Maximum likelihood geometry

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High school probability

n-sided die, probabilities $P = (p_1, \ldots, p_n)$, thrown N times
$\rightsquigarrow$ prob of $U = (u_1, \ldots, u_n) \in \mathbb{N}^n$ with $u_1 + \ldots + u_n = N$ is

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Example
If only constraints are $\sum_i p_i =: p_+ = 1$ and $p_i \geq 0$
$\rightsquigarrow$ maximum attained by $p_i := u_i/N$.

(Mixtures of) independence

$P = (p_{ij})_{ij} \in \mathbb{R}^{m \times n}$ joint distribution of *two* random variables
$\rightsquigarrow$ *independent* if p_{ij} can be written as $q_i t_j$, i.e., iff $\mathrm{rk}(P) = 1$

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Maximise $\ell_U(P)$ subject to $p_{ij} \geq 0, p_{++} = 1, \mathrm{rk}(P) = 1.$

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Mixture of r copies of independence
P convex combination of $P_1, \ldots, P_r$ as above
$\rightsquigarrow p_{++} = 1$ and $\mathrm{rk}(P) \leq r$

ML-problem much harder!

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ML-problem for manifold $M \subseteq (\mathbb{R}_{>0})^n$
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Necessary condition for P **to be the ML-estimate**
P *critical*: $d_P \ell_U$ vanishes identically on $T_P M$
$\Leftrightarrow \sum_i \frac{x_i}{p_i} u_i = 0$ for all $X \in T_P M \Leftrightarrow (p_1^{-1}, \ldots, p_n^{-1}) T_P M \subseteq U^\perp$

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Algebraic measure of complexity
Count number of critical points. . . easier over $\mathbb{C}$!

ML-degree

Setting

$M \subseteq (\mathbb{C}^*)^n$ smooth subvariety (locally closed) $\rightsquigarrow$ Crit(M):= $\{(P, U) \in M \times \mathbb{C}^n \mid P^{-1}T_P M \subseteq U^\perp\}$ *variety of critical points*

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Theorem (Huh, 2012; related Franecki-Kapranov, 2000)
M closed in addition to smooth (*very affine*)
$\rightsquigarrow$ ML-degree is $(-1)^{\dim_{\mathbb{C}} M}\chi(M)$, where χ is the Euler characteristic of M.

ML-degrees for matrices of given rank

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For small $r \le m \le n$ ML-degree of M is as follows:

		(m,n)						
		$(3,3)$	$(3,4)$	$(3,5)$	$(4,4)$	$(4,5)$	$(4,6)$	$(5,5)$
	1	1	1	1	1	1	1	1
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Conjecture (HRS)
ML-degree (M_r) = ML-degree (M_{m-r+1})

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$U \in \mathbb{N}^{m\times n}$ sufficiently general $\rightsquigarrow$ the map $P \mapsto Q'$ defined by $p_{ij}q'_{ij} = u_{i+}u_{ij}u_{+j}/(u_{++}^3)$ is a bijection between critical points of ℓ_U on M_r and those on M_{m-r+1}.

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Remark

- $\ell_U(P)\ell_U(Q')$ independent of P
- P positive real $\Leftrightarrow$ so is Q'
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- Rodriguez established a general ML-duality theory.

"M_r and M_{m-r+1} are ML-dual"

Rank-2 case

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Theorem (Botong-Rodriguez 2015)
For $r = 2$ and $m = 3 \leq n$ the ML-degree is equal to $2^{n+1} - 6$.

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The proof involves subtle topological counting. More generally, they prove a recurrence relation for the rank-two case with which a closed formula for any fixed m and running n can be found.

Algebraic varieties with ML-degree 1

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In general, consider a rational map $\Psi : \mathbb{C}^n \to (\mathbb{C}^*)^n$ which is a composition of a linear map $\mathbb{C}^n \to \mathbb{C}^r$ followed by a monomial map $\mathbb{C}^r \to (\mathbb{C}^*)^n$ which is homogeneous of degree zero. Define M as the smooth locus of the closure of $\mathrm{im}\Psi$.

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Theorem (Huh 2013)
The variety M has ML-degree 1, and Ψ is its ML-estimator. Moreover, every variety of ML-degree 1 arises like this.

Reintroducing inequalities

Forget about ML-degree.

$M_1 := \{P \in \mathbb{R}^{m\times n}_{\geq 0} \mid \mathrm{rk}(P) = 1, \sum_{ij} p_{ij} = 1\}$ independence

$M_r := \{c_1 P_1 + \ldots + c_r P_r \mid P_i \in M_1, c_i \in \mathbb{R}_{\geq 0}, c_1 + \ldots + c_r = 1\}$
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Theorem (Vavasis 2009, Shitov 2015/2016)
nonnegative rank is NP-hard and may depend on the field.

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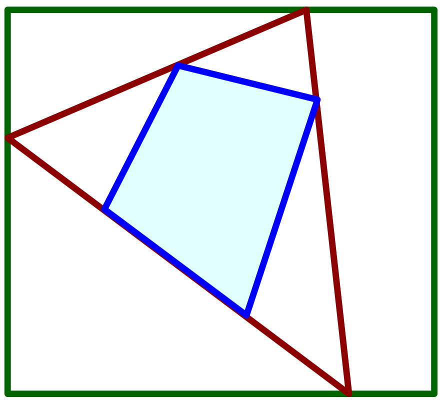
Theorem (K-R-S)
This boundary has three orbits of irreducible components under row and column permutations:

- one orbit where an entry of U is zero
- one orbit corresponding to the picture:
- and its transpose



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$Y := (u_{i+} \cdot u_{+j})_{ij}$ satisfies $Y \ker P \subseteq \mathrm{im} P$
P satisfies $P \ker P \subseteq \mathrm{im} P$

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$q_{ij} := u_{i+} \frac{u_{ij}}{p_{ij}} u_{+j}, q'_{ij} := q_{ij}/(u_{++}^3)$

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$q_{++} = u_{++}^3$

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$$\sum_{ij} q_{ij} = \sum_{ij} y_{ij} \frac{u_{ij}}{p_{ij}} = \sum_{ij} c p_{ij} \frac{u_{ij}}{p_{ij}} = (u_{++})^3$$

□

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In particular for $x \in \mathrm{im} Q$ or $y \perp \ker Q \rightsquigarrow Q'$ critical in M_s!

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- ψ_r injective
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Theorem (D-Rodriguez, 2012)

M_r and M_{m-r+1} are ML-dual. □

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Further work

symmetric/alternating matrices!

tensors? other ML-dual pairs of varieties?