algebra is really good at counting the number of solutions to a system of polynomial/rational equations!!

# Implicit models

## Problem

Given vector of counts  $u$ , we would like to maximize the log-likelihood function  $\ell(\theta|u) = \sum_{j=1}^r u_j \log p_j$  over the *intersection* of the interior of the probability simplex  $\Delta_{r-1}$  and the variety  $V(\text{polynomials defining the model})$ .

## Example

$$M_{X \perp\!\!\!\perp Y} = \left\{ \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{bmatrix} \in \Delta_3 : p_{11}p_{22} - p_{12}p_{21} = 0 \right\} \text{ and } u = \begin{bmatrix} 19 & 141 \\ 17 & 149 \end{bmatrix}.$$

- Maximize  $\ell(p|u) = 19 \log p_{11} + 141 \log p_{12} + 17 \log p_{21} + 149 \log p_{22}$  over  $M_{X \perp\!\!\!\perp Y}$ .
- The polynomial **constraints** are  $p_{11} + p_{12} + p_{21} + p_{22} = 1$  and  $p_{11}p_{22} - p_{12}p_{21} = 0$ .

→ Go to [lecture9-interlude-LangrangeMultipliers.pdf](#)

# Exponential families have concave likelihood functions

## Proposition

Let  $\mathcal{M}$  be an *exponential family* with minimal sufficient statistics  $T(x)$  and natural parameter  $\eta$ . ( $f_\eta(x) = h(x)e^{\eta^t T(x) - A(\eta)}$ .) Then the likelihood function is **strictly concave**.

- The MLE, if it exists, is the solution to  $T(x) = \mathbb{E}_\eta[T(X)]$ .
  - $x$  denotes the data vector.

- *iid* samples  $\implies$  sufficient statistic of the sample is  $T_n(X^{(1)}, \dots, X^{(n)}) = \sum_{i=1}^n T(X^{(i)})$ .

## Theorem (Prop 7.3.7)

**Exponential family**  $p_\theta(x) = h(x) \exp(\langle \theta, T(x) \rangle - A(\theta))$  with sufficient statistics  $T(x)$ , log-partition function  $A(\theta) = \log \int_{\mathcal{X}} h(x) \exp(\langle \theta, T(x) \rangle)$   
Then

$$\frac{\partial}{\partial \theta_i} A(\theta) = \mathbb{E}_\theta[T_i(X)] \quad \text{and} \quad \frac{\partial^2}{\partial \theta_i \partial \theta_j} A(\theta) = \text{Cov}_\theta[T_i(X), T_j(X)].$$

## Example: ML degree of (rescaled) binomial is 3

$$p(\theta) = (s, s\theta, s\theta^2, s\theta^3) \in \Delta_3 \subset \mathbb{R}^4.$$

where  $s = \frac{1}{1+\theta+\theta^2+\theta^3}$ . Sample size  $n = u_0 + u_1 + u_2 + u_3$ . We have

$$\begin{aligned} L(\theta|u) &= s^{u_0} (s\theta)^{u_1} (s\theta^2)^{u_2} (s\theta^3)^{u_3} \\ &= s^{u_0+u_1+u_2+u_3} \theta^{u_1+2u_2+3u_3} \end{aligned}$$

$$\ell(\theta|u) = n \log s + (u_1 + 2u_2 + 3u_3) \log \theta$$

The score equation is:

$$0 = \frac{\partial \ell}{\partial \theta} = -ns(1 + 2\theta + 3\theta^2) + (u_1 + 2u_2 + 3u_3) \frac{1}{\theta}$$

Thus  $3n\theta^3 + 2n\theta^2 + n\theta - (u_1 + 2u_2 + 3u_3)s^{-1} = 0$  and we arrive at

$$3(n - u_3)\theta^3 + 2(n - u_2)\theta^2 + (n - u_1)\theta - (u_1 + 2u_2 + 3u_3) = 0$$



## ML for discrete expo fam.

### Theorem (Prop 7.3.7)

*Exponential family*  $p_{\theta}(x) = h(x) \exp(\langle \theta, T(x) \rangle - A(\theta))$  with sufficient statistics  $T(x)$ , log-partition function  $A(\theta) = \log \int_{\mathcal{X}} h(x) \exp(\langle \theta, T(x) \rangle)$   
Then

$$\frac{\partial}{\partial \theta_i} A(\theta) = \mathbb{E}_{\theta}[T_i(X)] \quad \text{and} \quad \frac{\partial^2}{\partial \theta_i \partial \theta_j} A(\theta) = \text{Cov}_{\theta}[T_i(X), T_j(X)].$$

### Corollary (Cor 7.3.8)

The likelihood function for an exponential family is *strictly concave*. The MLE (if it exists) is the *unique* solution to the equation

$$\mathbb{E}_{\theta}[T(X)] = T(x)$$

where  $x$  denotes the data vector.

## Corollary [Birch's theorem]

Let  $A \subseteq \mathbb{Z}^{k \times r}$  such that  $1 \in \text{rowspan}(A)$ . Let  $u$  be a vector of counts from *iid* samples. Then the MLE of the log-linear model is **the unique solution**, if it exists, to

$$Au = nAp \text{ and } p \in \mathcal{M}_A.$$

- Inspires algorithms for computing MLE:
  - **Iterative proportional fitting**. Stephen Fienberg, [AMS 1970](<https://www.jstor.org/stable/2239244>).
- R can do this - it's super fast
  - some resources at end of these slides
  - IPF is usually embedded inside other functions

```
fm <- loglin(HairEyeColor, list(c(1, 2), c(1, 3), c(2, 3)))
```

```
5 iterations: deviation 0.04093795
```

```
## fm
```

## The following problem will appear on HW 3

- exercise 7.2. in the book

Let  $\mathcal{M}$  be the model of binomial random variables  $\text{Bin}(2, \theta)$ :

$$\mathcal{M} = \{(1 - \theta)^2, 2\theta(1 - \theta), \theta^2) \in \Delta_2 : \theta \in (0, 1)\}.$$

- What is the ML degree of  $\mathcal{M}$ ?
- Compute the MLE  $\hat{\theta}$  for the two data points  $u = (8, 6, 5)$  and  $v = (4, 20, 8)$ . Interpret your results

## Interlude: log-linear models Campuswire post #37.

Did anyone try and succeed to write out what it means that " $\log(p)$  is in the  $\text{rowspan}(A)$ " for the example of the independence model?

## Interlude: log-linear models Campuswire post #37.

### Observation

Let  $p \in \mathcal{M}_{X \perp\!\!\!\perp Y}$ . If  $p$  has all positive entries ( $p \in \text{int}(\Delta_{\mathcal{R}-1})$ ) then

$$\begin{aligned}\log p &= (\log p_{1+} p_{+1}, \log p_{1+} p_{+2}, \log p_{2+} p_{+1}, \log p_{2+} p_{+2}) \\ &= (\log p_{1+} + \log p_{+1}, \log p_{1+} + \log p_{+2}, \log p_{2+} + \log p_{+1}, \log p_{2+} + \log p_{+2}) \\ &= \log p_{1+}(1, 1, 0, 0) + \log p_{2+}(0, 0, 1, 1) + \log p_{+1}(1, 0, 1, 0) \\ &\quad + \log p_{+2}(0, 1, 0, 1).\end{aligned}$$

Thus  $\log p \in \mathcal{M}_A$ , where  $A \in \mathbb{Z}^{4 \times 4}$  is the matrix

$$A = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}.$$

- Answer by Miles:

In general (from slide 13 or lec. 7):

$$p_{\theta} = \frac{1}{Z(\theta)} h \prod_j \theta^{a_j} \text{ where } a_j \text{ is the } j^{\text{th}} \text{ row of } A \in \mathbb{Z}^{k \times r}.$$

If  $p_{\theta} \in \text{int}(\Delta_{\mathcal{R}-1})$  then  $(1, \dots, 1) = \mathbf{1} \in \text{rowspan}(\mathbf{A})$  i.e.  $\mathbf{1} = \mathbf{cA}$  for some vector  $c \in \mathbb{Z}^r$

$$\begin{aligned} \text{Assume } h = \mathbf{1}. \text{ Then } \log p_{\theta} &= \log(h) - \log(Z(\theta))\mathbf{1} + \sum_j \mathbf{a}_j \log \theta \\ &= \mathbf{0} - \log(\mathbf{Z}(\theta))\mathbf{cA} + \log \theta \mathbf{A} &= (-\log(Z(\theta))c + \log \theta) A \end{aligned}$$

Here  $-\log(Z(\theta))c + \log \theta$  is just a vector, in  $\mathbb{R}^r$  so this means  $\log p_{\theta} \in \text{rowspan}(A)$

# Exact testing!

this is our next topic!!

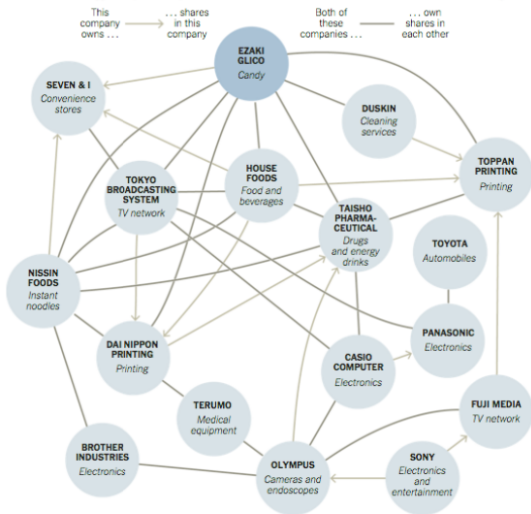
- Last slide from likelihood geometry said: “IPF is usually embedded inside other functions”
- ... which begs the question: What other questions might we have??

The following few slides are a **preview** of our next topic.

# Is the given set of shareowning relations expected or not?

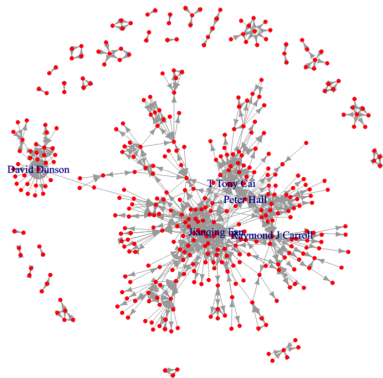
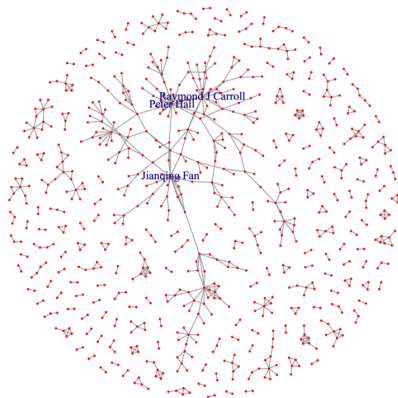
## Inside Japan Inc.

Many companies in Japan own shares in each other to create relationships that can protect them from outside interference. Here are some companies that have disclosed their connections, beginning with Ezaki Glico, a candy maker that has struggled to post steady returns even as it has resisted other shareholders' demands for change.





# Are degrees a good summary of a network?

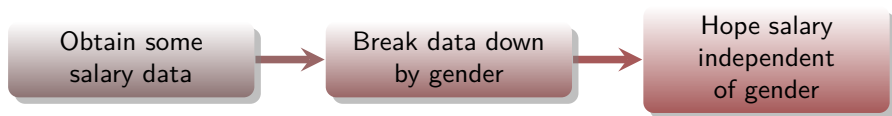


## At the heart of statistical reasoning

- Given: data, find out if it is usual/expected? surprising/outlier? quantify??

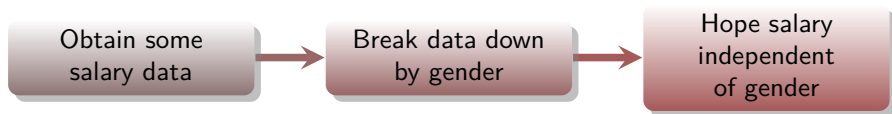
# At the heart of statistical reasoning

- Given: data, find out if it is usual/expected? surprising/outlier? quantify??
- Do all genders get fair salary in Tirana?



## At the heart of statistical reasoning

- Given: data, find out if it is usual/expected? surprising/outlier? quantify??
- Do all genders get fair salary in Tirana?



- We expect a certain 'shape' of the data. A certain... distribution!

**YOUR** everyday intuition  $\mapsto$  formal framework.

|                    | M  | F  | Other |          |
|--------------------|----|----|-------|----------|
| $\leq 1,2M$<br>LEK |    |    |       | 13       |
| $> 1,2M$<br>LEK    |    |    |       | 13       |
|                    | 10 | 10 | 6     | 26 total |

Figure 6: Small table format

# A simple search: Chicago data science salary data

glassdoor

data scientist

Chicago, IL



## Data Scientist Salaries Chicago, IL

F

Overview

Salaries

Interviews

Insights

Career Path

### How much does a Data Scientist make in Chicago, IL?

Experience

All years of Experience

Industry

All industries

**\$134,267** / yr

Total Pay

**\$110,139** / yr

Base Pay

**\$24,128** / yr

Additional Pay

**\$134,267** / yr



The estimated total pay for a Data Scientist is \$134,267 per year in the Chicago, IL area, with an average salary of \$110,139

### Total Pay Trajectory

For Data Scientist in Chicago, IL

\$134,267 / yr  
Data Scientist

\$176,030 / yr  
Senior Data Scientist

\$178,448 / yr  
Lead Data Scientist

[See Full Career Path](#)

[Download as data table](#)

### Related Job Titles

For Data Scientist in Chicago, IL

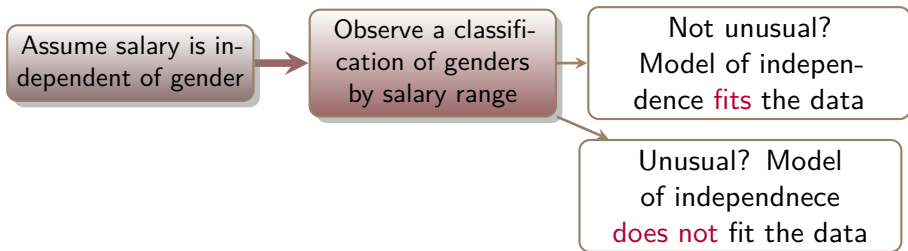
Some related job titles:

# Formal reasoning with data: independence example

- **Modeling:** Construct a statistical model for **independence**.
- **Question:** Does the model **fit** the observed set of gender vs. salary ranges?

(Can it adequately explain how the salary data was generated?)

- **Process:**



# Models with a design matrix

- $X_1, \dots, X_k$  discrete random variables,  $X_i \in \{1, \dots, d_i\}$
- $u$  = a **k-way contingency table**  $u \in \mathbb{Z}_{\geq 0}^{d_1 \times \dots \times d_k}$  [Draw a table!] Flatten  $u$  to vector.

## Log-linear model

Sufficient statistics = **marginals** of  $u$ :  $P_\theta(U = u) = \exp\{\langle \mathbf{A}u, \theta \rangle - \psi(\theta)\}$ .

## Example $X_1 \perp\!\!\!\perp X_2$

$$\left[ \begin{array}{cccc|cccc|ccc} 1 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & 1 & 1 & \cdots & 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & 1 & 1 & \cdots & 1 \end{array} \right]$$


---


$$\left[ \begin{array}{cccc|cccc|ccc} 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 & 0 & 1 & \cdots & 0 & \cdots & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 1 & \cdots & 0 & 0 & \cdots & 1 \end{array} \right]_{(d_1+d_2) \times d_1 d_2}$$

$$\cdot \begin{bmatrix} u_{11} \\ \vdots \\ u_{d_1 d_2} \end{bmatrix} = \begin{bmatrix} u_{1+} & \cdots & u_{+d_2} \end{bmatrix}.$$

# Conclusions

## Main take-aways about *likelihood geometry*

- Numerical algorithms for computing MLE, for example the EM algorithm implemented widely, are usually some form of hill-climbing. They have no way of telling you whether you are at a global or local optimum.
- Likelihood function in exponential families is strictly concave
  - However there can be local optima on the boundary of the model
- When you compute estimates numerically, it is a good idea to understand how many critical points there are
  - You can set up the system of score equations
  - You can count the number of (complex) solutions to those equations
    - This quantity, called the **ML degree** in algebraic statistics, is one measure of complexity of estimation.
- ML degree is one *if and only if* the MLE formula is a rational function of the data.
  - Birch's theorem.



## Additional material

- Here is a [vignette](#) about how IPF algorithm works in R.
- In `python`, I have not used this, but found this link which appears to be useful: [IPF in python](#)

# License

Parts of this presentation are from Kaie Kubjas' course lectures, used with permission; and Carlos Amendola's lecture in Bernd Sturmfel's short course on Algebraic Statistics in Berlin, fall 2022.

This document is created for Math/Stat 561, Spring 2023.

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