MLE DEGREE OF DISCRETE RANDOM CYCLES

Courtney R. Gibbons

August 4, 2017

Hamilton

arXiv:1703.02251 NSF Grant Number DMS 1321794

Joint work with Carlos Améndola, Nathan Bliss, Isaac Burke, Martin Helmer, Serkan Hoşten, Evan D. Nash, Jose Israel Rodriguez, Daniel Smolkin

Problem. Model to use is known and data is available $\Longrightarrow$ MLE.

Parametrize. Build a matrix A to parametrize the model.
“Statistical models are algebraic varieties.” – T. Kahle

Scale. Scale the the model in different ways to study ML degree.

Polytope. Study properties of the polytope Q of A.

Theorems. Prove theorems about the way c changes the number of solutions to the maximum likelihood equations for the model.

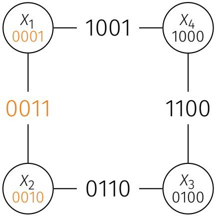
Four (binary) variables

Smoker; High blood pressure;
Family history of heart disease; High lipoprotein ratio;
X : Joint binary random variable (X_1, X_2, X_3, X_4).

$i, j, k, \ell \in \{0, 1\}$

$p_{ijk\ell} = \text{prob}(X_1 = i, X_2 = j, X_3 = k, X_4 = \ell)$

$u_{ijk\ell} = \text{data vector};\ u_{0000} = 297,\ u_{1000} = 275,\ \ldots\ u_+ := \sum u_{ijk\ell} = 1841.$



This graph encodes independence statements: X_1 and X_3 independent given X_2 and X_4 and vice versa.

Parametrize and build a matrix:

- For each vertex, record the "on states" of X_t in the joint random variable X. For each edge $X_t X_{t'}$, record the combinations of on states of both X_t and $X_{t'}$.

  Parameters: $\theta_{0001}, \theta_{0010}, \theta_{0100}, \theta_{1000}, \theta_{0011}, \theta_{0110}, \theta_{1100}, \theta_{1001}$

- Make a matrix...

- Label the rows of a matrix A by the θ parameters and the columns by the probabilities $p_{0000}, p_{0001}, \ldots, p_{1111}$.
- Place a 1 in an entry if the parameter label is termwise less than or equal to the probability label.

$$
A = \begin{array}{c} \\ s \\ s\theta_{1000} \\ s\theta_{0100} \\ s\theta_{0010} \\ s\theta_{0001} \\ s\theta_{1100} \\ s\theta_{1001} \\ s\theta_{0110} \\ s\theta_{0011} \end{array}
\begin{array}{c} \begin{array}{cccccccccccccccc} p_{0000} & p_{0001} & p_{0010} & p_{0011} & p_{0100} & p_{0101} & p_{0110} & p_{0111} & p_{1000} & p_{1001} & p_{1010} & p_{1011} & p_{1100} & p_{1101} & p_{1110} & p_{1111} \end{array} \\
\left(\begin{array}{cccccccccccccccc}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\
0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1
\end{array} \right) \end{array}
$$

Let V be the Zariski closure of the image of

$$\psi^c : (\mathbb{C}^*)^9 \longrightarrow (\mathbb{C}^*)^{16}$$
$$\psi^c(s, \theta_1, \ldots, \theta_8) \longmapsto (c_1 s\theta^{\mathrm{col}_1(A)}, c_2 s\theta^{\mathrm{col}_2(A)}, \ldots, c_8 s\theta^{\mathrm{col}_8(A)})$$

for some $c \in (\mathbb{C}^*)^{16}$.

Eg, for the matrix A on the previous slide,

$$\psi^{(c_1,\ldots,c_{16})}(\theta) = (c_{0000}s, \ldots, c_{0101}s\theta_{0100}\theta_{0001}, \ldots).$$

Let $f = \sum_{t=1}^{16} c_t\theta^{\mathrm{col}_t(a)}$. (The image of θ is in the hyperplane $\sum_{ijk\ell} p_{ijk\ell} - 1$.)

(Statisticians: these are probabilities, so $sf = 1$)

The Zariski closure $V^{(1,\dots,1)}$ of the image of this parametrization is a toric variety defined by the following prime ideal:

$$
\begin{aligned}
I = \langle\, & p_{1011}p_{1110} - p_{1010}p_{1111},\ p_{0111}p_{1101} - p_{0101}p_{1111},\\
& p_{1001}p_{1100} - p_{1000}p_{1101},\ p_{0110}p_{1100} - p_{0100}p_{1110},\ p_{0011}p_{1001} - p_{0001}p_{1011},\\
& p_{0011}p_{0110} - p_{0010}p_{0111},\ p_{0001}p_{0100} - p_{0000}p_{0101},\ p_{0010}p_{1000} - p_{0000}p_{1010},\\
& p_{0100}p_{0111}p_{1001}p_{1010} - p_{0101}p_{0110}p_{1000}p_{1011},\ p_{0010}p_{0101}p_{1011}p_{1100} - p_{0011}p_{0100}p_{1010}p_{1101},\\
& p_{0001}p_{0110}p_{1010}p_{1101} - p_{0010}p_{0101}p_{1001}p_{1110},\ p_{0001}p_{0111}p_{1010}p_{1100} - p_{0011}p_{0101}p_{1000}p_{1110},\\
& p_{0000}p_{0011}p_{1101}p_{1110} - p_{0001}p_{0010}p_{1100}p_{1111},\ p_{0000}p_{0111}p_{1001}p_{1110} - p_{0001}p_{0110}p_{1000}p_{1111},\\
& p_{0000}p_{0111}p_{1011}p_{1100} - p_{0011}p_{0100}p_{1000}p_{1111},\ p_{0000}p_{0110}p_{1011}p_{1101} - p_{0010}p_{0100}p_{1001}p_{1111}\,\rangle.
\end{aligned}
$$

Given a data vector u, let

$$\ell_u(p) = \frac{p_{0000}^{u_{0000}} \cdot p_{0001}^{u_{0001}} \cdots p_{1111}^{u_{1111}}}{(p_{0000} + \cdots + p_{1111})^{u_{0000}+\cdots+u_{1111}}}.$$

Goal: find a probability distribution $\hat{p} = (\hat{p}_1, \ldots, \hat{p}_n)$ in V which maximizes ℓ_u. Such a probability distribution $\hat{p}$ is a ***maximum likelihood estimate***, and $\hat{p}$ can be identified by computing all critical points of ℓ_u on V.

Let $u = (u_{0000}, \ldots, u_{1111})$ and recall $u_+ = \sum_{ijk\ell} u_{ijk\ell}$. Using Lagrange multipliers, we obtain the likelihood equations for the variety V:

$$1 = sf$$

$$\vdots$$

$$(Au)_t = u_+ s \theta_t \frac{\partial f}{\partial \theta_t} \text{ for } t = 1, \ldots, d-1.$$

The (only real) solution to the ML equations is the only real point in the variety over these polynomials.

The binary 4-cycle parametrized with $c = (1, \ldots, 1)$ has degree 64 (use your favorite software or theorem to prove this) and ML degree...13.[1]

1. For what c does $\text{MLdeg}(V^c) = \text{MLdeg}(V^{(1,\ldots,1)})$?
2. How does the choice of c affect how much $\text{MLdeg}(V^c)$ drops from $\deg(V^{(1,\ldots,1)})$?

[1] This was first computed in [GMS06, p. 1484]

The Main Idea: For A, the associated projective variety V, and polynomial $f = \sum_{t=1}^{16} c_t \theta^{\mathrm{col}_t(A)}$, define the variety

$$\nabla_A = \overline{\left\{ c \in (\mathbb{C}^*)^{16} \middle| \exists \theta \in (\mathbb{C}^*)^9 \text{ where } f \text{ and its partials by } \theta_t \text{ all vanish} \right\}},$$

and then look at an irreducible polynomial that vanishes on $\nabla(A)$. If this polynomial is unique (up to scalar multiple), then it is called the *A-**discriminant***, $\Delta_A(f)$.

When the toric variety V is smooth, and Q is the lattice polytope whose vertices are columns of A, the ***Principal*** A***-determinant*** is

$$E_A(f) = \prod_{\substack{\Gamma \text{ nonempty} \\ \text{face of } Q}} \Delta_{\Gamma \cap A}$$

where $\Gamma \cap A$ is the matrix whose columns correspond to the lattice points contained in Γ. The locus of $E_A(f)$ is denoted Σ_A.

When V is a toric hypersurface, $E_A(f) = \Delta_A(f)$ (and is easy to calculate).

The binary 3-cycle can be parametrized by

$$B = \begin{array}{c} \\ 1 \\ \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \\ \theta_5 \\ \theta_6 \end{array} \begin{array}{c} \begin{array}{cccccccc} p_{000} & p_{001} & p_{010} & p_{011} & p_{100} & p_{101} & p_{110} & p_{111} \end{array} \\ \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix} \end{array}$$

and has kernel $\ker(B) = (1, -1, -1, 1, -1, 1, 1, -1)^T$.

Thus B is a hypersurface generated by $p_{000}p_{011}p_{101}p_{110} - p_{001}p_{010}p_{100}p_{111}$, and $EBf = \Delta_B(f) = c_{000}c_{011}c_{101}c_{110} - c_{001}c_{010}c_{100}c_{111}$.

Theorem (MRC Likelihood Geometry Group)

Let $V^c \subset \mathbb{P}^{n-1}$ be the projective variety defined by the monomial parametrization $\psi^c : (\mathbb{C}^*)^d \longrightarrow (\mathbb{C}^*)^n$ where

$$\psi^c(s, \theta_1, \theta_2, \ldots, \theta_{d-1}) = (c_1 s\theta^{a_1}, c_2 s\theta^{a_2}, \ldots, c_n s\theta^{a_n}),$$

and $c \in (\mathbb{C}*)^n$ is fixed. Then $\mathrm{MLdeg}(V^c) < \deg(V)$ if and only if c is in the principal A-determinant of the toric variety $V = V^{(1,\ldots,1)}$.

Proposition (MRC Likelihood Geometry Group)

The ML degree of the binary 3*-cycle is* 4 *unless* $c \in (\mathbb{C}^*)^{d+1}$ *is in* Σ_A*. If* $c \in \Sigma_A$*, then* $\mathrm{MLdeg}(V^c) = 3$.

Proof.

Observe that V^c is a hypersurface with generator $g(p)$. Then $E_A(f) = g(c)$. Fix a useful monomial ordering.

Find a Gröbner basis for

$$I = \langle\, g\,,\ \Delta_A\,,\ \text{MLE equations}\,\rangle\,.$$

Use [GS] and a random data vector u to calculate a Gröbner basis $\{g_1 = \Delta_A, g_2, \dots, g_15\}$ for I.

Analyze degrees of the leading terms under the assumption that $c_{ijk} \in \mathbb{C}^*$ and satisfies the equation $g_1 = \Delta_A = 0$: g_2 is a univariate polynomial in p_{111} of degree 3, and the initial terms of g_3 through g_{15} have degree 1 in p_{ijk}. □

For the binary random 4-cycle, here is what we know:

- The polytope Q has 24 facets, of which 5 are simplices and 3 are hypersurfaes. There are 16 with nontrivial discriminants.
  - We calculated these yesterday in [GS]!
  - We have not analyzed them yet.
- There are 168 codimension two faces of Q, and 88 are not simplices. Of these:
  a) 24 faces have 8 vertices. They're all simplices or arise from hypersurfaces.
  b) 32 faces have 9 vertices. There is only one whose discriminant does not lie on coordinate hyperplanes. It's generated by

$$c_{0110}c_{1000}c_{1011}c_{1101} + c_{0100}c_{1001}c_{1011}c_{1110} - c_{0100}c_{1001}c_{1010}c_{1111}.$$

  c) 32 faces have 10 vertices and their discriminants all lay on coordinate hyperplanes.

Thanks!

- I. M. Gelfand, M. M. Kapranov, and A. V. Zelevinsky, *Discriminants, resultants, and multidimensional determinants*, Mathematics: Theory & Applications, Birkhäuser Boston, Inc., Boston, MA, 1994.
- Dan Geiger, Christopher Meek, and Bernd Sturmfels, *On the toric algebra of graphical models*, Ann. Statist. **34** (2006), no. 3, 1463–1492.
- Daniel R. Grayson and Michael E. Stillman, *Macaulay2, a software system for research in algebraic geometry*, Available at `http://www.math.uiuc.edu/Macaulay2/`.