Chipsplitting Games: A Combinatorial Approach to Classifying One-Dimensional Discrete Statistical Models with Rational Maximum Likelihood Estimator

by

Viet-Duc Nguyen

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Supervisors:

Professor Carlos Améndola Professor Christian Haase

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Die Satzung zur Sicherung guter wissenschaftlicher Praxis an der TU Berlin vom 8. März 2017 habe ich zur Kenntnis genommen.

Ich erkläre weiterhin, dass ich die Arbeit in gleicher oder ähnlicher Form noch keiner anderen Prüfungsbehörde vorgelegt habe.

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Zusammenfassung in deutscher Sprache

Die vorliegende Ausarbeitung setzt die Forschung von Arthur Bik und Orlando Marigliano zur Klassifizierung ein-dimensionaler diskreter statistischer Modelle mit rationalen Maximum Likelihood Schätzern unter Verwendung fundamentaler Modelle fort. Wir erzielen bedeutende Fortschritte beim Beweis zur endlichen Anzahl der fundamentalen Modelle im Wahrscheinlichkeitssimplex Δ_5 . Zudem bestimmen wir die Anzahl der fundamentalen Modelle im Simplex Δ_6 mit einem maximalen Grad von 11.

Abstract

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This paper continues the research of Arthur Bik and Orlando Marigliano on the classification of one-dimensional discrete statistical models with rational maximum likelihood estimators using fundamental models. We present a missing proof of an algorithm from their work. Furthermore, we make significant progress in proving the finite number of fundamental models in the probability simplex Δ_5 . We also determine the number of fundamental models in the simplex Δ_6 with a maximum degree of 11.

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Chapter 1

Introduction

In statistics we come across various collections of probability distributions, such as the normal distribution, Poisson distribution, and binomial distribution. These distributions are used to model random variables in applications, and are referred to as *statistical models*. Precisely, a statistical model is just a set of probability distributions. If the set contains only discrete distributions, we call it a *discrete statistical model*. In this case, discrete statistical models are just subsets of the probability simplex $\Delta_n := \{p \in \mathbb{R}^{n+1} \mid \sum p_i = 1\}$.

A discrete distribution $p \in \mathcal{M} \subset \Delta_n$ from a discrete statistical model encapsulates the probabilities of observing the states $0, \ldots, n$, i.e. if $X \in \{0, \ldots, n\}$ is a discrete random variable, then the state X = i occurs with probability p_i for all $i = 0, \ldots, n$. Say we have a binomial random variable X with n + 1 states, then $p_i = \binom{n}{i} \theta^i (1 - \theta)^{n-i}$ computes the probability of observing i successes in n trials with success probability $\theta \in [0, 1]$. The set \mathcal{M} of all probability distributions of that form, i.e. $\mathcal{M} = \{\binom{n}{i} \theta^i (1 - \theta)^{n-i}\}_{i=0}^n \mid \theta \in [0, 1]\}$, is our first example of a discrete statistical model, and is known as the binomial model.



Figure 1.1: This figure shows the probability simplex Δ_2 with the binomial model (red curve). Every point on the curve is a binomial distribution.

Given a statistical model $\mathcal{M} \subset \Delta_n$ and data $u \in \mathbb{N}^{n+1}$, a typical problem in statistics is to find a distribution from a statistical model that best describes the data. "Best" can mean a lot of things, but in maximum likelihood estimation it means finding the distribution that maximizes the probability of observing the data; the map $\Phi : \Delta_n \to \mathcal{M}, u \mapsto \hat{p}$ that assigns the data u to a distribution $\hat{p} \in \mathcal{M}$ from the statistical model is called the maximum likelihood estimator (MLE). This map is characterized by the property that \hat{p} maximizes the log-likelihood function $\ell(p) = \sum u_i \log p_i$ for all $p \in \mathcal{M}$.

We focus on one-dimensional discrete statistical models with rational MLE. These are models \mathcal{M} satisfying

- $\mathcal{M} = \text{image}(p)$ for some rational map $p = (p_0, \dots, p_n) : I \to \Delta_n$ where p_i is rational, $I \subset \mathbb{R}$ is a union of closed intervals and $p(\partial I) \subset \partial \Delta_n$,
- all the n+1 coordinates of the maximum likelihood estimator Φ are rational functions in the data u.

There are two intriguing questions to ask about statistical models with rational MLE: the first one is about which form do the maximum likelihood estimators take; the second one is more concerned with the classification of the statistical models, i.e. can we divide these models into easier to understand classes? An answer to the first question was given by June Huh. He showed that if Φ is rational, then each of its coordinates is an alternative product of linear forms with numerator and denominator of the same degree, see [3, 2]. For the second question, Arthur Bik and Orlando Marigliano classified all one-dimensional discrete statistical models with rational MLE using fundamental models [1].

This thesis continues the work of Arthur Bik and Orlando Marigliano. In the first half, we present their classification results on how fundamental models serve as the building blocks of one-dimensional discrete models with rational MLE. In the second half, we establish and extend their finding that there are only finitely many fundamental models within the probability simplices Δ_n for $n \leq 4$. Due to the complexity of the problem, the cases $n \geq 5$ were left open. For the first time, we make significant progress for n = 5. Other contributions of this thesis include a new result on the number of fundamental models in Δ_6 with a maximum degree of 11, and a missing proof of a key algorithm from their work.

Chapter 2

Classification with Fundamental Models

In this chapter we present the classification of one-dimensional discrete statistical models with rational maximum likelihood estimator (MLE) using fundamental models. The classification is due to Arthur Bik and Orlando Marigliano [1].

Problem statement: Can we find a class of easy to understand models that serve as building blocks for all one-dimensional discrete statistical models with rational MLE?

The answer to this question are reduced and fundamental models.

2.1 Parametrization

It turns out that one-dimensional discrete statistical models with rational MLE admit the following parametrization.

Proposition 2.1. Let \mathcal{M} be a one-dimensional discrete statistical models with rational maximum likelihood estimator. Then, there exists a map of the form

$$p: [0,1] \to \Delta_n, \quad \theta \mapsto (w_k \theta^{i_k} (1-\theta)^{j_k})_{k=0}^n$$

 $i_k, j_k \in \mathbb{Z}_{>0}, \ w_k \in \mathbb{R}_{>0} \quad \forall k = 0, \dots, n$

such that $\mathcal{M} = \text{image}(p)$.

We introduce some notation to simplify the proof of Proposition 2.1. Let $\mathcal{M} \subset \Delta_n$ be a one-dimensional discrete statistical model parametrized by rational functions $p_0 = \frac{g_0}{h_0}, \ldots, p_n = \frac{g_n}{h_n}$. Define b to be the least common multiple of h_0, \ldots, h_n and $a_i \coloneqq bp_i$. Since $\sum p_k = 1$, we can multiply by b to obtain $\sum a_k = b$. We see that the polynomials a_0, \ldots, a_n, b

determine the statistical model \mathcal{M} , and have no common factors. The log-likelihood function is then given by

$$\ell(p) = \sum u_i \log p_i$$

$$= \sum u_i \log \frac{a_i}{b}$$

$$= \sum u_i \log a_i - \sum u_i \log b.$$

To find the maximum likelihood estimator, we need find all critical points of the log-likelihood function. This is equivalent to finding the roots of the gradient of the log-likelihood function

$$\ell(p(\theta))' = \sum u_k \frac{a_k'}{a_k} - \sum u_k \frac{b'}{b} = 0.$$
 (2.1)

These equations are called the *score equations* in algebraic statistics, and the number of complex solutions to these equations for general data $u \in \mathbb{C}^{n+1}$ is called the *maximum likelihood degree* of the statistical model. This ML degree has an important meaning in algebraic statistics, as it determines the complexity of the model. We have the following relationship between the ML estimator and the ML degree.

Proposition 2.2. Having rational maximum likelihood estimator can be expressed equivalently by saying that the maximum likelihood degree of the statistical model is one.

To prove Proposition 2.1, we need the following lemma.

Lemma 2.3. If \mathcal{M} has rational MLE, then there are exactly two distinct complex linear factors in a_0, \ldots, a_n , and b.

Proof. We prove the lemma in three steps:

• Let f be the product of all distinct complex linear factors in a_0, \ldots, a_n, b . If we multiply the score equations (2.1) by f, we get

$$f \cdot \ell(p(\theta))' = \sum u_k f \frac{a'_k}{a_k} - \sum u_k f \frac{b'}{b} = 0.$$

Note that every linear factor of a_k with multiplicity m occurs in a'_k with multiplicity m-1; thus every summand of $\frac{a'_k}{a_k}$ is of the form $\frac{\lambda}{(x-\xi)}$, where $\lambda \in \mathbb{R}$ and $x-\xi$ is some linear factor of a_k ; hence $f \cdot \frac{\lambda}{(x-\xi)}$ is of degree $\deg(f)-1$, and therefore $f \cdot \ell(p(\theta))'$ is of degree $\deg(f)-1$.

- We claim that the roots of $\ell(p(\theta))'$ are the same as the roots of $f \cdot \ell(p(\theta))'$. Assume we have shown this claim. By Proposition 2.2 the ML degree is one. So, $\ell(p(\theta))'$ has one root. Thus, $f \cdot \ell(p(\theta))'$ has one root, and therefore $f \cdot \ell(p(\theta))'$ is of degree one. This implies that $\deg(f) = 2$ with the previous step. Thus, there are exactly two distinct complex linear factors in a_0, \ldots, a_n , and b.
- It remains to show that the roots stay the same. Clearly, every root of $\ell(p(\theta))'$ is a root of $f \cdot \ell(p(\theta))'$. Conversely, we want to show that no new roots are introduced when multiplying by f, i.e. roots of f are not roots of $f \cdot \ell(p(\theta))'$. To do so, we rewrite

$$f \cdot \ell(p(\theta))' = \sum_{k=0}^{n} u_k f \frac{a'_k}{a_k} - \sum_{k=0}^{n} u_k f \frac{b'}{b} = \sum_{k=0}^{n+1} v_k f \frac{c'_k}{c_k}$$
$$v_k = u_k, \ c_k = a_k \quad \text{for } k = 0, \dots, n,$$
$$v_{n+1} = -\sum_{k=0}^{n} u_k, \ c_{n+1} = b.$$

Let q be a complex linear factor of f. We define polynomials r_0, \ldots, r_{n+1} and r such that $c_k = q^{l_k} r_k$, f = qr, and r_0, \ldots, r_{n+1}, r do not have q as a factor. Then, we have for $k = 0, \ldots, n+1$ that

$$f\frac{c'_k}{c_k} = qr \cdot \frac{l_k q^{l_k - 1} q' r_k + q^{l_k} r'_k}{q^{l_k} r_k} = qr \frac{l_k q'}{q} + qr \frac{r'_k}{r_k} \equiv r l_k q' \pmod{q}.$$

Thus, we obtain

$$f \cdot \ell(p(\theta))' \equiv rq' \sum_{k=0}^{n+1} v_k l_k \equiv rq' \sum_{k=0}^{n} v_k (l_k - l_{n+1}) \pmod{q}.$$

Note that by definition of l_k , a value of $l_k = 0$ means that q is not a factor of c_k . By definition of f, at least one $l_k > 0$. On the other hand, not all l_k can be positive since a_0, \ldots, a_n, b share no common factors. Hence, not all $l_k - l_{n+1} = 0$ vanish. Hence, for generic data u we assume $\sum_{k=0}^{n} v_k (l_k - l_{n+1}) \neq 0$. This with $q'r \not\equiv 0 \pmod{q}$ implies that q is not a complex linear factor of $f \cdot \ell(p(\theta))'$. We showed that the roots of f are not roots of $f \cdot \ell(p(\theta))'$.

Equipped with the lemma, we can now prove Proposition 2.1.

Proof. We want to show the following parametrization of \mathcal{M} :

$$p:[0,1]\to\Delta_n,\quad\theta\mapsto(w_k\theta^{i_k}(1-\theta)^{j_k})_{k=0}^n$$

First, we show that I is a single closed real interval and not a union of closed intervals. For the sake of contradiction assume that $I = \bigcup_k I_k$ is a union of closed disjoint intervals. By definition of \mathcal{M} we know that $p(\partial I) \subset \partial \Delta_n$. Thus, there exist $\theta_1, \theta_2 \in \partial I_0$ and $\theta_3, \theta_4 \in \partial I_1$ with $p_i(\theta_1) = p_i(\theta_2) = 0$ and $p_j(\theta_3) = p_j(\theta_4) = 0$ for some $i, j = 0, \ldots, n$. Note that θ_1, θ_2 are roots of $\frac{a_i}{b}$ and θ_3, θ_4 are roots of $\frac{a_j}{b}$. By Lemma 2.3 exactly two distinct complex linear factors occur in a_0, \ldots, a_n, b . Hence, $\theta_3 = \theta_1$ or $\theta_3 = \theta_2$. Contradiction for I_0 and I_1 are disjoint.

The previous argument shows that $I = [\alpha, \beta]$ is a real single closed interval. Thus, the roots of a_0, \ldots, a_n, b are real and take values in $\partial I = \{\alpha, \beta\}$. By a suitable parametrization, we can assume without loss of generality that I = [0, 1]. We can now write the polynomials a_0, \ldots, a_n, b as

$$a_k(\theta) = w_k \theta^{i_k} (1 - \theta)^{j_k}$$
$$b(\theta) = w \theta^i (1 - \theta)^j$$

with $w_k, w \in \mathbb{R}_{>0}$, and $i_k, j_k, i, j \in \mathbb{Z}_{\geq 0}$ for all k = 0, ..., n. Since $a_0, ..., a_n, b$ share no common factors, there exists some $i_k = 0$ if i > 0; however this would contradict $0 < w_k \le a_0(0) + \cdots + a_n(0) = b(0) = 0$. So i = 0. Similarly, j = 0. Finally, we divide p by w to obtain $b \equiv 1$.

Corollary 2.4. Any one-dimensional discrete statistical models with rational MLE can be represented by $(w_k, i_k, j_k)_{k=0}^n$ for $w_k \in \mathbb{R}_{>0}$ and $i_k, j_k \in \mathbb{Z}_{\geq 0}$.

From now on, we only consider one-dimensional discrete statistical models with rational MLE; we call them *models* for short.

Definition 2.5. The degree $\deg(\mathcal{M})$ of a model \mathcal{M} represented by $(w_k, i_k, j_k)_{k=0}^n$ is defined as $\max\{i_k + j_k : k = 0, \dots, n\}$.

Remark 2.6. We view two models $(w_k, i_k, j_k)_{k=0}^n$ and $(w'_k, i'_k, j'_k)_{k=0}^n$ as the same model if they are equal up to a permutation of the coordinates.

Example 2.7. The sequence ((1,0,2),(2,1,1),(1,2,0)) represents the binomial model with two trials. It has degree two. Its parametrization is given by $\theta \mapsto ((1-\theta)^2, 2\theta(1-\theta), \theta^2)$. Also see Figure 1.1 for a visualization of the binomial model within the probability simplex Δ_2 .

Note that we view the sequences ((1,0,2),(2,1,1),(1,2,0)) or ((2,1,1),(1,0,2),(1,2,0)) as the same model as ((2,1,1),(1,2,0),(1,0,2)) since the order of the coordinates does not matter.

Definition 2.8. Let \mathcal{M} be a model represented by $(w_k, i_k, j_k)_{k=0}^n$. The set of exponent pairs $(i_k, j_k)_{k=0}^n$ is called the support of \mathcal{M} , denoted by $\sup(\mathcal{M})$.

This was our first step towards understanding the structure of models. The next step is to introduce the concept of reduced models.

2.2 Reduced Models

Models in this section refer to one-dimensional discrete statistical models with rational MLE.

Definition 2.9. We call a model represented by $(w_k, i_k, j_k)_{k=0}^n$ reduced if $(i_k, j_k) \neq \mathbf{0}$ for all $k = 0, \ldots n$, and $(i_k, j_k) \neq (i_l, j_l)$ for all $k \neq l$.

Due to $(i_k, j_k) \neq (i_l, j_l)$, we can use functions to represent reduced models.

Remark 2.10. A reduced model \mathcal{M} represented by $(w_k, i_k, j_k)_{k=0}^n$ can also be identified by a function $f: \mathbb{Z}^2 \to \mathbb{R}_{\geq 0}, (i, j) \mapsto w$, where $w = w_k$ if $(i_k, j_k) = (i, j)$ and w = 0 otherwise. The support of f is the set of all pairs (i, j) with f(i, j) > 0. It coincides with the support of \mathcal{M} .

Reduced models are our first building blocks for the classification of models. This statement is justified by the following two propositions. They show that every non-reduced model can be transformed into a reduced model by a sequence of linear embeddings.

Proposition 2.11. Let $n \in \mathbb{N}_{>0}$. Let \mathcal{M} be a model represented by $(w_k, i_k, j_k)_{k=0}^n$. If $(i_l, j_l) = \mathbf{0}$ for some index l, then there exist a model \mathcal{M}' , $\lambda \in [0, 1]$ and $k = 0, \ldots, n$ such that

$$\mathcal{M} = \Psi_{\lambda,k}(\mathcal{M}'),$$

where
$$\Psi_{\lambda,k}: \Delta_{n-1} \to \Delta_n$$
 is defined as $p_i \mapsto \begin{cases} \lambda p_i & \text{if } k \neq i, \\ 1 - \lambda & \text{if } k = i. \end{cases}$

Proof. Let $(i_l, j_l) = \mathbf{0}$ for some index l. If $w_l = 1$, then $w_m = 0$ for all $m \neq l$; this contradicts $w_m > 0$ by Proposition 2.1. Set $\lambda = 1 - w_l > 0$ and k = l. Define the model \mathcal{M}' represented by

$$\left(\frac{w_h}{1-w_l}, i_h, j_h\right)_{h=0, h\neq l}^n.$$

Then, $\mathcal{M} = \Psi_{\lambda,k}(\mathcal{M}')$.

Proposition 2.12. Let $n \in \mathbb{N}_{>0}$. Let \mathcal{M} be model represented by $(w_k, i_k, j_k)_{k=0}^n$. If $(i_m, j_m) = (i_l, j_l)$ for $m \neq l$, then there exist a model \mathcal{M}' , $\lambda \in [0, 1]$ and $k, h = 0, \ldots, n$ such that

$$\mathcal{M} = \Psi_{\lambda,k,h}(\mathcal{M}'),$$

where
$$\Psi_{\lambda,k,h}: \Delta_{n-1} \to \Delta_n$$
 is defined as $p_i \mapsto \begin{cases} p_i & \text{if } i \notin \{k,h\}, \\ \lambda p_k & \text{if } k = i, \\ (1-\lambda)p_k & \text{if } h = i. \end{cases}$

Proof. Define $\lambda = \frac{w_m}{w_m + w_l}$, k = m, and h = l. Define the model \mathcal{M}' represented by

$$(w_g + \delta_{gm} w_l, i_g, j_g)_{q=0, q \neq l}^n$$
.

Then,
$$\mathcal{M} = \Psi_{\lambda,k}(\mathcal{M}')$$
.

By repeatedly applying the two propositions, we can transform any model into a reduced model.

Corollary 2.13. If Δ_n contains a model of degree d, then there also exists a reduced model of degree d in Δ_m for some $m \leq n$.

2.3 Fundamental Models

As before, models refer to one-dimensional discrete statistical models with rational MLE. The main building blocks for the classification of models are *fundamental models*; we will see that reduced models come from fundamental models.

Definition 2.14. We call a model represented by $(w_k, i_k, j_k)_{k=0}^n$ fundamental if it is reduced and the equation $p_0 + \dots p_n \equiv 1$ for given $(i_k, j_k)_{k=0}^n$ uniquely determines the weights $(w_k)_{k=0}^n$.

Example 2.15. The binomial model with two trials is fundamental. Given $(i_0, j_0) = (0, 2)$, $(i_1, j_1) = (1, 1)$, and $(i_2, j_2) = (2, 0)$, the equation $p_0 + p_1 + p_2 = w_0 \theta^2 + w_1 \theta (1 - \theta) + w_2 (1 - \theta)^2 \equiv 1$ uniquely determines the weights $w_0 = 1$, $w_1 = 2$, $w_2 = 1$. To see this observe that this equation is equivalent to $w_0 \theta^2 + w_1 \theta - w_1 \theta^2 + w_2 - w_2 2\theta + w_2 \theta^2 = 1$ which is equivalent to solving $w_2 - 1 + \theta(w_1 - 2w_2) + \theta^2(w_0 - w_1 + w_2) = 0$ for all $\theta \in \mathbb{R}$.

Example 2.16. Consider the probability simplex Δ_0 . It only contains the model 1 which is fundamental.

Example 2.17. Now, consider the probability simplex Δ_1 . It only contains the models $\theta \mapsto (\theta, 1 - \theta)$ and $\theta \mapsto (1 - \theta, \theta)$ which are equivalent. They are fundamental.

We will see that fundamental models like the ones above are building blocks for all reduced models by *composition*.

Definition 2.18. Let \mathcal{M} and \mathcal{M}' be reduced models which are represented by functions $f, g: \mathbb{Z}^2 \to \mathbb{R}_{\geq 0}$, see Remark 2.10. Let $\mu \in (0,1)$. The *composite* $\mathcal{M} *_{\mu} \mathcal{M}'$ of \mathcal{M} and \mathcal{M}' is the reduced model represented by the function

$$(i,j) \mapsto \mu f(i,j) + (1-\mu)g(i,j).$$

We are about to show that every reduced model is the composite of finitely many fundamental models.

Proposition 2.19. Let \mathcal{M} be a reduced model. Then \mathcal{M} is the composite of finitely many fundamental models.

Proof. For Δ_0 and Δ_1 we know that they only contain fundamental models, see Examples 2.16 and 2.17.

Assume we are given Δ_n with $n \geq 2$, and let \mathcal{M} be a model that is not fundamental. We aim to show that \mathcal{M} can be expressed as a composite of two models, \mathcal{M}' and \mathcal{M}'' , whose supports are proper subsets of supp(\mathcal{M}). Assume this is indeed the case. Then, by applying the same argument to \mathcal{M}' and \mathcal{M}'' , we can recursively decompose each nonfundamental model into models with smaller supports. Since supp(\mathcal{M}) is finite, this recursive decomposition must eventually terminate, yielding a decomposition of \mathcal{M} into fundamental models. Thus, we have shown that any reduced model is the composite of a finite number of fundamental models.

Let us prove that \mathcal{M} is the composite of two models whose supports are proper subsets of $\operatorname{supp}(\mathcal{M})$. Since \mathcal{M} is not fundamental, the equation $p_0 + \cdots + p_n = 1$ has distinct solutions $\mathbf{w}, \mathbf{w}' \in \mathbb{R}^{n+1}_{>0}$. Define $\mathbf{v} := \mathbf{w} - \mathbf{w}' \neq \mathbf{0}$. Then,

$$\sum_{k=0}^{n} v_k \theta^{i_k} (1 - \theta)^{j_k} = 0 \quad \forall \theta \in (0, 1).$$

Observe that there exist strictly positive and negative coefficients v_k . Define

$$\lambda := \min \left\{ \frac{w_k}{|v_k|} : k = 0, \dots, n, \ v_k < 0 \right\},$$

$$u_k := w_k + \lambda v_k \quad \text{for } k = 0, \dots, n,$$

$$S_1 := \{ (i_k, j_k) : k = 0, \dots, n, \ u_k \neq 0 \}.$$

Note that $\lambda > 0$ since all the coefficients w_k are strictly positive by definition. Also observe that $u_k \geq 0$ if $v_k \geq 0$. Moreover, by definition $\frac{w_k}{|v_k|} \geq \lambda$ for all $k \geq 0$. Hence, if $v_k < 0$, we also have $\frac{u_k}{v_k} = \frac{w_k}{v_k} + \lambda \leq 0$. Multiplying by $v_k < 0$ we obtain $u_k \geq 0$. All in all, we have $u_k \geq 0$ for all $k = 0, \ldots, n$. Moreover, $u_k = 0$ if and only if $v_k < 0$ and $\lambda = \frac{w_k}{|v_k|}$. This shows that $S_1 \subseteq \text{supp}(\mathcal{M})$. Since $u_0 + \ldots u_n = 1$, we have found a reduced model \mathcal{M}' represented by $(u_k, i_k, j_k)_{(i_k, j_k) \in S_1}$.

For the second model, we define

$$\mu := \min \left\{ \frac{w_k}{u_k} : k = 0, \dots, n, \ u_k \neq 0 \right\},$$

$$t_k := \frac{w_k - \mu u_k}{1 - \mu} \quad \text{for } k = 0, \dots, n,$$

$$S_2 := \left\{ (i_k, j_k) : k = 0, \dots, n, \ t_k \neq 0 \right\}.$$

Similarly, $\mu > 0$. We have $\mu < 1$ because some v_k is positive implying $u_k > w_k$. By definition, we have $t_k \ge 0$, and $t_k = 0$ if and only if $u_k \ne 0$ and $\mu = \frac{w_k}{u_k}$. This shows that $S_2 \subsetneq \text{supp}(\mathcal{M})$

and $S_1 \cup S_2 = \text{supp}(\mathcal{M})$. Since $t_0 + \cdots + t_n = 1$, we have found a reduced model \mathcal{M}'' represented by $(t_k, i_k, j_k)_{(i_k, j_k) \in S_2}$.

Finally, we see that $w_k = \mu u_k + (1 - \mu)t_k$. This shows that $\mathcal{M} = \mathcal{M}' *_{\mu} \mathcal{M}''$.

By applying the previous proposition with Corollary 2.13, we obtain the following corollary.

Corollary 2.20. If Δ_n contains a non-fundamental model of degree d, then there exists a fundamental model of degree d in Δ_m for some m < n.

Example 2.21. For the two-dimensional probability simplex Δ_2 , we can classify all models. Again, models refer to one-dimensional discrete statistical models with rational MLE. Note that the model \mathcal{M} parametrized by $\theta \mapsto (\theta, 1 - \theta)$ satisfies $\mathcal{M} *_{\mu} \mathcal{M} = \mathcal{M}$ for all μ . Since Δ_1 only contains the model $\theta \mapsto (\theta, 1 - \theta)$, we can conclude that Δ_2 only contains fundamental models or models that are not reduced.

To find all the fundamental models in Δ_2 , we need to check for all sets $S = \{(i_k, j_k)\}_{k=0}^2 \subset \mathbb{Z}_{>0}^2$ of size three if the equation $p_0 + p_1 + p_2 = \sum_{k=0}^2 w_k \theta^{i_k} (1-\theta)^{j_k} = 1$ has a unique solution (w_0, w_1, w_2) . As we can see, a priori infinitely many sets S need to be checked. However, as we will see in the next section, only those sets S with max $\{i+j: (i,j) \in S\} \leq 2n-1=3$ need to be considered. Clearly, this reduces the number of sets S to be checked to a finite number.

We compute that only the following supports uniquely determine the weights (w_0, w_1, w_2) :

$$\{(0,3),(1,1),(3,0)\},\{(0,2),(1,1),(2,0)\},\{(0,1),(1,1),(2,0)\},\{(0,2),(1,0),(1,1)\}.$$

They correspond to the fundamental models $((1-\theta)^3, 3\theta(1-\theta), \theta^3)$, $((1-\theta)^2, 2\theta(1-\theta), \theta^2)$, $(1-\theta, \theta(1-\theta), \theta^2)$, and $((1-\theta)^2, \theta, \theta(1-\theta))$. The last model is equivalent to the second last model by a parametrization $\theta \mapsto 1-\theta$ and permutation of the coordinates.

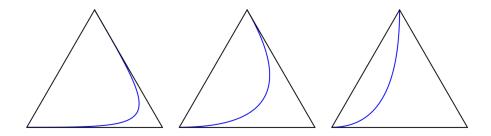


Figure 2.1: From left to right the illustration depicts the models parametrized $((1-\theta)^3, 3\theta(1-\theta), \theta^3)$, $((1-\theta)^2, 2\theta(1-\theta), \theta^2)$, $(1-\theta, \theta(1-\theta), \theta^2)$, and $((1-\theta)^2, \theta, \theta(1-\theta))$. The illustration is taken from [1].

We just computed all fundamental models of degree three or less in Δ_2 . We will see shortly that these are all models in the probability simplex Δ_2 . Of course, Δ_2 contains non-reduced models, too. These are models that come from linear embeddings $\Psi_{\lambda,k}$ and $\Psi_{\lambda,k,h}$, see Proposition 2.11 and Proposition 2.12. There are infinitely many of them, and for $\lambda = \frac{1}{3}$ we obtain the models $\theta \mapsto (\frac{2}{3}\theta, \frac{1}{3}, \frac{2}{3}(1-\theta))$ and $\theta \mapsto (1-\theta, \frac{1}{3}\theta, \frac{2}{3}\theta)$.



Figure 2.2: This illustration depicts two non-reduced models in Δ_2 for $\lambda = \frac{1}{3}$. They are parametrized by $\theta \mapsto (\frac{2}{3}\theta, \frac{1}{3}, \frac{2}{3}(1-\theta))$ and $\theta \mapsto (1-\theta, \frac{1}{3}\theta, \frac{2}{3}\theta)$. All other non-reduced models can be obtained by varying λ . The illustration is taken from [1].

Let us summarize the results of this section. It is the first part of our classification theorem.

Theorem 2.22. Every one-dimensional discrete statistical model with rational MLE in Δ_n is the image of a reduced model in Δ_m under a linear embedding $\Delta_m \to \Delta_n$ for some $m \le n$.

Moreover, every reduced model $\mathcal{M} \subset \Delta$ can be written as a composite of finitely many fundamental models

$$\mathcal{M} = \mathcal{M}_1 *_{\mu_1} (\cdots *_{\mu_{m-2}} (\mathcal{M}_{m-1} *_{\mu_{m-1}} \mathcal{M}_m))$$

for some m < n and $\mu_1, \ldots, \mu_m \in (0, 1)$.

Proof. See Proposition 2.19, Proposition 2.11, and Proposition 2.12.

2.4 On the Finiteness of Fundamental Models

We have established the first part of our classification theorem, namely that fundamental models are building blocks for all models. The second part is showing that there are only finitely many fundamental models in Δ_n given $n \in \mathbb{N}$. Artuhr Bik and Orlando Marigliano proved that there are only finitely many fundamental models in Δ_n for $n \leq 4$ [1]. We will

later make significant progress towards proving the case n = 5. For $n \ge 6$ no attempt has been made yet to the best of our knowledge.

Arthur Bik and Orlando Marigliano first proved the following proposition.

Theorem 2.23. Let \mathcal{M} be a one dimensional discrete statistical model with rational MLE in Δ_n . For $n \leq 4$ we have $\deg(\mathcal{M}) \leq 2n - 1$.

Given Theorem 2.23 it is easy to show the second part of our classification.

Theorem 2.24. There are only finitely many fundamental models in Δ_n for all $n \leq 4$.

Proof. By Theorem 2.23 we know that the degree of a fundamental model is at most 2n-1. Since the number of supports of a fundamental model of degree 2n-1 is finite, there are only finitely many fundamental models in Δ_n for all $n \leq 4$.

We will now spend the rest of this thesis on proving Theorem 2.23. The idea is to use the building blocks of fundamental models that we have established so far. Namely, it suffices to show the theorem for fundamental models.

Theorem 2.25. Let $N \in \mathbb{N}$. If for all $n \leq N$ and for all fundamental models $\mathcal{M} \in \Delta_n$ the upper bound $\deg(\mathcal{M}) \leq 2n - 1$ holds, then the upper bound also holds for all statistical models in $\Delta_{n'}$ for all $n' \leq N$.

Proof. Let $N \in \mathbb{N}$ and $n \leq N$. Assume there is some non-fundamental model \mathcal{M}' in Δ_n of degree greater than 2n-1. By Corollary 2.20 there exists a fundamental model \mathcal{M} in Δ_m for some m < n of degree greater than 2m-1. This contradicts the assumption that the degree of fundamental models is at most 2n'-1 for all $n' \leq N$.

Counting all fundamental models in Δ_n for $n \leq 4$ is our guiding objective. As a first step, we introduce a combinatorial game that aids in counting fundamental models. We know that every reduced model can be represented by the sequence of triples $(w_k, i_k, j_k)_{k=0}^n$, where $w_k \in \mathbb{R} > 0$ and $i_k, j_k \in \mathbb{Z}_{\geq 0}$. The model can be visualized in a directed graph with vertices in \mathbb{Z}^2 , where we can place values w_k on vertices (i_k, j_k) . Each vertex (i, j) is connected by directed edges to (i + 1, j) and (i, j + 1).

Surprisingly, we can derive a combinatorial game from this graph by defining a specific set of rules. This game, called the *chipsplitting game*, will be rigorously introduced in the next chapter. After that, we will explore the game's properties and show how it can be used to count fundamental models in Δ_n for $n \leq 4$.



Figure 2.3: The binomial model with two trials visualized in a directed graph with vertices in $\{0,1,2,3\}^2$.

Chapter 3

Chipsplitting Games

The notion of a chipsplitting game was introduced by [1] as a combinatorial approach to classifying one-dimensional discrete statistical models with rational maximum likelihood estimator. It was inspired by *chipfiring games* and for a subset of chipfiring games, the chipsplitting game is equivalent to the chipfiring game. We refer to [4] for a comprehensive introduction to chipfiring games.

3.1 Basic Definitions

Let us define the notion of a chipsplitting game.

Definition 3.1. Let (V, E) be a directed graph without loops.

- 1. A chip configuration is a vector $\mathbf{w} = (w_v)_{v \in V} \in \mathbb{Z}^V$ such that there are only finitely many nonzero components w_k .
- 2. The initial configuration is the chip configuration $\mathbf{0} \in \mathbb{Z}^V$.
- 3. A splitting move at $u \in V$ maps a chip configuration \mathbf{w} to some chip configuration \mathbf{w}' defined by

$$w'_{v} := \begin{cases} w_{v} - 1 & \text{if } v = u, \\ w_{v} + 1 & \text{if } (u, v) \in E \\ w_{v} & \text{otherwise.} \end{cases}$$

This map is denoted by split_u.

- 4. An unsplitting move at $u \in V$ maps \mathbf{w}' back to \mathbf{w} . This map is denoted by unsplit_u.
- 5. A chipsplitting game is a finite sequence of splitting and unsplitting moves.

- 6. An *outcome of a chipsplitting game* is the chip configuration obtained from applying the sequence of splitting and unsplitting moves defined by the game at the initial configuration.
- 7. Any outcome of a chipsplitting game is called an *outcome*.

Proposition 3.2. The order of the moves in a chipsplitting game does not affect the outcome.

Proof. This follows from commutativity of addition.

Note that all moves are reversible. Thus, we obtain the following corollary with Proposition 3.2.

Corollary 3.3. Let \mathbf{w} be an outcome. Then, there exists a chipsplitting game whose outcome is \mathbf{w} and where at no point both a splitting and an unsplitting move are applied at the same vertex.

Games that satisfy the condition in the corollary are called *reduced*. We will only consider reduced games in this thesis for simplicity. The map

{reduced games on
$$(V, E)$$
} / $\sim \rightarrow \{g : V' \to \mathbb{Z} : \#\{p \in V' : g(p) \neq 0\} < \infty\}$
 $f \mapsto (p \mapsto \text{number of moves at } p \text{ in game } f)$

is a bijection, where $V' \subset V$ is the subset of vertices with at least one outgoing edge. The equivalence relation \sim is defined by $f \sim g$ if f and g are the same up to reordering. Unsplitting moves are counted negatively by $p \mapsto$ number of moves at p in game f. Using the map above we identify a chipsplitting game with its corresponding function $V' \to \mathbb{Z}$. For every outcome $\mathbf{w} = (w_v)_{v \in V}$ we have

$$w_v = -f(v) + \sum_{u \in V', (u,v) \in E} f(u),$$

where we define f(v) = 0 for $v \notin V$.

Now, we define the directed graphs that we will consider in this thesis. For $d \in \mathbb{N} \cup \{\infty\}$ we write

$$V_d := \{(i, j) \in \mathbb{Z}^2_{\geq 0} \mid i + j \leq d\},$$

$$E_d := \{(v, v + e) \mid v \in V_{d-1}, e \in \{(1, 0), (0, 1)\}\}.$$

Definition 3.4. The degree $deg(\mathbf{v})$ of a vertex $\mathbf{v} = (i, j)$ is defined as i + j.

Example 3.5. A chip configuration $\mathbf{w} = (w_{i,j})_{(i,j)\in V_d} \in \mathbb{Z}^{V_d}$ can be illustrated as a triangle of numbers where $w_{i,j}$ is placed at the position (i,j) in the triangle. For example, $w_{2,4} = 4$ means that the value 4 is placed in the second column and fourth row of the triangle. The following is an example of a sequence of chip configurations for d = 3:

When $w_{i,j} = 0$, we omit the value in the triangle and write a dot instead. The sequence above starts with the initial configuration and then applies a splitting move at the vertex (0,0), (1,0), (0,1), (0,2) and (2,0). Finally, we apply an unsplitting move at the vertex (1,1) to obtain the final configuration. Coming back to figure 2.4, we see that it is represented as the third configuration of the triangle above.

Let us define some more terminology.

Definition 3.6. Let $\mathbf{w} = (w_{i,j})_{(i,j) \in V_d}$ be a chip configuration.

- 1. The positive support of **w** is defined as supp⁺(**w**) := { $(i,j) \in V_d \mid w_{i,j} > 0$ }.
- 2. The negative support of **w** is defined as supp⁻(**w**) := $\{(i,j) \in V_d \mid w_{i,j} < 0\}$.
- 3. The support of \mathbf{w} is defined as the union of the positive and negative support.
- 4. The degree of **w** is defined as $\deg(\mathbf{w}) := \max\{i+j \mid (i,j) \in \operatorname{supp}(\mathbf{w})\}.$
- 5. We say **w** is valid if its negative support is empty or only contains (0,0).

We are interested in *outcomes* that are *valid* since they will correspond to reduced models as we will see later. For that reason, it would be convenient to have a criterion for when a chip configuration is an outcome. The next section will provide such a criterion with the help of *Pascal equations*.

Example 3.7. Consider the following chip configuration:

```
. 1
1 . 5
. 5 . 2
1 . . 5 .
. 8 . . 2
-2 . . . . 2 .
```

We clearly see that this configuration is valid, but is it also an outcome of a chipsplitting game? Currently, the only way to answer this question is to apply all possible sequences of splitting and unsplitting moves to the initial configuration and check if the outcome is the given configuration. In the next section, we present an easily computable characterization to answer this question.

3.2 Pascal Equations

In this chapter we will establish that outcomes are roots of Pascal equations. So let us first define Pascal equations which are special cases of *linear forms*.

Definition 3.8. A linear form on \mathbb{Z}^{V_d} is a map of the form

$$\mathbb{Z}^{V_d} \to \mathbb{Z}, \quad \mathbf{w} \mapsto \sum_{(i,j) \in V_d} c_{i,j} w_{i,j}.$$

It is denoted by $\sum_{(i,j)\in V_d} c_{i,j} x_{i,j}$.

Definition 3.9. A Pascal form on \mathbb{Z}^{V_d} is a linear form $\sum_{(i,j)\in V_d} c_{i,j}x_{i,j}$ on \mathbb{Z}^{V_d} satisfying

$$c_{i,j} = c_{i+1,j} + c_{i,j+1}$$
 for all $(i,j) \in V_{d-1}$.

Example 3.10. We can visualize a Pascal form as a triangle of numbers where $c_{i,j}$ is placed at the position (i, j) in the triangle. Here are examples of Pascal forms for d = 2:

0			1			0			0	
1	1		1	0		0	0		1	1
2	1	0	1	0	0	1	1	1	0 .	-1 -2

Evaluating Pascal equations is invariant under splitting and unsplitting moves.

Proposition 3.11. Let $\mathbf{w} \in \mathbb{Z}^{V_d}$ be a chip configuration. Let $p = \sum c_{i,j} x_{i,j}$ be a Pascal equation on \mathbb{Z}^{V_d} . Then, we have $p(\mathbf{w}) = p(\mathrm{split}_u(\mathbf{w})) = p(\mathrm{unsplit}_v(\mathbf{w}))$ for all $u, v \in V_{d-1}$.

Proof. Let $u := (i', j') \in V_{d-1}$. By the Pascal property, we have

$$c_{i'+1,j'} + c_{i',j'+1} - c_{i',j'} = 0.$$

Thus, we have

$$p(\text{split}_{u}(\mathbf{w})) = \sum_{(i,j)\in V_{d}} c_{i,j}(\text{split}_{u}(\mathbf{w}))_{i,j}$$

$$= \sum_{(i,j)\in V_{d}} c_{i,j} \begin{cases} w_{i,j} - 1 & \text{if } (i,j) = u, \\ w_{i,j} + 1 & \text{if } (i,j) \in \{(i'+1,j'), (i',j'+1)\} \\ w_{i,j} & \text{otherwise} \end{cases}$$

$$= \sum_{(i,j)\in V_{d}} c_{i,j}w_{i,j} = p(\mathbf{w}).$$

Similarly, we can show that $p(\text{unsplit}_v(\mathbf{w})) = p(\mathbf{w})$ for all $v \in V_{d-1}$.

Corollary 3.12. Let $\mathbf{w} \in \mathbb{Z}^{V_d}$ be an outcome. Let $p = \sum c_{i,j} x_{i,j}$ be a Pascal equation on \mathbb{Z}^{V_d} . Then, $p(\mathbf{w}) = 0$.

Proof. Clearly, we have $p(\mathbf{0}) = 0$. Then, we use Proposition 3.11 and the fact that \mathbf{w} is obtained from the initial configuration $\mathbf{0}$ by a sequence of splitting and unsplitting moves. \square

This demonstrates that outcomes are roots of Pascal equations. The converse is also true as we will see now. This is one of the most important results; so let us state it now.

Theorem 3.13. Let $\mathbf{w} \in \mathbb{Z}^{V_d}$ be a chip configuration. Then, \mathbf{w} is an outcome if and only if \mathbf{w} is a root of all Pascal equations on \mathbb{Z}^{V_d} .

The direction left to right is the content of the previous corollary. For the other direction life would be easier if we had not to deal with infinitely many Pascal equations. So let us fix this first by introducing a basis from which we can generate all Pascal equations through linear combinations.

Example 3.14. Fix the degree d = 2. We later claim that the following set of Pascal forms is a basis:

Note that the first column of each Pascal form is a unit vector in \mathbb{R}^3 . We can also fix the first row of each Pascal form to be a unit vector in \mathbb{R}^3 :

We will denote the first set of Pascal forms by $\{col(0), col(1), col(2)\}$ and the second set by $\{row(0), row(1), row(2)\}$.

To generalize the example above to an arbitrary degree $d \in \mathbb{N}$ and to vectors beyond unit vectors, we assert that there exists a unique Pascal form whose first column is any chosen vector.

Proposition 3.15. Let $\mathbf{a} = (a_0, \dots, a_d)$ be any vector with integer entries. Then, the following two statements hold:

- 1. There exists a unique Pascal form $\sum c_{i,j}x_{i,j}$ such that $c_{0,\cdot}=\mathbf{a}$.
- 2. There exists a unique Pascal form $\sum c_{i,j}x_{i,j}$ such that $c_{i,0} = \mathbf{a}$.

Proof. Set $c_{0,\cdot} := \mathbf{a}$. Define $c_{i+1,j} := c_{i,j} - c_{i,j+1}$ for all $(i,j) \in V_d$ with i = 0. Then, we use the same formula to define $c_{i+1,j}$ for all $(i,j) \in V_d$ with i = 1. We repeat this process until we have defined all $c_{i,j}$ for $(i,j) \in V_d$.

For the second statement, we set $c_{\cdot,0} := \mathbf{a}$. Define $c_{i,j+1} := c_{i,j} - c_{i+1,j}$ for all $(i,j) \in V_d$ with j = 0. Then, we use the same formula to define $c_{i,j+1}$ for all $(i,j) \in V_d$ with j = 1. We repeat this process until we have defined all $c_{i,j}$ for $(i,j) \in V_d$.

Let us define our first two Pascal form bases.

Definition 3.16. Let k = 0, ..., d and $\mathbf{e}_k \in \mathbb{R}^{d+1}$ be the k-th unit vector.

- We define col(k) to be the unique Pascal form $\sum c_{i,j}x_{i,j}$ such that $c_{0,\cdot}=\mathbf{e}_k$.
- We define row(k) to be the unique Pascal form $\sum c_{i,j}x_{i,j}$ such that $c_{i,0}=\mathbf{e}_k$.

For examples of the Pascal forms col(k) and row(k) for d=2 see Example 3.14. We provide another example for d=7.

Example 3.17. Let us consider the Pascal form col(3) for d = 7. We visualize this Pascal form as follows:

The Pascal form row(3) is visualized as follows:

```
-35
-20
     15
     10
        -4
-10
-4
     6
        -4
     3
-1
       -3
             1
     1
       -2
             1
        -1
             1
```

Proposition 3.18. For all integers k = 0, ..., d the following formulas hold:

$$col(k) = (-1)^k \sum_{(i,j)\in V_d} (-1)^j \binom{i}{k-j} x_{i,j},$$
$$row(k) = (-1)^k \sum_{(i,j)\in V_d} (-1)^i \binom{j}{k-i} x_{i,j}.$$

Note that $\binom{a}{b} = 0$ for b < 0 or b > a.

Proof. We claim that $(-1)^k \sum_{(i,j) \in V_d} (-1)^j {i \choose k-j} x_{i,j}$ is a Pascal equation. To see that observe

$$(-1)^{j} \binom{i+1}{k-j} + (-1)^{j+1} \binom{i}{k-j-1} = (-1)^{j} \binom{i}{k-j}$$

for all $(i,j) \in V_d$ due to $\binom{a}{b+1} + \binom{a}{b} = \binom{a+1}{b+1}$ where we set a=i and b=k-j-1. Next, we see that $(-1)^{k+j} \binom{0}{k-j} = \delta_{jk}$. Thus, $(-1)^k \sum_{(i,j) \in V_d} (-1)^j \binom{i}{k-j} x_{i,j}$ is indeed $\operatorname{col}(k)$. By symmetry of the binomial coefficients, we can use the same argument to show the

second formula.

We now show that $\{\operatorname{col}(k)\}_{k=0}^d$ is indeed a basis for all Pascal forms on \mathbb{Z}^{V_d} .

Proposition 3.19. Let p be a Pascal form on \mathbb{Z}^{V_d} . The following statements hold:

- 1. There exist unique coefficients $\mu_0, \ldots, \mu_d \in \mathbb{Z}$ such that $p = \mu_0 \operatorname{col}(0) + \cdots + \mu_d \operatorname{col}(d)$.
- 2. There exist unique coefficients $\lambda_0, \ldots, \lambda_d \in \mathbb{Z}$ such that $p = \mu_0 \text{row}(0) + \cdots + \mu_d \text{row}(d)$.

Proof. Let $p = \sum c_{i,j} x_{i,j}$ be a Pascal form on \mathbb{Z}^{V_d} . If we try to solve the equation

$$\sum_{(i,j)\in V_d} c_{i,j} x_{i,j} = \lambda_0 \operatorname{col}(0) + \dots + \lambda_d \operatorname{col}(d)$$
(3.1)

for $\lambda_0, \ldots, \lambda_d$, then due to Proposition 3.18 we see for all $(i, j) \in V_d$ that we have

$$c_{i,j} = \lambda_0 (-1)^{0+j} \binom{i}{0-j} + \lambda_1 (-1)^{1+j} \binom{i}{1-j} + \dots + \lambda_d (-1)^{d+j} \binom{i}{d-j}$$
$$= \lambda_j (-1)^{2j} \binom{i}{0} + \lambda_{j+1} (-1)^{2j+1} \binom{i}{1} + \dots + \lambda_{i+j} (-1)^{2j+i} \binom{i}{i}.$$

We see $c_{0,\cdot} = (\lambda_0, \dots, \lambda_d)$. Thus we set the coefficients $\boldsymbol{\mu} \coloneqq c_{0,\cdot}$ and by Proposition 3.15 we see that $\sum_{(i,j)\in V_d} c_{i,j}x_{i,j} = \mu_0\operatorname{col}(0) + \cdots + \mu_d\operatorname{col}(d)$. Moreover, the same proposition shows that the coefficients $\lambda_0, \ldots, \lambda_d$ in Equation 3.1 are uniquely determined.

For the second statement we use the same argument.

Corollary 3.20. The set $\{\operatorname{col}(k)\}_{k=0}^d$ is a basis for all Pascal forms on \mathbb{Z}^{V_d} . The same holds for $\{\operatorname{row}(k)\}_{k=0}^d$.

Proof. This follows from the previous proposition.

Let us come back to Theorem 3.13. We can now prove the other direction; namely that roots of all Pascal equations on \mathbb{Z}^{V_d} are outcomes.

Proposition 3.21. Let $\mathbf{w} \in \mathbb{Z}^{V_d}$ be a chip configuration. If for all Pascal equations p on \mathbb{Z}^{V_d} we have $p(\mathbf{w}) = 0$, then \mathbf{w} is an outcome.

Proof. Let $\mathbf{w} \in \mathbb{Z}^{V_d}$ be a chip configuration. By assumption

$$\operatorname{col}(\operatorname{deg}(\mathbf{w}))(\mathbf{w}) = 0. \tag{3.2}$$

Note that by Proposition 3.18 for $\operatorname{col}(\operatorname{deg}(\mathbf{w})) = \sum c_{i,j} x_{i,j}$ we have $c_{i,\operatorname{deg}(\mathbf{w})-i} = (-1)^i$ for all $i = 0, \ldots, \operatorname{deg}(\mathbf{w})$. Moreover, we have

$$c_{i,j} = 0 \quad \text{for all } i + j < \deg(\mathbf{w})$$
 (3.3)

by Proposition 3.18. Together with Equation 3.2 and 3.3 we obtain

$$\sum_{i=0}^{\deg(\mathbf{w})} (-1)^i w_{i,\deg(\mathbf{w})-i} = 0.$$
(3.4)

Furthermore, we know that there exists a unique minimal set of splitting or unsplitting moves at vertices (i, j) of degree $\deg(\mathbf{w}) - 1$ such that applied to \mathbf{w} we obtain a chip configuration \mathbf{w}' with $w'_{i,j} = 0$ for all $i = 0, ..., \deg(\mathbf{w})$. We call applying these set of moves to \mathbf{w} retraction.

Thus, \mathbf{w}' has degree less than $\deg(\mathbf{w})$. By Proposition 3.11 \mathbf{w}' is also a root of all Pascal equations. We repeat the retraction process $\deg(\mathbf{w})$ many times until we obtain some chip configuration of degree 0. This chip configuration is the initial configuration due to Equation 3.4. Thus, \mathbf{w} is an outcome.

We have shown Theorem 3.13. Characterizing outcomes as roots of Pascal equations is a powerful tool to determine if a chip configuration is an outcome.

Algorithm 1 Validating outcomes

```
Require: chipsplitting configuration \mathbf{w} \in \mathbb{Z}^{V_d}
Ensure: True if w is an outcome, False otherwise
 1: function ISOUTCOME(A, n)
        initialize set S = \{ col(0), \ldots, col(deg(\mathbf{w})) \}
 2:
        for p of S do
 3:
 4:
            if p(\mathbf{w}) \neq 0 then
                return False
 5:
            end if
 6:
        end for
 7:
        return True
 9: end function
```

Proof of correctness of Algorithm 1. This follows from Theorem 3.13.

Example 3.22. Returning to Example 3.7, we see that the chip configuration is a root of all Pascal equations $col(0), \ldots, col(6)$ using Algorithm 1. Thus, the chip configuration is an outcome.

3.3 Valid Outcomes and Reduced Statistical Models

In the previous sections, we have established that outcomes are roots of Pascal forms. Now, we will demonstrate that a subset of *valid outcomes* are in one-to-one correspondence with

reduced statistical models. Thus, we obtain not only a combinatorial characterization of reduced statistical models through chip-splitting games but also an algebraic characterization through Pascal equations. As before, statistical models mean one-dimensional discrete statistical models with rational maximum likelihood estimator.

We remind that valid chipsplitting configurations are those where the negative support is empty or only contains the vertex (0,0). Hence, valid outcomes are roots of Pascal equations whose negative supports are empty or only contain the vertex (0,0).

The function $\mathbf{w}(\mathcal{M})$ maps reduced models $\mathcal{M} = (w_k, i_k, j_k)_{k=0}^n$ to chip configurations $\mathbf{w}(\mathcal{M}) = (w_{i,j})_{(i,j) \in V_{\infty}}$ by

$$w_{i,j} := \begin{cases} -1 & \text{if } (i,j) = (0,0), \\ w_k & \text{if } (i,j) = (i_k, j_k) \text{ for some } k, \\ 0 & \text{otherwise.} \end{cases}$$

Note that the map $\mathbf{w}(\mathcal{M})$ defines a *real* chipsplitting games; the rules of the game are the same as for integer chipsplitting games.

Example 3.23. The binomial model ((1,3,0),(3,2,1),(3,1,2),(1,0,3)) with three trials is mapped to the chip configuration below:

Example 3.24. Does the following valid real outcome from Example 3.7 induce a reduced statistical model through the inverse map \mathbf{w}^{-1} ?

The outcome would correspond to the reduced model

$$\mathcal{M} = ((0.5, 2, 0), (0.5, 4, 0), (2.5, 1, 3), (0.5, 1, 5), (4, 2, 1), (2.5, 2, 4),$$
$$(2.5, 3, 2), (1, 3, 3), (1, 5, 0), (1, 5, 1))$$

in the probability simplex Δ_9 . As it turns out \mathcal{M} is indeed a reduced statistical model by the next theorem.

Theorem 3.25. The map $\mathcal{M} \mapsto w(\mathcal{M})$ is a bijection between reduced statistical models and valid real outcomes $\mathbf{w} \in \mathbb{R}^{V_{\infty}}$ with $w_{0,0} = -1$.

reduced models « valid outcomes

Figure 3.1: Bijection between reduced models and valid real outcomes **w** with $w_{0,0} = -1$

To show this theorem, we need to do some preparations. Let $\mathbb{R}[\theta]_{\leq d}$ denote the vector space of polynomials in the variable θ of degree at most d with real coefficients. Similarly, we define $\mathbb{Z}[\theta]_{\leq d}$ and $\mathbb{Q}[\theta]_{\leq d}$. Next, we introduce the linear map $\alpha_d^{\mathbb{R}}$ that maps real chip configurations to real polynomials:

$$\alpha_d^{\mathbb{R}} : \mathbb{R}^{V_d} \to \mathbb{R}[\theta]_{\leq d},$$

$$\mathbf{w} \mapsto \sum_{(i,j)\in V_d} w_{i,j} \theta^i (1-\theta)^j.$$

We define the map $\alpha_d^{\mathbb{Z}}$ and $\alpha_d^{\mathbb{Q}}$ for integer and rational chip configurations analogously.

Lemma 3.26. The following statements hold true for all $d \in \mathbb{N} \cup \{\infty\}$:

- 1. $\{\mathbf{w} \in \mathbb{R}^{V_d} \mid \mathbf{w} \text{ is an outcome}\} = \text{kernel}(\alpha_d^{\mathbb{R}});$
- 2. $\{\mathbf{w} \in \mathbb{Z}^{V_d} \mid \mathbf{w} \text{ is an outcome}\} = \text{kernel}(\alpha_d^{\mathbb{Z}});$
- 3. $\{\mathbf{w} \in \mathbb{Q}^{V_d} \mid \mathbf{w} \text{ is an outcome}\} = \text{kernel}(\alpha_d^{\mathbb{Q}}).$

Proof. We only prove the first statement. The other two statements are proven analogously. Note that it suffices to show the statement for $d < \infty$ since $\alpha_{\infty}^{\mathbb{R}}$ is the direct limit of $\alpha_0^{\mathbb{R}}, \alpha_1^{\mathbb{R}}, \alpha_2^{\mathbb{R}}, \ldots$, and so on.

Let $d < \infty$. By Corollary 3.20, the codimension of the outcome space is d + 1, as it is defined by the roots of the Pascal forms $col(0), \ldots, col(d)$.

Let $f(\theta) = \lambda_0 + \lambda_1 \theta + \cdots + \lambda_d \theta^d$ be a polynomial in \mathbb{R} of degree at most d. Define a chipsplitting configuration \mathbf{w} by

$$w_{i,j} \coloneqq \begin{cases} \lambda_i & \text{if } j = 0, \\ 0 & \text{otherwise.} \end{cases}$$

Then, $\alpha_d^{\mathbb{R}}(\mathbf{w}) = f$, which shows that the map $\alpha_d^{\mathbb{R}}$ is surjective. Hence, the kernel of $\alpha_d^{\mathbb{R}}$ has codimension d+1; it has equal codimension as the space of outcomes.

Finally, we just need to show that the space of outcomes is contained in the kernel of $\alpha_d^{\mathbb{R}}$. Since their codimensions are equal, the two spaces must be equal. Let $\mathbf{w} \in \mathbb{R}^{V_d}$ be an

outcome. The value of $\alpha_d^{\mathbb{R}}(\mathbf{w})$ remains the same if apply splitting or unsplitting moves at arbitrary vertices $(i,j) \in V_{d-1}$ because we have

$$-\theta^{i}(1-\theta)^{j} + \theta^{i+1}(1-\theta)^{j} + \theta^{i}(1-\theta)^{j+1} = \theta^{i}(1-\theta)^{j}(-1+\theta+(1-\theta)) = 0.$$

The remaining claim follows from $\alpha_d^{\mathbb{R}}(\mathbf{0}) = 0$.

We now show Theorem 3.25.

Proof of Theorem 3.25. Let $\mathcal{M} = (w_k, i_k, j_k)_{k=0}^n$ be a reduced model.

- First, we need to show that $\mathbf{w} := w(\mathcal{M})$ is an outcome; a-priori we only know that it is some chip configuration. By definition of $w(\mathcal{M})$, we have that $w_{0,0} = -1$. Since \mathcal{M} is a statistical model, we know that $\sum_{k=0}^{n} w_k \theta^{i_k} (1-\theta)^{j_k} \equiv 1$. Thus, $\alpha_d^{\mathbb{R}}(\mathbf{w}) = \sum_{k=0}^{n} w_k \theta^{i_k} (1-\theta)^{j_k} 1 \equiv 0$. Thus, $\mathbf{w} \in \text{kernel}(\alpha_d^{\mathbb{R}})$. By Lemma 3.26, the chip configuration \mathbf{w} is an outcome.
- Injectivity: Let $\mathcal{M} = (w_k, i_k, j_k)_{k=0}^n$ and $\mathcal{M}' = (w'_k, i'_k, j'_k)_{k=0}^n$ be two distinct models. Then, $w(\mathcal{M}) \neq w(\mathcal{M}')$ (see Remark 2.6).
- Surjectivity: Let $\mathbf{w} \in \mathbb{R}^{V_{\infty}}$ be a valid real outcome with $w_{0,0} = -1$. We define

$$w_k \coloneqq w_{i_k,j_k}$$
 for all $k = 0, \dots, n$.

Then, $\mathcal{M} = (w_k, i_k, j_k)_{k=0}^n$ is a reduced model by Lemma 3.26. We see that $w(\mathcal{M}) = \mathbf{w}$. Hence, $\mathcal{M} \mapsto w(\mathcal{M})$ is surjective.

Next, we collect simple results.

Proposition 3.27. The following statements hold for all reduced models \mathcal{M} :

- 1. $\operatorname{supp}^+(w(\mathcal{M})) = \operatorname{supp}^+(\mathcal{M})$.
- 2. The map $\mathcal{M} \mapsto w(\mathcal{M})$ is degree-preserving.
- 3. The outcome $w(\mathcal{M})$ is a rational outcome if and only if all the coefficients of \mathcal{M} are rational.

Proof. All three statements follow directly from definitions.

Proposition 3.28. Let $\mathbf{w} \in \mathbb{Q}^{V_{\infty}}$ be a valid rational outcome. Then, there exist positive $\lambda \in \mathbb{Q}$ and integral valid outcome $\mathbf{z} \in \mathbb{Z}^{V_{\infty}}$ such that $\mathbf{w} = \lambda \mathbf{z}$.

Proof. Let **w** be a valid rational outcome. Its support is finite. Thus, there exist $\mu \in \mathbb{N}$ such that $\mu \mathbf{w} \in \mathbb{Z}^{V_{\infty}}$. Define $\lambda \coloneqq \frac{1}{\mu}$ and $\mathbf{v} \coloneqq \mu \mathbf{w}$. Clearly, $\alpha_{\deg(\mathbf{v})}^{\mathbb{Z}}(\mathbf{v}) = \mu \alpha_{\deg(\mathbf{w})}^{\mathbb{Q}}(\mathbf{w}) \equiv 0$. By Lemma 3.26, **v** is an outcome. It is valid because $\mu \mathbf{w}$ is valid.

Proposition 3.29. Let $\mathbf{w} \in \mathbb{R}^{V_{\infty}}$ be a valid real outcome. If $w_{0,0} = 0$, then $\mathbf{w} = \mathbf{0}$.

Proof. By Lemma 3.26, we have $\sum w_{i,j}\theta^i(1-\theta)^j \equiv 0$. By assumption, the negative support is empty. Hence, all the $w_{i,j}$ are non-negative. We evaluate at $\theta = \frac{1}{2}$ to conclude that the positive support of \mathbf{w} is empty. Hence, $\mathbf{w} = 0$.

Let us go back to Example 3.23.

Example 3.30. We have seen that the valid real outcome below induces a reduced statistical model by Theorem 3.25.

The outcome has degree three and positive support size four. Can we find another outcome with the same degree but smaller positive support size? Indeed we can unsplit at vertex (1,1) to get

```
1
. .
. 3 .
-1 . . 1.
```

Can we reduce the positive support size further? As it will turn out, we cannot. The positive support size is minimal for a degree three outcome.

Example 3.31. Let us fix the positive support size to be three. What is the largest degree of a valid real outcome with positive support size three? We have already found

```
1
. .
. 3 .
-1 · . 1.
```

However is there an even larger one? Once again, the answer is no: by the following theorem, the degree of a valid real outcome with positive support of size three is at most three.

Theorem 3.32. The following upper bound

$$\deg(\mathbf{w}) \le 2 \cdot |\mathrm{supp}^+(\mathbf{w})| - 3$$

holds for valid integral outcomes \mathbf{w} with $|\text{supp}^+(\mathbf{w})| \leq 5$.

Arthur Bik and Marigliano Orlando established this theorem in [1], and we will provide a proof in the following sections. The question of whether the upper bound extends to cases with larger positive support sizes, $|\sup^+(\mathbf{w})| > 5$, remains open. A primary contribution of this thesis is the significant advancement in proving this bound for the case $|\sup^+(\mathbf{w})| = 6$.

Pos. Support Size	Max Degree
2	1
3	3
4	5
5	7

Table 3.1: The following table shows the largest degree of a valid real outcome with positive support size 2, 3, 4 and 5.

Theorem 3.32 is of particular interest because it is equivalent to Theorem 2.23, i.e. proving that the degree of outcomes is bounded by their positive support size is equivalent to establishing that the degree of statistical models is bounded by their dimension.

degree of outcomes
$$\mathbf{w} \longleftrightarrow$$
 degree of statistical models \mathcal{M} $\operatorname{supp}^+(\mathbf{w}) \longleftrightarrow$ dimension of \mathcal{M}

Proposition 3.33. Theorem 2.23 and Theorem 3.32 are equivalent.

Proof. Assume Theorem 2.23 holds. We want to show Theorem 3.32. Let \mathbf{w} be a valid integral outcome of positive support size $n \leq 5$. Normalize \mathbf{w} such that $w_{0,0} = -1$. The degree and positive support size do not change. By Theorem 3.25, the outcome \mathbf{w} induces a reduced statistical model \mathcal{M} in Δ_{n-1} . Then, $\deg(\mathcal{M}) \leq 2(n-1) - 1 = 2n - 3$. Thus, applying Theorem 3.25 let us go back to the outcome \mathbf{w} , and Proposition 3.27 establishes $\deg(\mathbf{w}) \leq 2n - 3$.

For the converse direction, assume Theorem 3.32 holds. Let $n \leq 5$. We want to show Theorem 2.23. Let $\mathcal{M} = (w_k, i_k, j_k)_{k=0}^{n-1} \subset \Delta_{n-1}$ be a one-dimensional discrete statistical model with rational MLE. By Theorem 2.25 we may assume that \mathcal{M} is fundamental. We use Theorem 3.25 to map \mathcal{M} to some valid real outcome $\mathbf{w} = (w_{i,j})$ with $w_{0,0} = -1$. Note that \mathbf{w} is even a rational outcome because by Definition 2.14 the weights $(w_k)_{k=0}^{n-1}$ of the fundamental model \mathcal{M} are uniquely determined by the equation $p_0(\theta) + p_1(\theta) + \cdots + p_{n-1}(\theta) - 1 \equiv 0$, and for some $\theta \in [0, 1]$ this equation becomes rational. Next, we use Proposition 3.28 to find some integral valid outcome \mathbf{z} such that $\mathbf{w} = \mu \mathbf{z}$ for some positive scalar $\mu \in \mathbb{Q}_{>0}$. Again, scaling does not affect the degree or size of the positive support. By Proposition the integral valid outcome 3.27 \mathbf{z} has positive support size n. By Theorem 3.32 we have $\deg(\mathbf{z}) \leq 2n-3$. Thus, $\deg(\mathbf{w}) = \deg(\mu \mathbf{z}) = \deg(\mathbf{z}) \leq 2n-3$. Hence, the degree of \mathcal{M} is smaller or equal to 2(n-1)-1 by Proposition 3.27. We proved Theorem 2.23.

Recall that our goal is to demonstrate that only finitely many fundamental statistical models exist in Δ_n for $n \leq 4$. To achieve this, we originally aimed to prove Theorem 2.24 from Chapter 2. However, as established in Chapter 3, we can alternatively prove Theorem 3.32, which serves as an equivalent approach to resolving the problem. We have chosen to focus on Theorem 3.32 because it allows us to address the problem from a combinatorial perspective.

Chapter 4

On the Finiteness of Valid Integral Outcomes

Let us devote the remaining chapters to the study of Theorem 3.32, which for the sake of convenience we restate below.

Theorem. The following upper bound

$$\deg(\mathbf{w}) \le 2 \cdot |\mathrm{supp}^+(\mathbf{w})| - 3$$

holds for valid integral outcomes \mathbf{w} with $|\operatorname{supp}^+(\mathbf{w})| \leq 5$.

From now on, valid outcomes **w** refer to *integral* valid outcomes in \mathbb{Z}^{V_d} for *finite* $d \in \mathbb{N}$.

4.1 Invertibility Criterion

Let $d \in \mathbb{N}$. One of the most important tools in the study of valid outcomes is the *invertibility* criterion first introduced in [1]. By Theorem 3.13 we can characterize valid outcomes as the roots of all Pascal forms on \mathbb{Z}^{V_d} . In the previous chapter we have already found two bases for the space of Pascal forms, namely $(\text{row}(0), \ldots, \text{row}(d))$ and $(\text{col}(0), \ldots, \text{col}(d))$ (see Definition 3.16). Let us introduce a new basis for the space of Pascal forms.

Definition 4.1. Let k = 0, ..., d and $\mathbf{e}_k \in \mathbb{R}^{d+1}$ be the k-th unit vector. We define $\operatorname{diag}(k)$ to be the unique Pascal form $\sum c_{i,j} x_{i,j}$ such that $c_{k,d-k} = \mathbf{e}_k$.

Example 4.2. Fix the degree d = 7. We visualized diag(3) by

Proposition 4.3. For all integers k = 0, ..., d we have:

$$\operatorname{diag}(k) = \sum_{(i,j)\in V_d} {\binom{d-i-j}{k-i}} x_{i,j}.$$

Note that $\binom{a}{b} = 0$ for b < 0 or b > a.

Proof. Note that for all $(i,j) \in V_d$ with i+j=d we have $\binom{d-i-j}{k-i}=1$ if and only if k=i, and in all other cases $k \neq i$ the binomial coefficient is zero. Thus, it remains to show that $\sum_{(i,j)\in V_d} \binom{d-i-j}{k-i} x_{i,j}$ is a Pascal form. We have

$$\binom{d-i-j}{k-i} = \binom{d-i-1-j}{k-i-1} + \binom{d-i-j-1}{k-i}.$$

for all $(i, j) \in V_{d-1}$ because $\binom{a+1}{b+1} = \binom{a}{b+1} + \binom{a}{b}$.

Proposition 4.4. Let p be a Pascal form on \mathbb{Z}^{V_d} . There exist unique coefficients $\mu_0, \ldots, \mu_d \in \mathbb{Z}$ such that $p = \mu_0 \operatorname{diag}(0) + \cdots + \mu_d \operatorname{diag}(d)$.

Proof. Let $p = \sum c_{i,j} x_{i,j}$. Choose $\mu_k = c_{k,d-k}$ for $k = 0, \ldots, d$. Since p is a Pascal form, the coefficients $c_{i,j}$ satisfy the Pascal recurrence relation. Thus, the coefficients μ_k are uniquely determined.

The invertibility criterion uses the diagonal basis $(\text{diag}(0), \dots, \text{diag}(d))$ to determine whether a given outcome is valid.

Definition 4.5. Let $E \subset \{0, \ldots, d\}$ and $S \subset V_d$ with $|E| = |S| \neq 0$. The pairing matrix of (E, S) is definded as $A_{E, S}^{(d)} := \left[\binom{d-i-j}{k-i}\right]_{k \in E, (i,j) \in S}$.

Example 4.6. Let d = 2, $S = \{(1, 1), (0, 0)\}$ and $E = \{0, 1\}$. Then the pairing matrix is

$$A_{E,S}^{(d)} = \begin{bmatrix} \binom{2-1-1}{0-1} & \binom{2-0-0}{0-2} \\ 2-1-1 & \binom{2-0-0}{1-2} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.$$

Now, assume **w** is an outcome with support in S. Since it is an outcome, we have $diag(k)(\mathbf{w}) = 0$ for all k = 0, 1, 2, 3. Thus,

$$A_{E,S}^{(d)}\mathbf{w} = \mathbf{0}.$$

We make the following observation: if the matrix $A_{E,S}^{(d)}$ were invertible (it is not for the given example), then we would have $\mathbf{w} = \mathbf{0}$. This is the invertibility criterion.

Proposition 4.7 (Invertibility Criterion). Let \mathbf{w} be an outcome with supp $(\mathbf{w}) \subset S$. If $A_{E,S}^{(d)}$ is invertible, then $\mathbf{w} = \mathbf{0}$.

Proof by Contraposition. Let $\mathbf{w} \neq \mathbf{0}$. Its support is non-empty. Then, $\mathbf{w}' := (w_{i,j})_{(i,j) \in S} \neq \mathbf{0}$. So, $A_{E,S}^{(d)} \cdot \mathbf{w}' = \mathbf{0}$. The kernel of the pairing matrix is non-trivial. Hence, the pairing matrix $A_{E,S}^{(d)}$ is not invertible.

Given a non-zero outcome \mathbf{w} we try to construct sets $S \supset \operatorname{supp}(\mathbf{w})$ and E such that the pairing matrix $A_{E,S}^{(d)}$ is invertible. If we succeed, then \mathbf{w} is not a *valid* outcome since the initial configuration is the only valid outcome with support in S. If we fail, then \mathbf{w} may be or may not be a valid.

4.2 Divide and Conquer

The invertibility criterion is a powerful tool to determine whether a given outcome is valid. However, it is not always easy to find suitable sets S and E such that the pairing matrix is invertible. We will now introduce a method to construct such sets.

Divide

Instead of finding one large set S with supp $(\mathbf{w}) \subset S$, we divide S into smaller sets S_1, \ldots, S_l . These smaller sets S_1, \ldots, S_k will be implicitly defined by integers $\lambda_1, \ldots, \lambda_l \in \mathbb{N}$ as we will shortly see. We choose $l \in \mathbb{N}$ and integers $\lambda_1, \ldots, \lambda_l \in \mathbb{N}$ such that for all $i = 1, \ldots, d$ we have

$$|S_i| \in \{0, \lambda_i\}$$

$$S_i := \{(i, j) \in \operatorname{supp}(\mathbf{w}) : i = c_{k-1}, \dots, c_k - 1\}$$

$$c_i := \lambda_1 + \dots + \lambda_i,$$

$$\lambda_1 + \dots + \lambda_l = d + 1.$$

Such decomposition will always work when $|\{(i,j) \in \text{supp}(\mathbf{w}) : i \geq d-k\}| \leq k+1$ for all $k=0,\ldots,d$. This is because we can always choose λ_1 minimal such that $|S_1| \in \{0,\lambda_1\}$. We repeat this process until $c_l=d+1$. This decomposition is illustrated in the following example.

Example 4.8. Fix the degree d = 6. Assume we have some outcome $\mathbf{w} \in \mathbb{Z}^{V_6}$ with support in the positions marked with an * below.

The first column contains two non-zero entries. So we see $\lambda_1 = 2$. Then, we conclude that $\lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = \lambda_6 = 1$; otherwise $|S_i| \notin \{0, \lambda_i\}$ for i > 1.

Next with S_i defined, we define for all i = 1, ..., l the sets

$$E_i := \begin{cases} \{c_{i-1}, \dots, c_i - 1\} & \text{if } |S_i| = \lambda_i, \\ \emptyset & \text{if } |S_i| = 0. \end{cases}$$

We see that $|E_i| = |S_i|$ for all i = 1, ..., l. Define $E := E_1 \cup \cdots \cup E_l$.

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