A New Method for Computing Elimination Ideals of Likelihood Equations

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ABSTRACT

We develop a probabilistic algorithm for computing elimination ideals of likelihood equations. We show experimentally that it is far more efficient than directly computing Gröbner bases or the interpolation method proposed in [39, 40] for medium to large size models. Furthermore, we deduce discriminants of the elimination ideals, which play a central role in real root classification. In particular, we can compute the discriminant of one Jukes-Cantor model in phylogenetics (with size 8 GB text file).

CCS CONCEPTS

• **Computing methodologies** → **Symbolic and algebraic manipulation**; *Algebraic algorithms*.

KEYWORDS

Maximum likelihood estimation, Likelihood equation, Real root classification, Discriminant, Elimination ideal

ACM Reference Format:

Xiaoxian Tang, Timo de Wolff, and Rukai Zhao. 2019. A New Method for Computing Elimination Ideals of Likelihood Equations. In *International Symposium on Symbolic and Algebraic Computation (ISSAC '19)*, July 15–18, 2019, Beijing, China. ACM, New York, NY, USA, 8 pages. <https://doi.org/10.1145/3326229.3326241>

1 INTRODUCTION

This work is motivated by the *maximum likelihood estimation* problem in statistics:

Which probability distribution describes a given data set optimally for a chosen statistical model?

A standard way to answer this question is to determine a point in the model that maximizes a *likelihood function*; see (1). When the model is algebraic (see Definition 2.2) and the data is discrete, then one finds all critical points of the likelihood function by solving a system of *likelihood equations* (2) via applying Lagrange multipliers.

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ISSAC '19, July 15–18, 2019, Beijing, China

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ACM ISBN 978-1-4503-6084-5/19/07...\$15.00
<https://doi.org/10.1145/3326229.3326241>

Solving likelihood equations motivates an important branch in algebraic statistics [1, 13, 14, 24–27, 31].

Likelihood equations form an algebraic system in *probability variables* $p_0, \dots, p_n$, *Lagrange multipliers* $\lambda_1, \dots, \lambda_{s+1}$, and *parameters* $u_0, \dots, u_n$ representing the data obtained from statistical experiments. Given such a system with generically chosen data vector $(u_0, \dots, u_n)$, the number of complex solutions is a finite non-negative constant, called the *maximum-likelihood-degree (ML-degree)*; see Definition 2.5 and [27, 31]. Since the variables p_i represent probabilities, one is especially interested in a *real solution classification* [15, 33, 47] of likelihood equations. Unfortunately, this classification is very challenging, since it is a specific *real quantifier elimination* problem [2–5, 7–11, 16, 17, 23, 28–30, 34–38, 41, 42, 45], a fundamental problem in computational real algebraic geometry.

The number of real solutions only changes when the parameters (data) pass a set called the *discriminant variety*; see [33, Definition 1]. Hence, these discriminant varieties of likelihood equations play a core role in real solution classification. In [40], Rodriguez and the first author studied how to compute discriminant varieties for a likelihood equation system efficiently. Experiments [40, Tables 2–3] suggest that Gröbner bases [12, 21, 22] cannot be computed directly for medium to large size models. Rodriguez and the first author proposed in [40, Algorithm 2] a probabilistic algorithm based on evaluation/interpolation techniques, which, in theory, works for arbitrary general zero-dimensional systems. In practice, however, it is limited to small algebraic models with ML-degrees not greater than 6. The main bottleneck is that the size of the discriminants we are trying to compute are huge; for instance, a model with ML-degree 6 has a discriminant with total degree 12 and thousands terms.

The key idea of this article is to exploit the special structure of likelihood equations to both improve the computational efficiency and to allow ourselves to compute generators of elimination ideals instead of computing discriminants directly. We summarize the entire challenge in Figure 1. Thus, the **task** of this paper is to efficiently compute the elimination ideal with respect to all parameters (data) and one variable for a given system of likelihood equations. More precisely, we have the following **problem statement**:

Input: Likelihood equations

$$f_0, \dots, f_{n+s+1} \in \mathbb{Q}[u_0, \dots, u_n, p_0, \dots, p_n, \lambda_1, \dots, \lambda_{s+1}].$$

Output: A generator of the elimination ideal with respect to one probability variable p_i for some i between 0 and n

$$\sqrt{\langle f_0, \dots, f_{n+s+1} \rangle} \cap \mathbb{Q}[u_0, \dots, u_n, p_i].$$

Figure 1: An visualization of our motivation.

Models	# p_i	MLD	Timings		
			Standard	Interpolation	Algorithm 1
1	4	3	0.046 s	1.831 s	0.525 s
2	6	2	0.524 s	24.983 s	2.310 s
3	6	4	3.211 s	282.425 s	16.174 s
4	6	6	∞	7933.230 s	782.676 s
5	5	12	∞	10726.268 s	761.257 s
6	9	10	∞	> 1583 d	14 d
7	5	23	∞	9919.260 s	4624.575 s
8	8	14	∞	> 4667 d	> 15 d
9	8	9	∞	> 39 d	2 d

Table 1: Runtimes for computing elimination ideals (s: seconds; d: days). The models are sorted by the same order with [40, Table 3]. The column “standard” contains the runtimes via a regular Fgb Gröbner basis computation, the column “Interpolation” contains the runtimes for [40, Algorithm 2], and the last column contains the runtimes for our Algorithm 1.

Our **main contribution** is the development of a probabilistic algorithm, Algorithm 1, for computing elimination ideals of Lagrange likelihood equations. We implemented the algorithm in `Maple`. Our experiments, summarized in Table 1, show that Algorithm 1 is significantly more efficient than the standard approach of directly computing Gröbner bases, or the evaluation/interpolation method in [40] for statistical models beyond small size, see Table 1 and Section 6 for further details. Our crucial idea to save computational time is to exploit an observation that the elimination ideals have special structures; see (3).

In particular, we are able to compute the discriminant of one Jukes-Cantor model [27, P_{comb} , Example 15] in phylogenetics [44, Chapter 15]. This was impossible before. We point out that this is a gigantic polynomial, whose total degree is 176, and which take several GB memory when stored in a text file, see Table 2 (Model 9) for further details.

The article is organized as follows. Section 2 are preliminaries. In Section 3, we discuss the specialization properties of (radical) elimination ideals and multivariate factorization. In Section 4, we introduce general zero-dimensional systems. In Section 5, we introduce Algorithm 1 together with a list of sub-algorithms for computing elimination ideals of likelihood equations. In Section 6, we explain the implementation details and compare the efficiency of our code with existing methods.

2 PRELIMINARIES

We assume that the reader is familiar with the fundamental concepts of computational algebraic geometry. For a general overview, we refer the reader to [18] and [43].

2.1 Notation

Throughout the paper, we use bold letters for vectors or a finite set of polynomials, e.g., $\mathbf{z} = (z_1, \dots, z_n)$ and $\mathbf{H} = \{h_1, \dots, h_m\}$. For $h \in \mathbb{Q}[\mathbf{z}]$ we denote the *total degree* of h by $\deg(h)$ and the degree of f with respect to a particular variable z_j as $\deg(h, z_j)$. We denote by $\text{coeff}(h, z_j^i)$ the *coefficient* of h with respect to the monomial z_j^i . If $N = \deg(h, z_j)$, then simply denote $\text{coeff}(h, z_j^N)$ by $\text{lcoeff}(h, z_j)$. For $\mathbf{H} \subseteq \mathbb{Q}[\mathbf{z}]$, we denote by $\langle \mathbf{H} \rangle$ the *ideal* generated by $\mathbf{H}$ in $\mathbb{Q}[\mathbf{z}]$, and by $\mathcal{V}(\mathbf{H})$ the *affine variety* $\{\mathbf{z} \in \mathbb{C}^n \mid h(\mathbf{z}) = 0 \text{ for all } h \in \mathbf{H}\}$. For any ideal $I \subset \mathbb{Q}[\mathbf{z}]$, we denote by $\sqrt{I}$ the *radical ideal* of I , and we denote by $\mathcal{V}(I)$ the affine variety defined by the generator polynomials of I . For any subset $S \subseteq \mathbb{C}^n$, we denote by $I(S)$ the ideal generated by the polynomials vanishing on S , i.e., $I(S) = \{h \in \mathbb{Q}[\mathbf{z}] \mid h(\mathbf{z}^*) = 0 \text{ for all } \mathbf{z}^* \in S\}$, and denote by $\bar{S}$ the *Zariski closure* $\mathcal{V}(I(S))$ of S in $\mathbb{C}^n$. For a positive integer n , and for any $1 \leq i \leq n$, we denote the *canonical projection* by $\text{proj}_i : \mathbb{C}^n \rightarrow \mathbb{C}^i$. Finally, we denote by $\text{gcd}(a, b)$ the *greatest common divisor* of two integers a, b .

2.2 Algebraic Statistics

In this section we recall the basic notions from algebraic statistics, which we need in this article.

Definition 2.1 (Probability Simplex). We define the *n-dimensional probability simplex* as $\Delta_n = \{(p_0, \dots, p_n) \in \mathbb{R}^{n+1} \mid p_0 > 0, \dots, p_n > 0, p_0 + \dots + p_n = 1\}$.

Definition 2.2 (Algebraic Statistical Model and Model Invariant). Given homogenous polynomials $g_1, \dots, g_s \in \mathbb{Q}[p_0, \dots, p_n]$ such that $\mathcal{V}(g_1, \dots, g_s) \subseteq \mathbb{C}^{n+1}$ is irreducible and generically reduced, we define an *algebraic statistical model* as

$$\mathcal{M} = \mathcal{V}(g_1, \dots, g_s) \cap \Delta_n.$$

Each g_i is called a *model invariant* of $\mathcal{M}$. If $\mathcal{V}(g_1, \dots, g_s)$ has codimension s , then we say $\{g_1, \dots, g_s\}$ is a set of *independent model invariants*.

Given an algebraic statistical model $\mathcal{M}$ and a *data vector* $\mathbf{u} = (u_0, \dots, u_n) \in \mathbb{R}_{\geq 0}^{n+1}$, the *maximum likelihood estimation* (MLE) problem is the optimization problem

$$\max \prod_{k=0}^n p_k^{u_k} \text{ subject to } \mathbf{p} \in \mathcal{M}, \quad (1)$$

which is fundamental in statistics [20, Chapter 2]. One way to solve the MLE problem is to solve a system of likelihood equations [27] formulated by the Lagrange multiplier method. We give the explicit formulation of such a system:

Definition 2.3 (Lagrange Likelihood Equations). Given an algebraic statistical model $\mathcal{M}$ with a set of independent model invariants $\{g_1, \dots, g_s\} \subseteq \mathbb{Q}[p_0, \dots, p_n]$, the polynomial set $\mathbf{f} =$

$\{f_0, \dots, f_{n+s+1}\}$ below is said to be the system of *Lagrange likelihood equations* of $\mathcal{M}$ when set equal to zeros:

$$\begin{aligned} f_0(\mathbf{u}, \mathbf{p}, \boldsymbol{\lambda}) &= p_0 \cdot \left(\frac{\partial g_1}{\partial p_0} \lambda_1 + \dots + \frac{\partial g_s}{\partial p_0} \lambda_s + \lambda_{s+1} \right) - u_0, \\ &\vdots \\ f_n(\mathbf{u}, \mathbf{p}, \boldsymbol{\lambda}) &= p_n \cdot \left(\frac{\partial g_1}{\partial p_n} \lambda_1 + \dots + \frac{\partial g_s}{\partial p_n} \lambda_s + \lambda_{s+1} \right) - u_n, \\ f_{n+1}(\mathbf{u}, \mathbf{p}, \boldsymbol{\lambda}) &= g_1(p_0, \dots, p_n), \\ &\vdots \\ f_{n+s}(\mathbf{u}, \mathbf{p}, \boldsymbol{\lambda}) &= g_s(p_0, \dots, p_n), \\ f_{n+s+1}(\mathbf{u}, \mathbf{p}, \boldsymbol{\lambda}) &= g_{s+1}(p_0, \dots, p_n) := p_0 + \dots + p_n - 1, \end{aligned} \quad (2)$$

with indeterminates $\mathbf{u} = (u_0, \dots, u_n)$, $\mathbf{p} = (p_0, \dots, p_n)$, and $\boldsymbol{\lambda} = (\lambda_1, \dots, \lambda_{s+1})$. More specifically, $u_0, \dots, u_n$ are parameters, and $p_0, \dots, p_n, \lambda_1, \dots, \lambda_{s+1}$ are variables.

THEOREM 2.4. [27] *Given a system of Lagrange likelihood equations $f_0, \dots, f_{n+s+1}$ defined in (2), there exists an affine variety $V \subseteq \mathbb{C}^{n+1}$, and a non-negative integer N such that for any $\mathbf{b} \in \mathbb{C}^{n+1} \setminus V$, the equations*

$$f_0(\mathbf{b}, \mathbf{p}, \boldsymbol{\lambda}) = \dots = f_{n+s+1}(\mathbf{b}, \mathbf{p}, \boldsymbol{\lambda}) = 0$$

have N common complex solutions in $\mathbb{C}^{n+1} \times \mathbb{C}^{s+1}$.

Definition 2.5 (Maximum-Likelihood-Degree). [27] Given an algebraic statistical model $\mathcal{M}$ with a system of Lagrange likelihood equations defined as in (2), the non-negative integer N stated in Theorem 2.4 is called the *maximum-likelihood-degree*, short *ML-degree*, of $\mathcal{M}$.

Definition 2.6 (Mixed Discriminant). [40, Definition 4] Given an algebraic statistical model $\mathcal{M}$ with a system of Lagrange likelihood equations $\mathbf{f} = \{f_0, \dots, f_{n+s+1}\}$ defined in (2), we define

$$\mathcal{L}_{MJ} = \overline{\text{proj}_{n+1}(\mathcal{V}(\mathbf{f}) \cap \mathcal{V}(J))},$$

where J denotes the determinant of Jacobian matrix of $\mathbf{f}$ with respect to $(\mathbf{p}, \boldsymbol{\lambda})$:

$$\det \begin{bmatrix} \frac{\partial f_0}{\partial p_0} & \dots & \frac{\partial f_0}{\partial p_n} & \frac{\partial f_0}{\partial \lambda_1} & \dots & \frac{\partial f_0}{\partial \lambda_{s+1}} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_{n+s+1}}{\partial p_0} & \dots & \frac{\partial f_{n+s+1}}{\partial p_n} & \frac{\partial f_{n+s+1}}{\partial \lambda_1} & \dots & \frac{\partial f_{n+s+1}}{\partial \lambda_{s+1}} \end{bmatrix}.$$

If $I(\mathcal{L}_{MJ})$ is principal, then a generator polynomial of $I(\mathcal{L}_{MJ})$, denoted by $\mathcal{D}_{MJ}$, is said to be a *mixed discriminant* of $\mathbf{f}$.

It is important to highlight that $\mathcal{L}_{MJ}$ is a component of the *discriminant variety* [33] of Lagrange likelihood equations, which plays a central role of real root classification; see e.g., [40, Theorem 2]. Notice that if $\mathcal{L}_{MJ}$ is principal, then the mixed discriminant $\mathcal{D}_{MJ}$ is homogenous in $\mathbb{Q}[\mathbf{u}]$; see [40, Proposition 2]. By Definition 2.6, $\mathcal{D}_{MJ}$ can be computed by computing the elimination ideal $\langle \mathbf{f}, J \rangle \cap \mathbb{Q}[\mathbf{u}]$. That means to compute a Gröbner base of $\langle \mathbf{f}, J \rangle$ with respect to a lexicographic order, where the determinant J of the Jacobian matrix, defined as in Definition 2.6, can be huge. So, computing $\mathcal{D}_{MJ}$ is usually challenging in practice; see [40, Tables 2–3].

According to [40, Algorithm 2, Strategy 3], one way to improve the efficiency for computing $\mathcal{D}_{MJ}$ is to compute the elimination ideal with respect to one probability variable first; for instance, $\langle \mathbf{f} \rangle \cap \mathbb{Q}[\mathbf{u}, p_0]$. If $\sqrt{\langle \mathbf{f} \rangle \cap \mathbb{Q}[\mathbf{u}, p_0]} = \langle E_f \rangle$, then it is well known that $\mathcal{D}_{MJ}$ is a factor of the discriminant of E_f with respect to p_0 ; see

[40, Lemma 3]. However, E_f is hard to obtain via directly computing Gröbner bases; see the column “standard” in Table 1. Therefore, the goal of the rest of paper is to compute E_f more efficiently.

3 SPECIALIZATION PROPERTIES

In this section, we discuss a selection of specialization properties, which guarantee the correctness of our Algorithm 1 in Section 5. Roughly speaking, elimination ideals (and their radicals) “specialize well” over a Zariski open set (see Proposition 3.2), and frac In what follows, we consider polynomial rings with at least two variables, i.e., $\mathbb{Q}[z_1, \dots, z_n]$ with $n \geq 2$. Given $h \in \mathbb{Q}[z_1, \dots, z_n]$, we denote for every $1 \leq i < n$, by $\text{lm}_i(h)$ and $\text{lcoeff}_i(h)$ the *leading monomial* and *leading coefficient of h with respect to $z_{i+1}, \dots, z_n$* , when h is considered in $\mathbb{Q}(z_1, \dots, z_i)[z_{i+1}, \dots, z_n]$ with the lexicographic order $z_{i+1} < \dots < z_n$. For every $\mathbf{b} = (b_1, \dots, b_i) \in \mathbb{C}^i$, we define the polynomial $h(\mathbf{b}) = h|_{z_1=b_1, \dots, z_i=b_i} \in \mathbb{C}[z_{i+1}, \dots, z_n]$. For every polynomial set $H \subseteq \mathbb{Q}[z_1, \dots, z_n]$, we define $H(\mathbf{b}) = \{h(\mathbf{b}) \in \mathbb{C}[z_{i+1}, \dots, z_n] \mid h \in H\}$.

Definition 3.1. [32, Definition 4.1] Given $H \subseteq \mathbb{Q}[z_1, \dots, z_n]$, for any $1 \leq i < n$, a subset $\mathbf{g}$ of H is a *noncomparable subset of H with respect to $z_{i+1}, \dots, z_n$* if

- (1) for every $h \in H$, there exists a $g \in \mathbf{g}$ such that $\text{lm}_i(h)$ is a multiple of $\text{lm}_i(g)$, and
- (2) for any $g_1, g_2 \in \mathbf{g}$, with $g_1 \neq g_2$, the leading monomial $\text{lm}_i(g_1)$ is not a multiple of $\text{lm}_i(g_2)$, and $\text{lm}_i(g_2)$ is not a multiple of $\text{lm}_i(g_1)$.

PROPOSITION 3.2. *Given $H \subseteq \mathbb{Q}[z_1, \dots, z_n]$, for any $1 \leq i < n$, if the elimination ideal*

$$\langle H \rangle \cap \mathbb{Q}[z_1, \dots, z_i, z_{i+1}] = \langle q \rangle \text{ with } \deg(q, z_{i+1}) > 0,$$

and if $\sqrt{\langle q \rangle} = \langle g \rangle$, then

- (1) *there exists an affine variety $V \subseteq \mathbb{C}^i$ such that for any $\mathbf{b} \in \mathbb{C}^i \setminus V$, $\langle H(\mathbf{b}) \rangle \cap \mathbb{C}[z_{i+1}] = \langle g(\mathbf{b}) \rangle$, and*
- (2) *there exists an affine variety $W \subseteq \mathbb{C}^i$ such that for any $\mathbf{b} \in \mathbb{C}^i \setminus W$, $\sqrt{\langle H(\mathbf{b}) \rangle \cap \mathbb{C}[z_{i+1}]} = \langle g(\mathbf{b}) \rangle$.*

PROOF. Let $\mathcal{G}$ be a Gröbner basis of $\langle H \rangle$ with respect to the lexicographic order $z_1 < \dots < z_n$. For any $1 \leq i < n$, let $\mathcal{N}$ be a noncomparable set of $\mathcal{G}$ with respect to $z_{i+1}, \dots, z_n$.

Part (1): If $\langle H \rangle \cap \mathbb{Q}[z_1, \dots, z_{i+1}] = \langle q \rangle$, then by [18, page 121, Theorem 2], $\mathcal{G} \cap \mathbb{Q}[z_1, \dots, z_{i+1}]$ is a Gröbner basis of $\langle q \rangle$. So $\mathcal{G} \cap \mathbb{Q}[z_1, \dots, z_{i+1}]$ contains only one element, say h , and hence $h = c \cdot q$ where $c \in \mathbb{Q}$. Also, $\mathcal{G}_i = \mathcal{G} \cap \mathbb{Q}[z_1, \dots, z_i] = \emptyset$ since $\deg(h, z_{i+1}) = \deg(q, z_{i+1}) > 0$, and hence, $\mathcal{V}(\mathcal{G}_i) = \mathbb{C}^i$. By [32, Theorem 4.3], there exists $V \subseteq \mathbb{C}^i$ such that for any $\mathbf{b} \in \mathbb{C}^i \setminus V$, $\mathcal{N}(\mathbf{b})$ is a Gröbner basis of $\langle H(\mathbf{b}) \rangle$. By [18, page 121, Theorem 2], $\mathcal{N}(\mathbf{b}) \cap \mathbb{C}[z_{i+1}]$ is a Gröbner basis of $\langle H(\mathbf{b}) \rangle \cap \mathbb{C}[z_{i+1}]$. Notice that $\mathcal{N}(\mathbf{b}) \cap \mathbb{C}[z_{i+1}] = \{h(\mathbf{b})\}$. So, we have $\mathcal{N}(\mathbf{b}) \cap \mathbb{C}[z_{i+1}] = \langle h(\mathbf{b}) \rangle = \langle g(\mathbf{b}) \rangle$.

Part (2): If $\sqrt{\langle q \rangle} = \langle g \rangle$, then $\mathcal{V}(q) = \mathcal{V}(g)$. So, for any $\mathbf{b} \in \mathbb{C}^i$, $\mathcal{V}(q(\mathbf{b})) = \mathcal{V}(g(\mathbf{b}))$. Hence, we have $\sqrt{\langle q(\mathbf{b}) \rangle} = \sqrt{\langle g(\mathbf{b}) \rangle}$. Note that $\langle g \rangle$ is a radical ideal. Then it is a basic fact that there exists an affine variety $V_1 \subseteq \mathbb{C}^i$ such that for any $\mathbf{b} \in \mathbb{C}^i \setminus V_1$, $\langle g(\mathbf{b}) \rangle$ is still radical, and hence $\sqrt{\langle q(\mathbf{b}) \rangle} = \sqrt{\langle g(\mathbf{b}) \rangle} = \langle g(\mathbf{b}) \rangle$. By part (1), there exists an affine variety $V_2 \subseteq \mathbb{C}^i$ such that for any $\mathbf{b} \in \mathbb{C}^i \setminus V_2$, we have the equality in part (1). Let $W = V_1 \cup V_2$. Then for any $\mathbf{b} \in \mathbb{C}^i \setminus W$, we have the equality in part (2). $\square$

PROPOSITION 3.3. *Let $g \in \mathbb{Q}[z_1, \dots, z_n]$. If $g = \prod_{k=1}^r g_k^{m_k}$, where every g_k is irreducible in $\mathbb{Q}[z_1, \dots, z_n]$, and $g_j \neq g_k$ for any $j \neq k$, then for any $1 \leq i < n$ there exists an infinite subset $\Gamma \subseteq \mathbb{Q}^i$ such that for any $\mathbf{b} \in \Gamma$ we have $g(\mathbf{b}) = \prod_{k=1}^r g_k(\mathbf{b})^{m_k}$, where $g_k(\mathbf{b})$ is irreducible in $\mathbb{Q}[z_{i+1}, \dots, z_n]$, and $g_j(\mathbf{b}) \neq g_k(\mathbf{b})$ for any $j \neq k$.*

PROOF. Given that $g_1, \dots, g_r$ are irreducible, by Hilbert's irreducibility theorem, see e.g., [46, Theorem 1], for any $1 \leq i < n$, there exists an infinite subset $\Theta \subseteq \mathbb{Q}^i$ such that for any $\mathbf{b} \in \Theta$, $g_1(\mathbf{b}), \dots, g_r(\mathbf{b})$ are irreducible in $\mathbb{Q}[z_{i+1}, \dots, z_n]$. Now consider an arbitrary pair g_j, g_k with $j \neq k$ and thus $g_j \neq g_k$. Without loss of generality, let

$$W_{j,k} = \{\mathbf{b} \in \mathbb{C}^i \mid g_j(\mathbf{b}) - g_k(\mathbf{b}) = 0\}.$$

Obviously, $W_{j,k}$ is an affine variety, which does not equal $\mathbb{C}^i$. Then let $\Gamma = \Theta \cup \bigcup_{k=1}^r \bigcup_{j=1}^{k-1} (\mathbb{Q}^i \setminus W_{j,k})$, and we are done. $\square$

4 GENERAL ZERO-DIMENSIONAL SYSTEMS

Throughout the rest of the paper, we always assume that a system of Lagrange likelihood equations is general zero-dimensional; see Definition 4.1. A general zero-dimensional system has a nice structure, see [19, Theorem 6.10], which leads us to analyze their elimination ideals further. The relation between the Shape Lemma [6] and [19, Theorem 6.10] was discussed in [19].

Definition 4.1 (General Zero-Dimensional System). A polynomial set $\mathbf{H} = \{h_1, \dots, h_m\} \subseteq \mathbb{Q}[a_1, \dots, a_k, y_1, \dots, y_m]$ is called a *general zero-dimensional system* if there exists an affine variety $V \subseteq \mathbb{C}^k$ such that for any $\mathbf{b} = (b_1, \dots, b_k) \in \mathbb{C}^k \setminus V$, the equations $h_1(\mathbf{b}) = \dots = h_m(\mathbf{b}) = 0$ satisfy:

- (1) the number of complex solutions is a positive constant, denoted by $N(\mathbf{H})$;
- (2) all complex solutions are distinct;
- (3) every pair of distinct complex solutions $\mathbf{y}^* = (y_1^*, \dots, y_m^*)$ and $\mathbf{z}^* = (z_1^*, \dots, z_m^*)$ it holds that $y_1^* \neq z_1^*$.

PROPOSITION 4.2. *Consider a general zero-dimensional system $\mathbf{H} \subset \mathbb{Q}[a_1, \dots, a_k, y_1, \dots, y_m]$. If the elimination ideal*

$$\langle \mathbf{H} \rangle \cap \mathbb{Q}[a_1, \dots, a_k, y_1]$$

is principal, then its radical ideal is generated by a polynomial $g \in \mathbb{Q}[a_1, \dots, a_k, y_1]$ such that $\deg(g, y_1) = N(\mathbf{H})$.

PROOF. Let $\mathcal{G}$ be a Gröbner basis of $\langle \mathbf{H} \rangle$ with respect to the lexicographic order $a_1 < \dots < a_k < y_1 < \dots < y_m$. Since $\mathbf{H}$ is general zero-dimensional, by [19, Theorem 6.10], there exists

$$T_1 = C_N y_1^N + C_{N-1} y_1^{N-1} + \dots + C_1 y_1 + C_0 \in \mathcal{G},$$

where $N = N(\mathbf{H})$, and $C_i \in \mathbb{Q}[a_1, \dots, a_k]$. By [18, page 121, Theorem 2], $\mathcal{G} \cap \mathbb{Q}[a_1, \dots, a_k, y_1]$ is a Gröbner basis of $\langle \mathbf{H} \rangle \cap \mathbb{Q}[a_1, \dots, a_k, y_1]$. By the hypothesis that $\langle \mathbf{H} \rangle \cap \mathbb{Q}[a_1, \dots, a_k, y_1]$ is principal, $\mathcal{G} \cap \mathbb{Q}[a_1, \dots, a_k, y_1]$ contains only one element. Notice $T_1 \in \mathcal{G} \cap \mathbb{Q}[a_1, \dots, a_k, y_1]$. So, we know $\{T_1\} = \mathcal{G} \cap \mathbb{Q}[a_1, \dots, a_k, y_1]$. And hence, $\langle \mathbf{H} \rangle \cap \mathbb{Q}[a_1, \dots, a_k, y_1] = \langle T_1 \rangle$. By [18, page 187, Proposition 12], $\sqrt{\langle T_1 \rangle} = \langle g \rangle$, where $g = \frac{T_1}{\gcd(T_1, \frac{\partial T_1}{\partial a_1}, \dots, \frac{\partial T_1}{\partial a_k}, \frac{\partial T_1}{\partial y_1})}$. Hence,

$$\deg(g, y_1) \leq \deg(T_1, y_1) = N(\mathbf{H}).$$

Below, we prove $\deg(g, y_1) \geq N(\mathbf{H})$. By Definition 4.1, there exists an affine variety $V_1 \subsetneq \mathbb{C}^k$ such that for any $\mathbf{b} \in \mathbb{C}^k \setminus V_1$, $\mathcal{V}(\mathbf{H}(\mathbf{b}))$ has $N(\mathbf{H})$ distinct complex points with distinct y_1 -coordinates. By Proposition 3.2 (2), there exists $V_2 \subsetneq \mathbb{C}^k$ such that for any $\mathbf{b} \in \mathbb{C}^k \setminus V_2$,

$$\sqrt{\langle \mathbf{H}(\mathbf{b}) \rangle \cap \mathbb{Q}[y_1]} = \langle g(\mathbf{b}) \rangle.$$

Let $\mathbf{b} \in \mathbb{C}^k \setminus (V_1 \cup V_2)$. Then $g(\mathbf{b}) = 0$ has $N(\mathbf{H})$ distinct complex solutions, which are the y_1 -coordinates of points in $\mathcal{V}(\mathbf{H}(\mathbf{b}))$. So $\deg(g, y_1) \geq \deg(g(\mathbf{b}), y_1) \geq N(\mathbf{H})$. $\square$

5 ALGORITHM

Given an algebraic model $\mathcal{M}$, let its Lagrange likelihood equation system be $\mathbf{f} = \{f_0, \dots, f_{n+s+1}\} \subseteq \mathbb{Q}[\mathbf{u}, \mathbf{p}, \boldsymbol{\lambda}]$. Assuming $\langle \mathbf{f} \rangle \cap \mathbb{Q}[\mathbf{u}, p_0]$ is principal, we propose a probabilistic algorithm for computing the polynomial $E_{\mathbf{f}}$ generating $\sqrt{\langle \mathbf{f} \rangle \cap \mathbb{Q}[\mathbf{u}, p_0]}$. We simply denote $\text{coeff}(E_{\mathbf{f}}, p_0^i)$ by $A_i(\mathbf{u})$. Then $E_{\mathbf{f}} = \sum_{i=0}^N A_i(\mathbf{u}) p_0^i$, where by Theorem 2.4, Definition 4.1 and Proposition 4.2, N is the ML-degree of $\mathcal{M}$. First, we highlight a fact:

(F1) $E_{\mathbf{f}}$ is homogenous with respect to $\mathbf{u}$, and hence each A_i is homogenous with the same total degree in $\mathbb{Q}[\mathbf{u}]$.

We omit the proof of **(F1)** since the argument is similar to [40, Proposition 2], which is based on a basic fact implied by (2): for every $(\mathbf{u}, p_0) \in \text{proj}_{n+2}(\mathcal{V}(\mathbf{f}))$ and for any complex scalar $\gamma \neq 0$, $(\gamma \mathbf{u}, p_0)$ is also in $\text{proj}_{n+2}(\mathcal{V}(\mathbf{f}))$.

Besides observing **(F1)**, we make the following assumptions to simplify our algorithm:

- (A1)** Assume $\deg(A_N, u_0) = \deg(A_N)$, i.e., A_N contains a term $u_0^{\deg(A_N)} \in \mathbb{Q}[u_0]$.
- (A2)** Assume A_N is monic with respect to u_0 , which unifies our output polynomial $E_{\mathbf{f}}$.

If **(A1)** does not hold, then we apply an invertible linear change to the parameters u_j such that **(A1)** holds for the new parameters (similar to [40, Algorithm 4]). For instance, obtain new parameters v_j as

$$v_0 = u_0, \text{ and } v_j = b_j u_j + u_0 \text{ for } j = 1, \dots, n,$$

where b_j are randomly chosen rational numbers. By [40, Lemmas 1–2], $\deg(A_N(\mathbf{v}), v_0)$ will be equal to $\deg(A_N(\mathbf{v}))$.

Let

$$\mathcal{S}(\mathbf{u}) = \sum_{i=0}^n u_i.$$

The key idea of our algorithm is an observation from experiments: $\mathcal{S}(\mathbf{u})$ appears in some coefficients of $E_{\mathbf{f}}$ with respect to p_0 . So, we further write

$$E_{\mathbf{f}}(\mathbf{u}, p_0) = \sum_{i=0}^N A_i(\mathbf{u}) p_0^i = \sum_{i=0}^N \mathcal{S}(\mathbf{u})^{\alpha_i} R_i(\mathbf{u}) p_0^i, \quad (3)$$

where $R_i \in \mathbb{Q}[\mathbf{u}] \setminus \langle \mathcal{S}(\mathbf{u}) \rangle$. In a separate paper, we intend to prove for a general model that at least one α_i in (3) is nonzero. The main algorithm has three steps; see Algorithm 1:

Step 1 Compute $N, (\alpha_0, \dots, \alpha_N)$, and the degree of every u_j in each A_i .

Algorithm 1: (Main Algorithm)

input : Lagrange likelihood equations $f_0, \dots, f_{n+s+1} \in \mathbb{Q}[u, p, \lambda]$
output : A generator of $\sqrt{\langle f_0, \dots, f_{n+s+1} \rangle} \cap \mathbb{Q}[u, p_0]$; $E_f(u, p_0) = \sum_{i=0}^N A_i(u) p_0^i$

- 1 $N, (\alpha_0, \dots, \alpha_N), \mathcal{L}, \Omega \leftarrow \text{Degrees}(f_0, \dots, f_{n+s+1})$
- 2 $A_N(u) \leftarrow \text{LeadingCoefficient}(f_0, \dots, f_{n+s+1}, \alpha_N, \mathcal{L})$
- 3 $A_0(u), \dots, A_{N-1}(u) \leftarrow \text{Coefficients}(f_0, \dots, f_{n+s+1}, A_N(u), \alpha_0, \dots, \alpha_{N-1}, \Omega)$
- 4 **Return** $\sum_{i=0}^N A_i(u) p_0^i$

Algorithm 2: (Sub-Algorithm of Algorithm 1) Degrees

input : Lagrange likelihood equations $f_0, \dots, f_{n+s+1} \in \mathbb{Q}[u, p, \lambda]$
output : $N, (\alpha_0, \dots, \alpha_N), \mathcal{L}, \Omega$, where

- $N = \deg(E_f, p_0)$,
- α_i is the multiplicity of the factor $\sum_{k=0}^n u_k$ appearing in $\text{coeff}(E_f, p_0^i)$,
- $\mathcal{L}$ is a list with length $n+1$, whose $(j+1)$ -th entry is $\deg(\text{lcoeff}(E_f, p_0), u_j)$ for $j = 0, \dots, n$,
- Ω is an $N \times (n+1)$ matrix, whose $(i+1, j+1)$ -entry is $\deg(\text{coeff}(E_f, p_0^i), u_j)$ for $i = 0, \dots, N-1$ and for $j = 0, \dots, n$.

- 1 $f_0^*, \dots, f_{n+s+1}^* \leftarrow$ replace $u_1, \dots, u_n$ in $f_0, \dots, f_{n+s+1}$ with some rational numbers $b_1, \dots, b_n$
- 2 $g(u_0, p_0) \leftarrow$ generator of $\sqrt{\langle f_0^*, \dots, f_{n+s+1}^* \rangle} \cap \mathbb{Q}[u_0, p_0]$
- 3 $N \leftarrow \deg(g, p_0)$
- 4 **for** i **from** 0 **to** N **do**
- 5 $\alpha_i \leftarrow$ multiplicity of the factor $u_0 + \sum_{k=0}^n b_k$ in $\text{coeff}(g, p_0^i)$
- 6 $\mathcal{L}(1) \leftarrow \deg(\text{lcoeff}(g, p_0), u_0)$
- 7 **for** i **from** 0 **to** $N-1$ **do**
- 8 $\Omega(i+1, 1) \leftarrow \deg(\text{coeff}(g, p_0^i), u_0)$
- 9 **for** j **from** 1 **to** n **do**
- 10 $f_0^*, \dots, f_{n+s+1}^* \leftarrow$ replace $u_0, \dots, u_{j-1}, u_{j+1}, \dots, u_n$ in $f_0, \dots, f_{n+s+1}$ with some rational numbers
- 11 $g(u_j, p_0) \leftarrow$ generator of $\sqrt{\langle f_0^*, \dots, f_{n+s+1}^* \rangle} \cap \mathbb{Q}[u_j, p_0]$
- 12 $\mathcal{L}(j+1) \leftarrow \deg(\text{lcoeff}(g, p_0), u_j)$
- 13 **for** i **from** 0 **to** $N-1$ **do**
- 14 $\Omega(i+1, j+1) \leftarrow \deg(\text{coeff}(g, p_0^i), u_j)$
- 15 **return** $N, (\alpha_0, \dots, \alpha_N), \mathcal{L}, \Omega$

Step 2 Compute the leading coefficient $A_N(u)$ by interpolating $R_N(u)$.

Step 3 Compute the coefficients $A_i(u)$ by interpolating $R_i(u)$ for $i = 0, \dots, N-1$.

We present the pseudocode in Algorithm 1 and its sub-algorithms Algorithms 2–6, and a running example in Section 5.1. Algorithm 1 is guaranteed to terminate since we only have finite loops. The algorithm is probabilistic, but Propositions 3.2–3.3 guarantee that it provides the correct output for a generical choice of random rational numbers.

5.1 Running Example

In this subsection, we illustrate how Algorithm 1 works by the linear model $\mathcal{M}$ below given by a weighted four-sided die [40, Example 1], for which we know the ML-degree is 3:

$$\mathcal{M} = \mathcal{V}(p_0 + 2p_1 + 3p_2 - 4p_3) \cap \Delta_3,$$

where $\Delta_3 = \{(p_0, p_1, p_2, p_3) \in \mathbb{R}_{\geq 0}^4 \mid p_0 + p_1 + p_2 + p_3 = 1\}$. The input Lagrange likelihood equations (2) are

$$\begin{aligned} f_0 &= p_0 \lambda_1 + p_0 \lambda_2 - u_0 & f_1 &= p_1 \lambda_1 + 2p_1 \lambda_2 - u_1 \\ f_2 &= p_2 \lambda_1 + 3p_2 \lambda_2 - u_2 & f_3 &= p_3 \lambda_1 - 4p_3 \lambda_2 - u_3 \\ f_4 &= p_0 + 2p_1 + 3p_2 - 4p_3 & f_5 &= p_0 + p_1 + p_2 + p_3 - 1 \end{aligned}$$

Algorithm 3: (Sub-Algorithm of Algorithm 1) LeadingCoefficient

input : Lagrange likelihood equations $f_0, \dots, f_{n+s+1}$, and $a_N, \mathcal{L}$, where

- α_N is the multiplicity of the factor $\sum_{k=0}^n u_k$ appearing in $\text{lcoeff}(E_f, p_0)$,
- $\mathcal{L}$ is a list, whose $(j+1)$ -th entry is $\deg(\text{lcoeff}(E_f, p_0), u_j)$ for $j = 0, \dots, n$.

output : $\text{lcoeff}(E_f, p_0): A_N(u)$

- 1 $d \leftarrow \mathcal{L}(1) - \alpha_N$ *Here, $d = \deg(R_N, u_0)$, and by (A1), $\deg(R_N, u_0) = \deg(R_N)$*
- 2 **for** i **from** 0 **to** $d-1$ **do**
- 3 Enumerate all the monomials in the set
 $\{u_1^{\beta_1} \dots u_n^{\beta_n} \mid \sum_{j=1}^n \beta_j = d-i, 0 \leq \beta_j \leq \mathcal{L}(j+1) - \alpha_N\}$ as $U_{i,1}, \dots, U_{i,t_i}$
- 4 $t \leftarrow \max(t_0, \dots, t_{d-1})$
- 5 **for** k **from** 1 **to** t **do**
- 6 $b_{k,1}, \dots, b_{k,n} \leftarrow$ some rational numbers
- 7 $q(u_0) \leftarrow \text{IntersectForLC}(f_0, \dots, f_{n+s+1}, b_{k,1}, \dots, b_{k,n}, \alpha_N)$
- 8 $C_{0,k}^*, \dots, C_{d-1,k}^* \leftarrow$ the coefficients of $q(u_0)$ with respect to $u_0^0, \dots, u_0^{d-1}$
- 9 **for** i **from** 0 **to** $d-1$ **do**
- 10 $\mathcal{M}_i \leftarrow$ the $t_i \times t_i$ matrix whose (k, r) -entry is $U_{i,r} \mid u_1 = b_{k,1}, \dots, u_n = b_{k,n}$
- 11 $C_i(u_1, \dots, u_n) \leftarrow (U_{i,1}, \dots, U_{i,t_i}) \mathcal{M}_i^{-1} (C_{i,1}^*, \dots, C_{i,t_i}^*)^T$
- 12 **Return** $\left(\sum_{k=0}^n u_k\right)^{\alpha_N} \left(u_0^d + \sum_{i=0}^{d-1} C_i(u_1, \dots, u_n) u_0^i\right)$

Algorithm 4: (Sub-Algorithm of Algorithm 3) IntersectForLC

input : Lagrange likelihood equations $f_0, \dots, f_{n+s+1}$, some rational numbers $b_1, \dots, b_n$ and α_N , where a_N is the multiplicity of the factor $\sum_{k=0}^n u_k$ appearing in $\text{lcoeff}(E_f, p_0)$.

output : $\text{lcoeff}(E_f, p_0) \mid_{u_1=b_1, \dots, u_n=b_n}$

- 1 $f_0^*, \dots, f_{n+s+1}^* \leftarrow$ replace $u_1, \dots, u_n$ in $f_0, \dots, f_{n+s+1}$ with $b_1, \dots, b_n$, respectively
- 2 $g(u_0, p_0) \leftarrow$ generator of the radical of elimination ideal $\langle f_0^*, \dots, f_{n+s+1}^* \rangle \cap \mathbb{Q}[u_0, p_0]$
- 3 $q(u_0) \leftarrow$ divide $\text{lcoeff}(g, p_0)$ by $(u_0 + \sum_{i=1}^n b_i)^{\alpha_N}$
- 4 Make $q(u_0)$ monic with respect to u_0 , and **return** $q(u_0)$

Algorithm 5: (Sub-Algorithm of Algorithm 1) Coefficients

input : Lagrange likelihood equations $f_0, \dots, f_{n+s+1}$, and $A_N(u), \alpha_0, \dots, \alpha_{N-1}, \Omega$, where

- $A_N(u) = \text{lcoeff}(E_f, p_0)$,
- α_i is the multiplicity of the factor $\sum_{k=0}^n u_k$ appearing in $\text{coeff}(E_f, p_0^i)$,
- Ω is an $N \times (n+1)$ matrix, whose $(i+1, j+1)$ -entry is $\deg(\text{coeff}(E_f, p_0^i), u_j)$.

output : $\text{coeff}(E_f, p_0^i)$ for $i = 0, \dots, N-1: A_0(u), \dots, A_{N-1}(u)$

- 1 $d \leftarrow \deg(A_N(u))$
- 2 **for** i **from** 0 **to** $N-1$ **do**
- 3 Enumerate all the monomials in
 $\{u_0^{\beta_0} \dots u_n^{\beta_n} \mid \sum_{j=0}^n \beta_j = d - \alpha_i, 0 \leq \beta_j \leq D(i+1, j+1) - \alpha_i\}$ as $U_{i,1}, \dots, U_{i,t_i}$
- 4 $t \leftarrow \max(t_0, \dots, t_{N-1})$
- 5 **for** k **from** 1 **to** t **do**
- 6 $b_{k,0}, \dots, b_{k,n} \leftarrow$ some rational numbers
- 7 $g(p_0) \leftarrow \text{Intersect}(f_0, \dots, f_{n+s+1}, b_{k,0}, \dots, b_{k,n})$
- 8 $C_{0,k}^*, \dots, C_{N-1,k}^* \leftarrow$ the coefficients of $g(p_0)$ with respect to $p_0^0, \dots, p_0^{N-1}$
- 9 **for** i **from** 0 **to** $N-1$ **do**
- 10 $\mathcal{M}_i \leftarrow t_i \times t_i$ matrix whose (k, r) -entry is $\frac{U_{i,r}}{A_N(u)} \mid_{u_0=b_{k,0}, \dots, u_n=b_{k,n}}$
- 11 $R_i(u) \leftarrow (U_{i,1}, \dots, U_{i,t_i}) \mathcal{M}_i^{-1} (C_{i,1}^*, \dots, C_{i,t_i}^*)^T$
- 12 **Return** $\left(\sum_{k=0}^n u_k\right)^{\alpha_0} R_0(u), \dots, \left(\sum_{k=0}^n u_k\right)^{\alpha_{N-1}} R_{N-1}(u)$

where $p_0, p_1, p_2, p_3, \lambda_1, \lambda_2$ are variables, and u_0, u_1, u_2, u_3 are parameters. The output is a generator of $\sqrt{\langle f_0, \dots, f_5 \rangle} \cap \mathbb{Q}[u, p_0]$. We write the generator as in the form (3).

Step 1. First, we compute $N, (\alpha_0, \dots, \alpha_N)$, and $\deg(A_i, u_j)$ for $j = 0, \dots, 3$ and for $i = 0, \dots, N$. For each $u_j \neq u_0$, substitute $u_j = b_j$ into $f_0, \dots, f_5$, where b_j is a random rational number. For instance,

Algorithm 6: (Sub-Algorithm of Algorithm 5) Intersect

input : Lagrange likelihood equations $f_0, \dots, f_{n+s+1}$, and some rational numbers $b_0, b_1, \dots, b_n$

output: $\frac{E_f(\mathbf{u}, p_0)}{\text{lcoeff}(E_f, p_0)} | u_0=b_0, \dots, u_n=b_n$

- 1 $\tilde{f}_0, \dots, \tilde{f}_{n+s+1} \leftarrow$ replace $u_0, \dots, u_n$ in $f_0, \dots, f_{n+s+1}$ with $b_0, \dots, b_n$, respectively
- 2 $g(p_0) \leftarrow$ generator of the radical of elimination ideal $\langle \tilde{f}_0, \dots, \tilde{f}_{n+s+1} \rangle \cap \mathbb{Q}[p_0]$
- 3 Make $g(p_0)$ monic with respect to p_0 , and **return** $g(p_0)$

we choose $\mathbf{b} = (b_1, b_2, b_3) = (2, 12, 7)$. We substitute $u_j = b_j$, and rename the resulting polynomials as $f_0^*, \dots, f_5^*$. Note that $f_k^* = f_k(u_0, \mathbf{b}, \mathbf{p}, \lambda)$. We obtain a generator of $\sqrt{\langle f_0^*, \dots, f_5^* \rangle \cap \mathbb{Q}[u_0, p_0]}$ by computing a Gröbner basis: $g^*(u_0, p_0) = 10(u_0 + 21)^2 p_0^3 - (u_0 + 21)(43u_0 + 276)p_0^2 + 2u_0(29u_0 + 396)p_0 - 24u_0^2$. If $\mathbf{b}$ is generic in the parameter space $\mathbb{C}^3$, then by Proposition 3.2 (2), $g^*(u_0, p_0) = E_f(u_0, \mathbf{b}, p_0)$. So, we have

$$N = \deg(E_f(\mathbf{u}, p_0), p_0) = \deg(E_f(u_0, \mathbf{b}, p_0), p_0) = \deg(g^*, p_0) = 3.$$

And, for $i = 0, \dots, N (= 3)$, we have

$$\deg(A_i(\mathbf{u}), u_0) = \deg(A_i(u_0, \mathbf{b}), u_0) = \deg(\text{coeff}(g^*, p_0^i), u_0) = 2.$$

So, we record $\mathcal{L}(1) = \deg(A_3, u_0) = 2$ and $\Omega(i+1, 1) = \deg(A_i, u_0) = 2$ for $i = 0, 1, 2$. Similarly, we compute the degrees of other parameters, and have

$$\mathcal{L} = [2, 2, 2, 2], \text{ and } \Omega = \begin{bmatrix} 2 & 0 & 0 & 0 \\ 2 & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 \end{bmatrix},$$

where $\mathcal{L}(j+1)$ records $\deg(A_3, u_j)$, and $\Omega(i+1, j+1)$ records $\deg(A_i, u_j)$ for $i = 0, 1, 2$. Notice $\mathcal{S}(u_0, \mathbf{b}) = u_0 + 21$. By Proposition 3.3, checking the multiplicity of the factor $u_0 + 21$ in each $\text{coeff}(g^*, p_0^i)$ for $i = 0, \dots, 3$, we have $\alpha_0 = \alpha_1 = 0$, $\alpha_2 = 1$, and $\alpha_3 = 2$.

Step 2. The second step is to recover the leading coefficient $A_N(\mathbf{u})$. By **Step 1**, we know $N = 3$ and $\alpha_3 = 2$. We write A_N as $A_3(\mathbf{u}) = \mathcal{S}(\mathbf{u})^2 R_3(\mathbf{u})$. By the degrees recored in $\mathcal{L}$, we know the degrees of u_0, u_1, u_2, u_3 in $A_3(\mathbf{u})$ are all 2. So, $R_3(\mathbf{u}) \in \mathbb{Q}$. According to the assumption (A2), $A_3(\mathbf{u})$ is monic with respect to u_0 . Hence, $R_3(\mathbf{u}) = 1$ and $A_3(\mathbf{u}) = \mathcal{S}(\mathbf{u})^2$.

Step 3. The last step is to interpolate $A_0(\mathbf{u}), A_1(\mathbf{u})$ and $A_2(\mathbf{u})$. As an example, we show how to interpolate $A_2(\mathbf{u})$ in details. By **Step 1**, we have $\alpha_2 = 1$. So we write $A_2(\mathbf{u}) = \mathcal{S}(\mathbf{u}) R_2(\mathbf{u})$. By the last row of Ω , the degrees of u_0, u_1, u_2, u_3 in $A_2(\mathbf{u})$ are 2, 2, 2, 2. Thus, the degrees of u_0, u_1, u_2, u_3 in $R_2(\mathbf{u})$ are 1, 1, 1, 1, respectively. By (F1), A_2 is homogenous, and we have $\deg(A_2) = \deg(A_3) = 2$. So R_2 is also homogenous, and $\deg(R_2) = \deg(A_2) - \deg(\mathcal{S}(\mathbf{u})) = 1$. Then we can assume $R_2(\mathbf{u}) = \sum_{k=0}^3 C_k u_k$, where $C_k \in \mathbb{Q}$. In order to determine the four coefficients C_k , we establish four linear equations by sampling four times. The correctness of this sampling step is guaranteed by Proposition 3.2 (2). We show below how to do the sampling and establish the first linear equation (4) in details. The other equations in (5) are similarly obtained.

For every u_j , substitute $u_j = b_j$ into $f_0, \dots, f_5$, where b_j is a random rational number. For instance, we choose $\mathbf{b} = (b_0, b_1, b_2, b_3) =$

$(5, 6, 11, 32)$. We substitute $u_j = b_j$, and rename the resulting polynomials as $\tilde{f}_0, \dots, \tilde{f}_5$. Note $\tilde{f}_k = f_k(\mathbf{b}, \mathbf{p}, \lambda)$. We compute a generator of $\sqrt{\langle \tilde{f}_0, \dots, \tilde{f}_5 \rangle \cap \mathbb{Q}[p_0]}$ and make it monic:

$$\tilde{g}^{(1)}(p_0) = p_0^3 - \frac{7}{5}p_0^2 + \frac{481}{1458}p_0 - \frac{5}{243}.$$

By Proposition 3.2 (2), if $\mathbf{b}$ is generic in $\mathbb{C}^4$, then $\tilde{g}^{(1)}(p_0) = \frac{E_f(\mathbf{b}, p_0)}{A_3(\mathbf{b})}$.

So $\text{coeff}(\tilde{g}^{(1)}, p_0^2) = \frac{A_2(\mathbf{b})}{A_3(\mathbf{b})}$. By the discussion above, we have $A_2(\mathbf{u}) = \mathcal{S}(\mathbf{u}) \sum_{k=0}^3 C_k u_k$, and by **Step 2**, $A_3(\mathbf{u}) = \mathcal{S}(\mathbf{u})^2$. So, we obtain

$$-\frac{7}{5} = \text{coeff}(\tilde{g}^{(1)}, p_0^2) = \frac{A_2(\mathbf{b})}{A_3(\mathbf{b})} = \frac{5C_0 + 6C_1 + 11C_2 + 32C_3}{54}. \quad (4)$$

Similarly, we obtain the other linear equations by samplings:

$$-\frac{311}{120} = \frac{11C_0 + 2C_1 + 3C_2 + 8C_3}{24}, \quad -\frac{244}{115} = \frac{7C_0 + 2C_1 + 5C_2 + 9C_3}{23}, \quad (5)$$

$$-\frac{181}{110} = \frac{7C_0 + 3C_1 + 13C_2 + 21C_3}{44}. \quad (6)$$

Solving $C_0, \dots, C_3$ from the 4 equations (4)–(5), we have

$$C_0 = -\frac{43}{10}, \quad C_1 = -2, \quad C_2 = -\frac{3}{2}, \quad C_3 = -\frac{4}{5},$$

and hence $A_2(\mathbf{u}) = -\mathcal{S}(\mathbf{u})(\frac{43}{10}u_0 + 2u_1 + \frac{3}{2}u_2 + \frac{4}{5}u_3)$. One can similarly interpolate $A_0(\mathbf{u})$ and $A_1(\mathbf{u})$. Finally, the output is $E_f = \mathcal{S}(\mathbf{u})^2 p_0^3 - \mathcal{S}(\mathbf{u})(\frac{43}{10}u_0 + 2u_1 + \frac{3}{2}u_2 + \frac{4}{5}u_3)p_0^2 + \frac{1}{5}u_0(29u_0 + 23u_1 + 21u_2 + 14u_3)p_0 - \frac{12}{5}u_0^2$. Also, it is straightforward to check the discriminant of E_f with respect to p_0 is

$$4u_0^2(u_0 + u_1 + u_2 + u_3)^2(441u_0^4 + 4998u_0^3u_1 + 20041u_0^2u_1^2 + 33320u_0u_1^3 + 19600u_1^4 - 756u_0^3u_2 + 20034u_0^2u_1u_2 + 83370u_0u_1^2u_2 + 79800u_1^3u_2 - 5346u_0^2u_2^2 + 55890u_0u_1u_2^2 + 119025u_1^2u_2^2 + 4860u_0u_2^3 + 76950u_1u_2^3 + 18225u_2^4 - 1596u_0^3u_3 - 11116u_0^2u_1u_3 - 17808u_0u_1^2u_3 + 4480u_1^3u_3 + 7452u_0^2u_2u_3 - 7752u_0u_1u_2u_3 + 49680u_1^2u_2u_3 - 17172u_0u_2^2u_3 + 71460u_1u_2^2u_3 + 27540u_2^3u_3 + 2116u_0^2u_3^2 + 6624u_0u_1u_3^2 - 4224u_1^2u_3^2 - 9528u_0u_2u_3^2 + 15264u_1u_2u_3^2 - 1216u_0u_3^3 - 512u_1u_3^3 + 3264u_2u_3^3 + 256u_3^4),$$

where the last factor is the mixed discriminant of $f_0, \dots, f_5$.

6 COMPUTATIONAL RESULTS

In this section, we explain the implementation details, and compare the timings of Algorithm 1 and existing methods by testing a list of interesting algebraic models.

6.1 Implementation

First, we explain the implementation and experimental details. Testing models, Maple code and computational results are available online via:

<https://sites.google.com/site/rootclassification/publications/supplementary-materials/1le2018>.

Software We implemented Algorithm 1 in Maple 2018, where we use the Fgb command `fgb_gbasis_elim` for computing elimination ideals, for instance, in Algorithm 2-Lines 2, 11, Algorithm 4-Line 2 and Algorithm 6-Line 2.

Hardware and System We used a 3.2 GHz Intel Core i5 processor (8 GB of RAM) under OS X 10.9.3.

Testing Models Testing Models are chosen from the literatures [20, 27] and have been tested by both standard elimination method and Algorithm 1.

6.2 Computing elimination ideals

We have computed the radical elimination ideals E_f for testing models by standard elimination, [40, Algorithm 2] and Algorithm 1. Table 1 compares the timings of the three methods.

Conclusion from Table 1: For smaller models with ML-degree less than 5, computing Gröbner bases directly (standard elimination) is the fastest method; for larger models with ML-degree greater than 5, Algorithm 1 is the fastest. Particularly, comparing columns “Interpolation” and “Algorithm 1”, we see the structure of elimination ideals indeed improves the efficiency significantly.

Instruction for Table 1:

- (1) The columns “ $\#p_i$ ” and “ML-Degree” give the number of probability variables n and ML-degree N , respectively.
- (2) In the column “standard” we record the time to compute the elimination ideal $\langle f \rangle \cap \mathbb{Q}[\mathbf{u}, p_0]$. When FGB returned no output until we run out the memory, we record “ ∞ ”.
- (3) We record timings of [40, Algorithm 2] and Algorithm 1 in the columns “Interpolation” and “Algorithm 1”. Timings in *italics font* means the computation did not finish within two weeks, but we estimate the sampling timing providing a lower bound; see Example 6.1.

Example 6.1. In Table 1, the estimated total timings for sampling, see **Step 3** in Section 5.1, are displayed in *italic*. We explain how to estimate these timings by the running example in Section 5.1. There are 4 parameters u_i ($i = 0, 1, 2, 3$). We know $\deg(A_2, u_i)$ are all 2. Also by (F1) and (A1), A_2 is homogenous and $\deg(A_2) = \deg(A_2, u_0) = 2$. So A_2 is a linear combination of 10 monomials. [40, Algorithm 2] interpolates $A_2(\mathbf{u})$ directly without any structure, so we need to sample 10 times. However, Algorithm 1 interpolates $R_2(\mathbf{u})$, which is a factor of $A_2(\mathbf{u})$ as shown in the running example, so we only need to sample 4 times since there are 4 possible monomials in $R_2(\mathbf{u})$. We check by Maple the timing for doing sample once in **Step 3** is 0.02 second. Then we estimate the timing of sampling in [40, Algorithm 2] and Algorithm 1 are $0.02 \times 10 = 2$ (seconds) and $0.02 \times 4 = 0.08$ (second), respectively.

6.3 Computing discriminants

Given $E_f(\mathbf{u}, p_0)$, we can directly compute the discriminant of E_f with respect to p_0 , denoted by $\text{discr}(E_f; p_0)$, by eliminating p_0 from E_f and $\frac{\partial E_f}{\partial p_0}$. We summarize the computational timing of this method for computing discriminants in Table 2. Here, we have a list of remarks on Table 2:

- (1) We can not save the large result for Model 6 into a text file. The size of a temporary file when we interrupt the saving process is 32 GB.
- (2) For Model 6 and Model 9, the estimated timings for [40, Algorithm 2] to compute $\mathcal{D}_{MJ}$ s are 13374 and 454833 days, respectively. Note that $\mathcal{D}_{MJ}$ is a factor of $\text{discr}(E_f; p_0)$.

ACKNOWLEDGMENTS

We thank David A. Cox, Hoon Hong, Anne Shiu, Frank Sottile, and Bernd Sturmfels for their support and advice. TdW was partially supported by the DFG grant WO 2206/1-1. XT was partially supported by the NSF (DMS-1513364, DMS-1752672, and CCF-1708884).

Models	Degree	Size	Our Method		
			E_f	$\text{discr}(E_f; p_0)$	Total
Model 4	110	7.5 MB	782.676 s	0.027 s	783 s
Model 6	342	> 32 GB	14 d	11.379 s	14 d
Model 9	176	8.68 GB	2 d	81.015 s	2 d

Table 2: Runtimes for computing discriminants

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