

Information Geometry and its Applications III

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Finite generation of cumulants

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Summary

Algebraic Statistics

Elimination in polynomial ideals

Finite generation

Toric statistical models

Reversible Markov chains

Toric and differential ideals

- **Markov bases of toric ideals** Persi Diaconis and Bernd Sturmfels. Algebraic algorithms for sampling from conditional distributions. *Ann. Statist.*, 26(1): 363–397, 1998. ISSN 0090-5364 preprint 1993
- **Gröbner bases in Design of Experiments** Giovanni Pistone and Henry P. Wynn. Generalised confounding with Gröbner bases. *Biometrika*, 83(3): 653–666, March 1996. ISSN 0006-3444
- **The name of the game** Giovanni Pistone, Eva Riccomagno, and Henry P. Wynn. *Algebraic statistics. Computational commutative algebra in statistics*, volume 89 of *Monographs on Statistics and Applied Probability*. Chapman & Hall/CRC, Boca Raton, FL, 2001. ISBN 1-58488-204-2

Ideals, bases

- $R = k[x_1, \dots, x_d]$ is the ring of polynomials in the indeterminates x_1, \dots, x_d with coefficients in field k .
- Polynomials f_1, \dots, f_m generate the ideal

$$\langle f_1, \dots, f_m \rangle = \left\{ \sum_{j=1}^m g_j f_j : g_j \in R \right\}$$

- Every ideal has many finite generating set or **bases**
- A **monomial order** is a type of total order on monomials which is compatible with product. Given a monomial order it is possible to write every polynomial in decreasing order and to identify its **leading term**.
- The **elimination ideal** is the ideal

$$\langle f_1, \dots, f_m \rangle \cap k[x_1, \dots, x_l], \quad l \leq d$$

- **CCA** Martin Kreuzer and Lorenzo Robbiano. *Computational commutative algebra. 1*. Springer-Verlag, Berlin, 2000. ISBN 3-540-67733-X

```

Use R:= Q[x[1..4],t,y[1..2]], Lex; -- ring
Eqs:=[x[1]-(1-x[2])*x[2], -- first bernoulli
      x[3]-(1-x[4])*x[4], -- second bernoulli
      y[1]-x[2]-x[4], -- sum of k'
      y[2]-x[1]-x[3], -- sum of k''
      t-x[2]+x[4]]; -- parameter
I:=Ideal(Eqs);
GBasis(I); -- Groebner basis
Elim(x,I); -- Elimination ideal

```

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[-x[2] - x[4] + y[1],
 x[3] + x[4]^2 - x[4],
 x[1] + x[2]^2 - x[2],
 -2x[4] - t + y[1],
 -1/2t^2 - 1/2y[1]^2 + y[1] - y[2]]

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Ideal(-1/2t^2 - 1/2y[1]^2 + y[1] - y[2])

```

Multivariate cumulant

Definition (Moment and cumulant generating function)

- X is a random vector in \mathbb{R}^m .
- For $\theta \in \mathbb{R}^m$, $\theta \cdot X = \sum_{i=1}^m \theta_i X_i$ is the scalar product.
- D_X is the *interior* of the convex set

$$\left\{ \theta \in \mathbb{R}^m : E[e^{\theta \cdot X}] < +\infty \right\}.$$

- If $D_X \neq \emptyset$, then the *moment (generating) function* M_X and *cumulant (generating) function* K_X of X are the functions defined for each $t \in D_X$ by the equations

$$M_X(\theta) = E[e^{\theta \cdot X}],$$

$$K_X(\theta) = \log M_X(\theta).$$

Monomial and moment aliasing

- Let D be a finite set of points in \mathbb{R}^m , $I(D)$ the **design ideal** in $\mathbb{R}[x_1, \dots, x_m]$, g_1, \dots, g_k a polynomial basis of $I(D)$, x^α , $\alpha \in L$, a linear monomial basis of $\mathbb{R}[x_1, \dots, x_m]/I(D)$. Given a Gröbner basis, the monomials that are not divider by a leading term for such a (linear) basis.
- This is the usual setting of the algebraic theory of Design of Experiments. Each equation $g(x) = 0$, $g \in I(D)$, is an **aliasing** relation between terms.
- Let

$$H(x) = \exp\left(\sum_{i=1}^n s_i x_i\right) = \sum_{\alpha \in L} b_\alpha(s) x^\alpha.$$

$$\text{Therefore } M_X(s) = \sum_{\beta \geq 0} \frac{s^\beta \mu_\beta}{\beta!} = \sum_{\alpha \in L} b_\alpha(s) \mu_\alpha,$$

$$\mu_\beta = \sum_{\alpha \in L} b_{\alpha, \beta} \mu_\alpha, \quad b_{\alpha, \beta} = D_\beta b_\alpha(s)|_{s=0}$$

- The monomial basis is computed by CoCoA
- the coefficients $b_\alpha(s)$ are obtained by interpolation

Cumulant aliasing

For a discrete distribution and monomial order τ every cumulant $\mu_\beta, \beta \geq 0$ is expressible as a linear function of the moments $\mu_\alpha, \alpha \in L$, whose coefficients depend only the support and choice of monomial ordering, not the $p(x)$.

Theorem (Cumulants aliasing)

For a discrete distribution and monomial order τ every cumulant $\kappa_\beta, \beta \geq 0$ is expressible as a polynomial function of the cumulant $\kappa_\alpha, \alpha \in L$, whose form is only dependent of the support and monomial ordering.

- Giovanni Pistone and Henry P. Wynn. Cumulant varieties. *Journal of Symbolic Computation*, 41(2):210–221, 2006. ISSN 0747-7171

Finite generation

Definition

The cumulants of X are called *finitely generated* if there exist polynomials

$$F_{hk}(\eta_i : i = 1, \dots, m; \gamma_{ij} : i \leq j = 1, \dots, m) \quad , \quad h \leq k = 1, \dots, m \quad ,$$

such that the corresponding system of equations can be uniquely solved for $\gamma = (\gamma_{ij})_{1 \leq h \leq k \leq m}$ as a function of $\eta = (\eta_i)_{1 \leq i \leq m}$, around the point

$$\eta_0 = K'_X(0) \quad , \quad \gamma_0 = K''_X(0) \quad ,$$

and the equations

$$F_{hk}(K'_X(t), K''_X(t)) = 0 \quad , \quad h \leq k = 1, \dots, m \quad ,$$

hold in a neighborhood of 0. The polynomials $F = (F_{hk})_{h \leq k = 1, \dots, m}$ are called *generating polynomials of X* .


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Variance function: Morris

- The following table is adapted from [Morris, 1982, Table 1], where all the distributions such as the variance function is a quadratic polynomial in the mean are studied.
- In our terms, the variance $K''(\theta)$ and the mean $K'(\theta)$ are related by a *generating polynomial* of degree 2.

Distribution	Parameters	Generating polynomial
Normal $N(\mu, \sigma^2)$	μ, σ^2	$K'' - \sigma^2$
Poisson $P(\lambda)$	λ	$K'' - K'$
Gamma $\Gamma(\alpha, \lambda)$	α, λ	$\alpha K'' - (K')^2$
Binomial $\text{Bin}(n, p)$	n, p	$nK'' - K'(n - K')$
Negative Binomial $\text{NegBin}(r, p)$	r, p	$rK'' - K'(r + K')$
Generalised Hyperbolic Secant	$r, \lambda = \tan t$	$rK'' - (K')^2 - r^2$

Finite generation; example

- The generating polynomial uniquely defines the corresponding distribution. E.g. the differential equation for $\eta(\theta) = K'(\theta)$ in the GHS case is

$$r\eta'(\theta) = \eta(\theta)^2 + r^2, \quad \eta(0) = 0$$

The unique solution is

$$\eta(\theta) = r \tan t$$

so that

$$K(\theta) = r \int_0^t \tan \tau d\tau = r \log \sec t.$$

- All cumulants are polynomials in the mean parameter. E.g. for the GHS distribution

$$r^n K^{(n)}(\theta) = f_n(K'(\theta)), \quad n = 2, 3, \dots$$

where

$$f_{n+1}(\eta) = f_n'(\eta)(\eta^2 + r^2).$$

Finite generation

- The *Laplace (double exponential) density* with parameter 1 has cumulant function $K(t) = -\log(1 - t^2)$. Then the first and second derivatives are

$$K'(t) = \frac{2t}{1 - t^2},$$
$$K''(t) = 2 \frac{1 + t^2}{(1 - t^2)^2}.$$

The generating polynomial is

$$(K'')^2 - 2(1 + (K')^2)K'' + (K')^2 + (K')^4.$$

- The uniform density on $\{0, 1, 2\}$ has generating polynomial

$$3(K')^4 + 2K' - 2K'' + 11(K')^2 - 12K'K'' - 12(K')^3 + 6(K')^2(K'') + 3(K'')^2$$

Finite generation

Theorem

The FGC property is stable for

- 1 *joining independent components, in particular sampling;*
- 2 *invertible linear transformations;*
- 3 *convolutions of the same distribution.*

Theorem

- *Every discrete distribution supported on an equally spaced set of reals has the FGC property.*
- *Every finite mixture of exponential random variables has the FGC property.*
- *Let $p_X(x)$ be the density function of a random variable with the FGC property. Then if Y is a random variable with density $g(y)p_X(y)$ where $g(y)$ is polynomial then Y also has the FGC property.*

Finite generation: discussion

- For $U[0, 1]$ the MGF is $M(\theta) = \frac{e^\theta - 1}{\theta}$.
- This involves θ and e^θ . We set $z = \frac{1}{e^\theta - 1}$ and $t = \frac{1}{\theta}$, so that $z' = -(1+z)z$ $t' = -t^2$ and

$$K' = 1 + z - t$$

$$K'' = -z - z^2 + t^2$$

$$K''' = z + 3z^2 + 2z^3 - 2t^3$$

- Algebraic elimination of t and z gives

$$\begin{aligned} & (K')^6 - 5(K')^5 - 3(K')^4 K'' + 17/2(K')^4 + 2(K')^3 K'' - 4(K')^3 K''' \\ & - 6(K')^3 + 3(K')^2 (K'')^2 + (K')^2 K'' + 6(K')^2 K''' + 3/2(K')^2 \\ & - 5K'(K'')^2 - 3K' K''' - (K'')^3 + 5/2(K'')^2 - 1/2K'' + 1/2K''' \end{aligned}$$

Toric ideals

- Let be given an integer **model matrix** X with rows $x \in \mathcal{D}$ and d columns.
- Consider the ring $k[y_x : x \in \mathcal{D}]$ and the Laurent ring $k(t_1, \dots, t_d)$, together with their homomorphism A defined by

$$A: y_x \mapsto \prod_{j=1}^d t_j^{A_{x,j}} = t^{A(x)},$$

- The kernel $I(A)$ of h is called the *toric ideal* of A ,

$$I(A) = \left\{ f \in k[y_x : x \in \mathcal{D}] : f(t^{A(x)} : x \in \mathcal{D}) = 0 \right\}.$$

- The toric ideal $I(A)$ is a prime ideal and the binomials

$$P^{z^+} - P^{z^-}, \quad z \in \mathbb{Z}^D, \quad A^T z = 0,$$

are a generating set of $I(A)$ as a k -vector space.

- In particular, Hilbert says that a finite generating set of the ideal is formed by selecting a finite subset of such binomials.

- Bernd Sturmfels. *Gröbner bases and convex polytopes*. American Mathematical Society, Providence, RI, 1996. ISBN 0-8218-0487-1

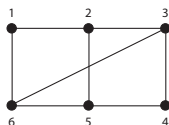
Toric ideals in statistics

- For the 2×2 independence model parameterized as $p_{x_1, x_2} = t_0 t_1^{x_1} t_2^{x_2}$, one computes the invariant:

$$A = \begin{array}{c} \\ ++ \\ +- \\ -+ \\ -- \end{array} \begin{array}{c} 1 \quad x_1 \quad x_2 \\ \left[\begin{array}{ccc} +1 & +1 & +1 \\ +1 & +1 & -1 \\ +1 & -1 & +1 \\ +1 & -1 & -1 \end{array} \right], \quad z = \begin{bmatrix} +1 \\ -1 \\ -1 \\ +1 \end{bmatrix}, \quad p_{++}p_{--} - p_{+-}p_{-+} \in I(A)$$

- Mathias Drton, Bernd Sturmfels, and Seth Sullivant. *Lectures on Algebraic Statistics*. Number 39 in Oberwolfach Seminars. Birkhäuser, 2009. ISBN 978-3-7643-8904-8
- Viceversa, one could go from the invariants to the parameterization.
- Giovanni Pistone and Maria Piera Rogantin. Algebra of reversible Markov chains. arXiv:1007.4282v1, 2010

CoCoA elimination



```
Use S:=Q[t,k[1..6],p[1..6,1..6]];
Set Indentation;
NI:=6; M:=[];
Define Lista(L,NI);
  For I:=1 To NI Do
    For J:=1 To I-1 Do
      Append(L,k[I]p[I,J]-k[J]p[J,I]); EndFor;
    EndFor; Return L; EndDefine;
N:=Lista(M,NI);
LL:=t*Product([k[I]|I In 1..NI])-1; Append(N,LL);
P0:=[p[1,3],p[1,4],p[1,5],p[2,4],p[2,6], p[3,1],p[3,5],
p[4,1],p[4,2],p[4,6],p[5,1],p[5,3],p[6,2],p[6,4]];
N:=Concat(N,P0);
E:=Elim(k,Ideal(N)); GB:=ReducedGBasis(E); GB;
```

GB;

[

$$p[1,3], p[1,4], p[1,5], p[2,4], p[2,6], p[3,1], p[3,5],$$

$$p[4,1], p[4,2], p[4,6], p[5,1], p[5,3], p[6,2], p[6,4],$$

$$p[2,3]p[3,4]p[4,5]p[5,2] - p[2,5]p[3,2]p[4,3]p[5,4],$$

$$p[1,2]p[2,3]p[3,6]p[6,1] - p[1,6]p[2,1]p[3,2]p[6,3],$$

$$p[1,2]p[2,5]p[5,6]p[6,1] - p[1,6]p[2,1]p[5,2]p[6,5],$$

$$p[2,5]p[3,2]p[5,6]p[6,3] - p[2,3]p[3,6]p[5,2]p[6,5],$$

$$p[3,4]p[4,5]p[5,6]p[6,3] - p[3,6]p[4,3]p[5,4]p[6,5],$$

$$p[1,2]p[2,5]p[3,6]p[4,3]p[5,4]p[6,1] -$$

$$p[1,6]p[2,1]p[3,4]p[4,5]p[5,2]p[6,3],$$

$$p[1,2]p[2,3]p[3,4]p[4,5]p[5,6]p[6,1] -$$

$$p[1,6]p[2,1]p[3,2]p[4,3]p[5,4]p[6,5]]$$

Toric model and Weyl

- Consider the **design** (sample space) $\mathcal{D} \subset \mathbb{Z}_+^d$ with reference measure μ , e.g. $\mu = 1$.
- The **design ideal** is

$$I(\mathcal{D}) = \{f \in \mathbb{Q}[x_1, \dots, x_d] : f(x) = 0, x \in \mathcal{D}\}.$$

- Consider the **toric statistical model**

$$p(x; t) \propto \prod_{j=1}^d t_j^{x_j}, \quad x \in \mathcal{D}, \quad t_j \geq 0, \quad j = 1, \dots, d,$$

- The normalizing constant (partition function) is

$$Z(t) = \sum_{x \in \mathcal{D}} t^x \mu(x)$$

- There exists a polynomial $p(t, x) \in \mathbb{Q}[t, x]$ such that $p(t, x) = t^x, x \in \mathcal{D}$.

Weyl differential algebra

- The **Weyl algebra** is the ring of differential operators $\mathbb{C}\langle t_1 \dots t_d, \partial_1 \dots \partial_d \rangle$ where everything commutes but

$$\partial_i t_i - t_i \partial_i = 1$$

- Define the operators

$$A(i, x) = t_i \partial_i - x_i = \partial_i t_i - (1 + x_i), \quad i = 1, \dots, d, \quad x \in \mathcal{D},$$

where the second equality follows from the commutation relation.

- For all $x \in \mathcal{D}$ we have

$$A(i, x) \bullet t^x = \partial_i \bullet (t_i t^x) - (1 + x_i) t^x = 0,$$

so that $t_i \partial_i \bullet t^x = x_i t^x$ and, by iteration, $(t_i \partial_i)^\alpha \bullet t^x = x_i^\alpha t^x$, $\alpha \in \mathbb{N}$.

The operator $(t_i \partial_i)^\alpha$ applied to the polynomial $Z(t) \in \mathbb{C}[t_1, \dots, t_d]$ gives

$$(t_i \partial_i)^\alpha \bullet Z(t) = \sum_{x \in \mathcal{D}} (t_i \partial_i)^\alpha \bullet t^x = \sum_{x \in \mathcal{D}} x_i^\alpha t^x.$$

- S. C. Coutinho. *A primer of algebraic D-modules*, volume 33 of *London Mathematical Society Student Texts*. Cambridge University Press, Cambridge, 1995. ISBN 0-521-55119-6; 0-521-55908-1. doi10.1017/CBO9780511623653. URL <http://dx.doi.org/10.1017/CBO9780511623653>

- Note the commutativity

$$(t_i \partial_i)(t_j \partial_j) = (t_j \partial_j)(t_i \partial_i),$$

hence we have an action of multivariate monomials:

$$\prod_{i=1}^d (t_i \partial_i)^{\alpha_i} \bullet Z(t) = \sum_{x \in \mathcal{D}} \prod_{i=1}^d (t_i \partial_i)^{\alpha_i} \bullet t^x = \sum_{x \in \mathcal{D}} \left(\prod_{i=1}^d x_i^{\alpha_i} \right) t^x \mu(x).$$

- By dividing by the normalizing constant we obtain the following expression for the moments:

$$Z(t)^{-1} \prod_{i=1}^d (t_i \partial_i)^{\alpha_i} \bullet Z(t) = \sum_{x \in \mathcal{D}} \prod_{i=1}^d (t_i \partial_i)^{\alpha_i} \bullet t^x \mu(x) = E_t [X^\alpha].$$

- By consider the ring homomorphism

$$A: \quad \mathbb{C}[x] \quad \rightarrow \quad \mathbb{C}\langle t_1 \dots t_d, \partial_1 \dots \partial_d \rangle \\ x_i \quad \mapsto \quad t_i \partial_i$$

We have

$$A(f(x)) \bullet Z(t) = \sum_{x \in \mathcal{D}} f(x) t^x \mu(x)$$

Theorem

- 1 Let x^α , $\alpha \in M$, be a monomial basis for \mathcal{D} . Then $Z(t)$ satisfies the following system of $\#M = \#\mathcal{D}$ linear non-omogeneous differential equations:

$$A(x^\alpha) \bullet Z(t) = \sum_{x \in \mathcal{D}} x^\alpha t^x \mu(x), \quad \alpha \in M.$$

- 2 Let $f_a(x)$ be the (reduced) indicator polynomial of $a \in \mathcal{D}$. Then $Z(t)$ satisfies the following system of $\#\mathcal{D}$ linear non-omogeneous differential equations:

$$A(f_a(x)) \bullet Z(t) = \mu(a)t^a, \quad a \in \mathcal{D}$$

- 3 Let $g(p_a: a \in \mathcal{D})$ be a polynomial in the toric ideal of the monomial homomorphism $p_a \mapsto t^a$. Then

$$g(\mu(x)^{-1} A(f_a(x)) \bullet Z(t): a \in \mathcal{D}) = 0$$

- 4 Also for cumulants.

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We appreciate! Thanks!