Solvability Threshold for Random Binary 3XOR Games

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Abstract

This honors thesis arose from an undertaking to determine the critical threshold of 3XOR game (if it exists). A game amounts to a special system of m equations with $3n$ unknowns over binaries. We fix m, n and randomly generate games (game equations). For large m, n, one suspects there is a critical threshold $c_?$ so that:

if $\frac{m}{n} < c_?$, then the equations have a solution with high probability.
if $\frac{m}{n} > c_?$, then the equations have no solution with high probability.

The thesis progresses towards finding $c_?$ if it exists. It is a work in progress and has many different types of mathematical parts. The thesis describes several of them, selected to some extent because of their mathematical character and completeness. Other components of this investigation, some complete, are being written as a preprint [HH24], and one part of the work is still in progress. In this thesis we carefully distinguish between these three stages of development: what is proved in the thesis, what is proved and currently being written into a preprint, and what is work progressing hopefully toward a proof.

The thesis has two parts. One part is the problem of determining when a particular one-parameter family of functions is non-positive over a particular region and determining its global maximizers. The other addresses a long argument taking a discrete combinatorics setup to the continuous maximization problem. The combinatorics part is proven, as are some Stirling-type asymptotics included in detail. The other analytical part, "the Discrete Laplace Asymptotic Method" is just sketched. This omitted part follows a path used in some areas of applied math which often is not fully rigorous. For our particular problem, we are making good progress at making it rigorous, and this is the subject of future work. The current stage of work gives strong evidence that a sharp threshold of exactly 3 exists for "nondegenerate" 3-XOR-games.

Contents

1 Introduction

This paper concerns the critical threshold for a 3XOR game, effectively a linear algebra problem over the binaries (integers modulo 2). A similar-looking structure is found in the classical 3XORSAT problem. There has been heavy study of the critical threshold for the 3XORSAT problem, with the celebrated paper of Dubois-Mandler [DM02a] and subsequent results for k-XORSAT in [PS14] showing that a critical threshold exists and giving its exact value as the solution to an explicit transcendental equation. This thesis will give serious evidence for the conjecture that the critical threshold for a non-degenerate 3XOR game equals that for non-degenerate 3XORSAT, corresponding to the system being square.

It is culturally interesting that XOR games seem to be studied little in the computer science community, while XORSAT is a paradigm in the field of classical computational complexity. History sheds light on this; XOR games arose in quantum physics rather than from computer science. The first XOR game to be studied is now called the CHSH game and with associated experiments (in 1972), it underlays the 2022 Nobel Prize [Nob22] for establishing that "quantum entanglement" exists. CHSH is a 2-player cooperative game.

Subsequently, people studied 3XOR games. Some of these have "perfect strategies" and some do not. It was not known if determining which is the case for a given 3XOR game is decidable. In 2023 an explicit polynomial time construction settled this, see [BH23] and computer experiments in [WHZ22] motivated this thesis.

The introduction starts with a statement of the key linear-algebra-type problem over binaries, which comes about in studying 3XOR games. Ironically, we shall not actually state exactly what 3XOR games are, since the linear algebra is simpler and contains the full mathematical issue. One can find a description of cooperative games elsewhere, in particular k-XOR GAMES c.f. [Wat+18].

The introduction then continues with definitions we need, our main conjecture, the main outline of a potential proof based on [DM02a], and finally a guide to the reader.

1.1 Set up: critical thresholds for 3XOR SAT and 3XOR games and their critical thresholds

1.1.1 Definition of 3-XOR-game matrices and two-cores.

A **3-XOR-game matrix** is a matrix $\Gamma = (A\ B\ C) \in \mathbb{Z}_2^{m\times 3n}$, where $A, B, C \in \mathbb{Z}_2^{m\times n}$ are blocks with 1 one in each row (the rest of the entries being zero). The key problem is solving linear equations over the binaries:

Given $\Gamma \in \mathbb{Z}_2^{m\times 3n}$ and b a vector in $\mathbb{Z}_2^m$ solve

$$\Gamma x = b \tag{1.1.1}$$

over $x \in \mathbb{Z}_2^{3n}$.

An example of a 3-XOR-GAME system with $m = 4$ and $n = 2$ is (Γ, b) as defined in the following display. In this case, there are several solutions, one being $x =$

$(0\ 1\ 1\ 0\ 0\ 1)^\top$:

$$\Gamma = \begin{pmatrix} 0 & 1 & & 0 & 1 & & 1 & 0 \\ 1 & 0 & & 0 & 1 & & 1 & 0 \\ 1 & 0 & & 1 & 0 & & 1 & 0 \\ 0 & 1 & & 1 & 0 & & 0 & 1 \end{pmatrix}, \qquad b = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}. \tag{1.1.2}$$

As motivation, we state loosely that a game matrix vector pair (Γ, b) defines a '3XOR game'. It has a 'perfect strategy' iff there exists a solution x to the linear equations.

The classical 3XORSAT problems have a similar form. Call $\Gamma \in \mathbb{Z}_2^{m\times 3n}$ a **3XOR-SAT matrix** provided each row has exactly 3 ones on it; informally stated, there is no A, B, C partitioning.

Next we consider degenerate cases of this linear algebra problem:

1. If a column of Γ is identically zero, then that column does not influence whether or not a solution of the equation exists; so the column could be deleted.

2. If a column has a single one, then that column corresponds to an unknown x_j on which there is only one constraint; hence x_j could be chosen to eliminate that constraint. Thus we eliminate the column and row to get a new system which is solvable if and only if the original linear equations are solvable.

This leads us to define a class of matrices, which yield a non-degenerate solvability problem.

Define a **two-core matrix** (non-degenerate matrix) to be a matrix where each column has at least 2 ones. In particular, a **two-core 3-XOR-game matrix** Γ is a matrix in $\mathbb{Z}_2^{m\times 3n}$ satisfying the block structure $\Gamma = (A\ B\ C)$, such that each column has at least 2 ones. Denote by $\Psi_{m,3n}$ the set of **two-core 3-XOR-games**, i.e. the set of pairs (Γ, s) such that Γ is a two-core 3-XOR-game matrix and $s \in \mathbb{Z}_2^m$. Note we assume $m > 2n$ to ensure $\Psi_{m,3n}$ is nonempty (see Section 7.3).

The following 3-XOR-game matrix is not a two-core because a column has fewer than two 1s (in fact, two columns are problematic).

$$\Gamma = \begin{pmatrix} 0 & 1 & & 1 & 0 & & 1 & 0 \\ 1 & 0 & & 1 & 0 & & 1 & 0 \\ 0 & 1 & & 0 & 1 & & 1 & 0 \\ 1 & 0 & & 1 & 0 & & 1 & 0 \\ 0 & 1 & & 1 & 0 & & 1 & 0 \end{pmatrix}.$$

The following is its 2-core reduction, obtained after removing the 4th and 6th columns, and the 3rd row.

$$\Gamma' = \begin{pmatrix} 0 & 1 & & 1 & & 1 \\ 1 & 0 & & 1 & & 1 \\ 1 & 0 & & 1 & & 1 \\ 0 & 1 & & 1 & & 1 \end{pmatrix}.$$

1.1.2 Randomly-generated linear equations

Fix a size m, n, and generate a 3-XOR-game matrix $\Gamma \in \mathbb{R}^{m \times 3n}$ uniformly on the set of 3-XOR-game matrices. Also, generate $b \in \mathbb{Z}_2^m$ uniformly from the set of such vectors, to get a randomly-generated set of binary equations $\Gamma x = b$. A goal is to understand the probability that there is a solution to these equations. This probability is heavily dependent on the ratio $\frac{m}{3n}$ of constraints to unknowns.

Indeed, a dramatic piece of structure, which one sees in similar situations ([DM02a] [BFU93]) is there exists some "sharp threshold" constant $c_{\mathbb{Z}_2}$ such that

- If $\frac{m}{n} > c_{\mathbb{Z}_2}$, then with high probability, $m \times 3n$ 3-XOR-game problems have a solution in $\mathbb{Z}$ mod 2, and
- If $\frac{m}{n} < c_{\mathbb{Z}_2}$, then with high probability, $m \times 3n$ 3-XOR-game have no solution in $\mathbb{Z}$ mod 2.

In this thesis, an event that occurs **with high probability (w.h.p.)** is one whose probability depends on c, m, n and goes to 1 as n goes to infinity with c fixed and $m = n(c+o(1))$, i.e. the probability of the event occurring can be made as close to 1 as desired by making n big enough with $m \sim cn$. Recall **little-o notation**: $y(n) = o(1)$ means $\lim_{n\to\infty} y(n) = 0$. Hence $m = n(c + o(1))$ is equivalent to stating $\lim_{n\to\infty} \frac{m}{n} = c$.

1.2 Conjecture: critical threshold for 3XOR-game two-cores is $c = 3$

The goal of this thesis and work-in-progress is to support (or refute) the following conjecture.

Conjecture 1.2.1. *As $n \to \infty$ with $m = n(c+o(1))$, random (uniformly distributed) 3-XOR-game two-core problems:*

1. *have at least one solution in $\mathbb{Z}_2$ w.h.p. provided $c < 3$.*
2. *have no solution in $\mathbb{Z}_2$ w.h.p. provided $c > 3$.*

Argument: The following brief argument provides an overview of the strategy for proving this conjecture. The strategy is the same overall approach as [DM02a].

Let N be a random variable denoting the number of solutions to a random 3-XOR-game problem on $3n$ unknowns with m equations.

A simple counting argument (Lemma 7.1.1) states the behavior for $c > 3$. As a quick summary: If $c > 3$, then $\mathbb{E}(N) = 2^{3n-m} \sim 2^{(3-c)n} \to 0$ as $n \to \infty$ and proves Item 2 since $N \geq 0$ is an integer.

The reverse direction is a long march. It begins with a counting argument in Section 7.4 to write the ratio $\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2}$ exactly as a single large summation of the form

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} = \sum_{\boldsymbol{x} \in \mathcal{U}_{m,n}^{01}} \breve{\mathscr{S}}_{m,n}(\boldsymbol{x}) \tag{1.2.1}$$

where $\mathcal{U}_c \subseteq (0,1)^6$ is a certain 6 dimensional polytope (defined later), and $\mathcal{U}_{m,n}^{01}$ (which has on the order of n^6 points) is the intersection of $\mathcal{U}_c$ with a certain discrete lattice $\mathscr{L}_{m,n}$. Section 8 provides a formula which asymptotically approximates the summand:

$$\breve{\mathscr{S}}_{m,n}(\boldsymbol{x}) \sim \frac{1}{n^3} \overline{g}_c e^{nh_c} \tag{1.2.2}$$

where the functions $\overline{g}_c$ and h_c are first introduced in Section 3.3. If the function h_c is non-positive on $\mathcal{U}_c$, then the Laplace Asymptotic Method from Section 9 [1] suggests

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} \sim \frac{c^3}{2} (2\pi)^3 \frac{\overline{g}_c(\boldsymbol{x}_0)}{\sqrt{\det(-\mathcal{H}\{h_c\}(\boldsymbol{x}_0))}} \tag{1.2.3}$$

where $\mathcal{H}\{h_c\}$ denotes the Hessian of h_c, and $\boldsymbol{x}_0$ is the maximizer of h_c. Much of this thesis and a companion paper [HH24] in preparation (devoted to interval arithmetic arguments) rigorously calculate that the unique global maximizer of h_c is at $\boldsymbol{x}_0 = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ provided $c < 3$. Subject to $\boldsymbol{x}_0 = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ being the unique global maximizer of h_c, then we rigorously show in Proposition 4.3.3 that the right-hand-side of Equation (1.2.3) equals 1, so $\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} \sim 1$. At this point we have

$$\Pr(N \geq 1) \geq \frac{\mathbb{E}(N)^2}{\mathbb{E}(N^2)} \tag{1.2.4}$$

tends to 1, so systems with $c < 3$ have at least one solution in $\mathbb{Z}_2$ with high probability. □

The proof above relied on Equation (1.2.4). Though it is well-known, its importance here leads us to put in the proof.

Lemma 1.2.2 (Second Moment Inequality)**.** *The inequality* $\Pr(N \geq 1) \geq \frac{\mathbb{E}(N)^2}{\mathbb{E}(N^2)}$ *holds for any non-negative integer random variable* N*.*

Proof. Follows from the Cauchy-Schwarz inequality

$$\begin{aligned}\mathbb{E}(N) &= \sum_{n=1}^{\infty} n \Pr(N = n) \leq \left(\sum_{n=1}^{\infty} n^2 \Pr(N = n)\right)^{\frac{1}{2}} \left(\sum_{n=1}^{\infty} \Pr(N = n)\right)^{\frac{1}{2}} \\ &= \mathbb{E}(N^2)^{\frac{1}{2}} \Pr(N \geq 1)^{\frac{1}{2}}, \quad \textit{so} \quad \frac{\mathbb{E}(N)^2}{\mathbb{E}(N^2)} \leq \Pr(N \geq 1).\end{aligned}$$

□

1.3 Reader's guide

The asymptotic techniques mentioned briefly before Equation (1.2.3) depend on showing h_c has a global maximum at $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$, so that e^{nh_c} is concentrated near $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$. Proving this is the main thrust of the thesis (together with [HH24]), so we now give a guide to how this is presented.

The key h_c is defined in Section 3.3. We shall prove that $h_c\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = 0$ regardless of c. As we saw in the outline above, proving that this is indeed the global maximum of h_c is one major part of proving Conjecture 1.2.1.

[1] This section currently relies on some heuristic traditional applied mathematics. Formalizing this is work we have in progress.

This requires an argument long enough that some arguments (which require interval arithmetic) are split into the in-preparation [HH24]. Interval arithmetic is a computer approach used to prove behavior of functions rigorously without needing too much analysis. However, implementing the algorithms requires care to give useful results with manageable amounts of computation.

Since h_c is a function of six variables, proving the global maximum property directly by using interval arithmetic is not practical, so we reduce the dimensionality of the problem. In Section 5.2, we reduce the problem of maximizing the 6-dimensional function h_c to maximizing the 3-dimensional function $\widehat{h}_c$, obtained by maximizing over de-coupled variables $\alpha_1, \alpha_2, \alpha_3$. In Section 2, we reduce the 3-dimensional maximization problem on a tetrahedron $\mathcal{T}$ to 1-dimensional problems on a few individual line segments. These 1-dimensional problems are discussed in Section 5.3.

Key properties of h_c are proved in Section 4 that allow for maximizing over α_i and enable computation of $\overline{g}_c(\boldsymbol{x}_0)$ and $h_c(\boldsymbol{x}_0)$ as required for computing Equation (1.2.3).

Prerequisite to Section 4 are standard properties of continuity and differentiability for the function $\widehat{h}_c$. Since this has a different flavor (implicit function theorem) from most of the thesis, we collect these proofs in Section 6.

The treatment of the 1-dimensional problems in Section 5.3 and one small piece of the analysis in Section 6 is illustrated by graphical plots which support their claims. These claims will be validated by interval arithmetic in the forthcoming work [HH24].

The argument outlined after Conjecture 1.2.1 gives a guide to parts of the thesis which do not focus on analysing global maximizers of h_c. Section 10 states a weaker version of Conjecture 1.2.1 that the theorems here, in combination with work well-underway, are likely to prove.

2 A special class of functions on a tetrahedron, and its properties

The proof of our main critical threshold theorem depends on proving that a certain class of functions on the unit tetrahedron in $\mathbb{R}^3$ is nonpositive. While special, this class possibly arises in some other context, and it has an elegant form, so we present it early in the thesis.

2.1 Definition of tetrahedron and barycentric-decoupled functions

Start by defining $\mathcal{T}$ to be the **closed tetrahedron** in $\mathbb{R}^3$ of points (r_1, r_2, r_3) satisfying the system of linear inequalities

$$\begin{aligned} t_0(\vec{r}) &:= (-1 + r_1 + r_2 + r_3)/2 \geq 0 \\ t_1(\vec{r}) &:= (1 + r_1 - r_2 - r_3)/2 \geq 0 \\ t_2(\vec{r}) &:= (1 - r_1 + r_2 - r_3)/2 \geq 0 \\ t_3(\vec{r}) &:= (1 - r_1 - r_2 + r_3)/2 \geq 0 \end{aligned} \tag{2.1.1}$$

This definition in Equation (2.1.1) implies $t_0 + t_1 + t_2 + t_3 = 1$ and

$$\begin{aligned} r_1 &= t_0 + t_1, & r_2 &= t_0 + t_2, & r_3 &= t_0 + t_3 \\ 1 - r_1 &= t_2 + t_3, & 1 - r_2 &= t_1 + t_3, & 1 - r_3 &= t_1 + t_2. \end{aligned}$$

Hence these are Normalized Barycentric Coordinates, with $\vec{r} \in \mathcal{T}$ represented by

$$\vec{r} = (r_1, r_2, r_3) = t_0\,(1,1,1) + t_1\,(1,0,0) + t_2\,(0,1,0) + t_3\,(0,0,1).$$

Note the four points $(1,1,1), (1,0,0), (0,1,0), (0,0,1)$ are the vertices of the regular tetrahedron $\mathcal{T}$, which is plotted in Figure 2.1.

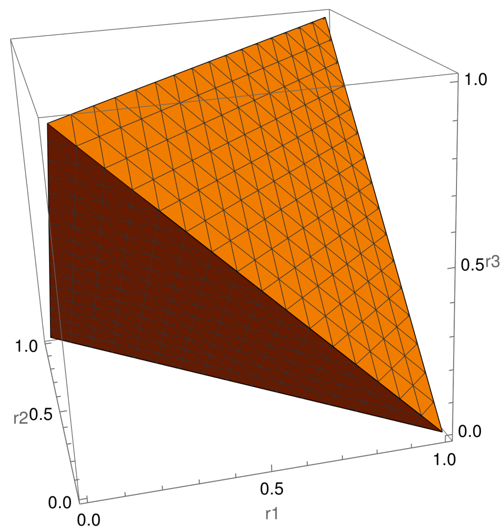

Figure 2.1: The tetrahedron $\mathcal{T}$ as defined in Equation (2.1.1)

We state a function $\mathfrak{D} \colon \mathcal{T} \to \mathbb{R}$ is **barycentric-decoupled** if it is of the following form, for some pair of functions $w, E \colon [0,1] \to \mathbb{R}$ satisfying $w(r) = w(1-r)$:

$$\mathfrak{D}(\vec{r}) = w(r_1) + w(r_2) + w(r_3) + E(t_0) + E(t_1) + E(t_2) + E(t_3). \tag{2.1.2}$$

Note this implies $\mathfrak{D}$ is a symmetric function of (t_0, t_1, t_2, t_3) since

$$w(r_1) + w(r_2) + w(r_3) \tag{2.1.3}$$
$$= \frac{1}{2}(w(r_1) + w(1-r_1) + w(r_2) + w(1-r_2) + w(r_3) + w(1-r_3)) \tag{2.1.4}$$
$$= \frac{1}{2}(w(t_0+t_1) + w(t_2+t_3) + w(t_0+t_2) + w(t_1+t_3) + w(t_0+t_3) + w(t_1+t_2)). \tag{2.1.5}$$

Lemma 2.1.1. *Fix a constant $\tau_0 \in [0,1]$ and barycentric-decoupled $\mathfrak{D}$.*

Then on the planar subset of $\mathcal{T}$ where $t_0 = \tau_0$ (i.e. $r_1 + r_2 + r_3 = 1 + 2\tau_0$), the function $\mathfrak{D}$ can be written in an r-decoupled form

$$\mathfrak{D}(r_1, r_2, r_3) = G^{\tau_0}(r_1) + G^{\tau_0}(r_2) + G^{\tau_0}(r_3),$$

where we define

$$G^{\tau_0}(r) := w(r) + E\,(r - \tau_0) + \frac{1}{3}E(\tau_0).$$

Note $G^{\tau_0}(r_i)$ is a function of r_i only.

Proof. For $i = 1, 2, 3$, then $r_i = t_0 + t_i$, so $t_i = r_i - t_0$. □

2.2 Four-lines Theorem

Theorem 2.2.1 (Four-lines theorem)**.** *Suppose* $\mathfrak{D}$ *is a barycenteric-decoupled function as in Equation* (2.1.2) *with* w *and* E *continuously differentiable. Recall* $w(r) = w(1-r)$*. Let* G^{τ_0} *be as in Lemma 2.1.1, and suppose* $\frac{dG^{\tau_0}(r)}{dr} = y$ *has at most two solutions in* r *for each* y*.*

If $\vec{r}$ *in the interior of* $\mathcal{T}$ *is a critical point of* $\mathfrak{D}$*, then* $\vec{r}$ *is either on:*

1. *a diagonal of* $\mathcal{T}$ *(segment through* $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ *and a vertex of* $\mathcal{T}$*):*

$$(r, r, r)\,,\ \text{or}\ (r, 1-r, 1-r)\,,\ \text{or}\ (1-r, r, 1-r)\,,\ \text{or}\ (1-r, 1-r, r)\,; \quad (r \in (0,1)).$$

2. *a central vertical segment of* $\mathcal{T}$*:*

$$\left(\frac{1}{2}, \frac{1}{2}, r\right),\ \text{or}\ \left(\frac{1}{2}, r, \frac{1}{2}\right),\ \text{or}\ \left(r, \frac{1}{2}, \frac{1}{2}\right); \qquad (r \in (0,1)).$$

   These are segments between the midpoint of two opposite edges (a pair of edges that have no vertices in common).

If $\vec{r}$ *in the interior of a face of* $\mathcal{T}$ *is a local maximum for* $\mathfrak{D}$*, then* $\vec{r}$ *is on*

3. *the centerline of a face, e.g.,*

$$(r, r, 1-2r); \qquad \left(r \in \left(0, \frac{1}{2}\right)\right).$$

Hence a local maximizer $\vec{r}$ *for* $\mathfrak{D}$ *on* $\mathcal{T}$ *must lie on one of the three sets of lines above, or*

4. *an edge of the tetrahedron, e.g.*

$$(r, r, 1); \qquad (r \in [0,1]).$$

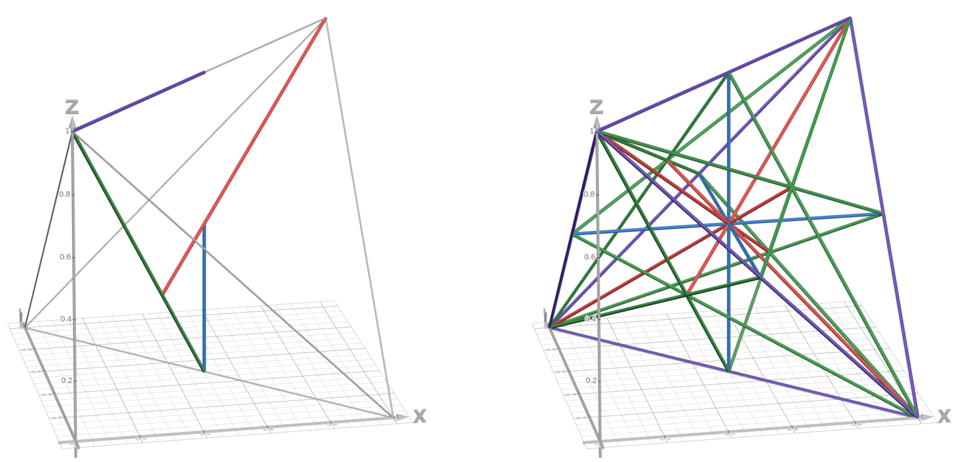

Figure 2.2: Left: the four segments from Corollary 2.2.2. Right: orbits of the segments under the tetrahedron symmetries.

Due to the symmetries of $\mathfrak{D}$ discussed in Lemma 2.2.4, it suffices to check the maximum of $\mathfrak{D}$ on one segment of each type above. This is practical for computation.

Corollary 2.2.2. *Suppose $\mathfrak{D}$ is a barycenteric-decoupled function as in Equation* (2.1.2) *with w and E continuously differentiable. Recall $w(r) = w(1-r)$.*

0. *Let $G^{\mathcal{T}_0}$ be as in Lemma 2.1.1, and suppose $\frac{dG^{\mathcal{T}_0}(r)}{dr} = y$ has at most two solutions in r for each y.*

Then, up to the symmetries described in Lemma 2.2.4, any local maximizer for $\mathfrak{D}$ on $\mathcal{T}$ must lie on one of these four segments:

1. *Diagonal: (r, r, r) for $r \in \left(\frac{1}{3}, 1\right)$.*
2. *Central vertical segment: $\left(\frac{1}{2}, \frac{1}{2}, r\right)$ for $r \in \left(0, \frac{1}{2}\right)$.*
3. *Centerline of face: $(r, r, 1-2r)$ for $r \in \left(0, \frac{1}{2}\right)$.*
4. *Edge of tetrahedron: $(r, r, 1)$ for $r \in \left[0, \frac{1}{2}\right]$.*

Reference Figure 2.2 for plots of these segments.

To prove Theorem 2.2.1, we begin by proving several lemmas.

Lemma 2.2.3. *Suppose $G(r)$ is any continuously-differentiable function $G\colon (0,1) \to \mathbb{R}$. Fix $\Lambda \in (0,3)$. Let P^Λ be the plane*

$$P^\Lambda = \{(r_1, r_2, r_3) \in (0,1)^3 \mid r_1 + r_2 + r_3 = \Lambda\}\}.$$

Suppose $\mathcal{T}^\Lambda \subseteq P^\Lambda$ is open in P^Λ. Define $F\colon \mathcal{T}^\Lambda \to \mathbb{R}$ by

$$F(r_1, r_2, r_3) = G(r_1) + G(r_2) + G(r_3).$$

Suppose $\vec{r}^* = (r_1^*, r_2^*, r_3^*) \in \mathcal{T}^\Lambda$ is a local maximizer of F in $\mathcal{T}^\Lambda$. Then

$$G'(r_1^*) = G'(r_2^*) = G'(r_3^*). \tag{2.2.1}$$

If furthermore $G'(r) = y$ has at most two solutions in r for each y, then either

$$r_1^* = r_2^*, \quad \text{or} \quad r_1^* = r_3^*, \quad \text{or} \quad r_2^* = r_3^*.$$

Proof. Suppose $\vec{r}^* = (r_1^*, r_2^*, r_3^*) \in \mathcal{T}^\Lambda$.

Let $D_{(1,-1,0)}F(\vec{r}^*)$ be the directional derivative in the $(1,-1,0)$ direction, so

$$D_{(1,-1,0)}F(\vec{r}^*) = \boldsymbol{\nabla} F(\vec{r}^*) \cdot (1,-1,0) = G'(r_1^*) - G'(r_2^*) = 0.$$

Thus $G'(r_1^*) = G'(r_2^*)$. Likewise, taking the directional derivative in the $(0,1,-1)$ direction shows $G'(r_3^*) = G'(r_2^*)$. Hence

$$G'(r_1^*) = G'(r_2^*) = G'(r_3^*). \tag{2.2.2}$$

The hypothesis on G' means it maps at most two inputs to each output. Thus

$$|\{r_1^*, r_2^*, r_3^*\}| \leq 2.$$

The pigeonhole principle implies some pair must be equal, so either

$$r_1^* = r_2^*, \quad \text{or} \quad r_1^* = r_3^*, \quad \text{or} \quad r_2^* = r_3^*.$$

□

Lemma 2.2.4. *Suppose $\mathfrak{D}$ is a barycentric-decoupled function on $\mathcal{T}$ as in Equation* (2.1.2)*. Then $\mathfrak{D}$ is invariant under permuting its arguments:*

$$\mathfrak{D}(r_1, r_2, r_3) = \mathfrak{D}(r_2, r_1, r_3) = \mathfrak{D}(r_1, r_3, r_2) = \cdots . \tag{2.2.3}$$

In addition, $\mathfrak{D}$ is invariant under double-reflections:

$$\mathfrak{D}(r_1, r_2, r_3) = \mathfrak{D}(1 - r_1, 1 - r_2, r_3) = \mathfrak{D}(1 - r_1, r_2, 1 - r_3) = \mathfrak{D}(r_1, 1 - r_2, 1 - r_3). \tag{2.2.4}$$

Proof. By definition of the t_i in Equation (2.1.1), the double-reflection

$$(r_1, r_2, r_3) \mapsto (1 - r_1, 1 - r_2, r_3)$$

corresponds to permuting the (t_0, t_1, t_2, t_3) tuple as

$$(t_0, t_1, t_2, t_3) \mapsto (t_3, t_1, t_2, t_0).$$

Similarly, the permutation of r_i

$$(r_1, r_2, r_3) \mapsto (r_2, r_1, r_3)$$

corresponds to permuting (t_0, t_1, t_2, t_3) as

$$(t_0, t_1, t_2, t_3) \mapsto (t_0, t_2, t_1, t_3).$$

In similar ways, all of the claimed symmetries correspond to permuting the (t_0, t_1, t_2, t_3) tuple. Since $\mathfrak{D}$ is barycentric-decoupled, it is a symmetric function of (t_0, t_1, t_2, t_3) (see Equation (2.1.5)), so permuting the tuple (t_0, t_1, t_2, t_3) does not affect its value. □

Proof of Theorem 2.2.1. Suppose $\vec{r}^* = (r_1^*, r_2^*, r_3^*)$ is a local maximizer of $\mathfrak{D}$.
Interior case:

Suppose $\vec{r}^*$ is on the interior of $\mathcal{T}$. Let $\Lambda = r_1^* + r_2^* + r_3^*$. Then (r_1^*, r_2^*, r_3^*) is a local maximizer of $\mathfrak{D}$ on the interior of the plane $r_1 + r_2 + r_3 = \Lambda$. The function $\mathfrak{D}$ decouples on that plane as in Lemma 2.1.1, so by Lemma 2.2.3, one pair of r_i^* must be equal. Without loss of generality, assume $r_1^* = r_2^*$ (otherwise permute r_i, which would take one central vertical segment to another central vertical segment, or a diagonal to another diagonal).

Since $r_1^* = r_2^*$, we note (r_1^*, r_1^*, r_3^*) is a local maxmimizer of $\mathfrak{D}$. By the symmetries in Lemma 2.2.4, then $(1 - r_1^*, r_1^*, 1 - r_3^*)$ is also a local maximizer of $\mathfrak{D}$. Let $\widetilde{\Lambda} = (1 - r_1^*) + r_1^* + (1 - r_3^*)$, so we have $(1 - r_1^*, r_1^*, 1 - r_3^*)$ is a local maximizer of $\mathfrak{D}$ on the interior of the plane $r_1 + r_2 + r_3 = \widetilde{\Lambda}$. By Lemma 2.2.3, at least one of the following must hold:

1. $r_1^* = 1 - r_1^*$. Then $r_1^* = r_2^* = \frac{1}{2}$, and $r_3^* \in (0, 1)$.
2. $1 - r_1^* = 1 - r_3^*$. Then $r_1^* = r_2^* = r_3^* \in (0, 1)$.
3. $r_1^* = 1 - r_3^*$. Then $r_1^* = r_2^* = 1 - r_3^* \in (0, 1)$.

Case 1 implies $\vec{r}^*$ is on a central vertical segment, and Cases 2 and 3 imply $\vec{r}^*$ is on a diagonal of the tetrahedron. Hence all critical points of $\mathfrak{D}$ in the interior of $\mathcal{T}$ are on either a diagonal or vertical segment of $\mathcal{T}$.

Face interior case:

Suppose $\vec{r}^*$ is on a face of $\mathcal{T}$. Without loss of generality, assume this is the face $\{\vec{r} \mid t_0(\vec{r}) = 0\}$ (otherwise perform a double-reflection to map to this face; the double-reflection maps centerlines to centerlines).

Then $\vec{r}$ is a local maximizer of $\mathfrak{D}$ on the interior of the plane $r_1 + r_2 + r_3 = 1$. By Lemma 2.2.3, one pair of r_i^* must be equal, so $\vec{r}$ is on a centerline of the face $\mathcal{F}_0$.

Edge case:

The above two cases narrow down the set of points that could possibly be local maxima on the interior of $\mathcal{T}$ and the interior of faces of $\mathcal{T}$. The only points left remaining in $\mathcal{T}$ are its edges (including its 4 vertices). □

2.3 More general decoupling understanding

While these are not essential to the later proofs, we note three remarks that show this barycentric-decoupling is natural in some sense.

Remark 2.3.1. We now give a more-general class of functions which must be barycentric-decoupled. Suppose $\mathfrak{D}$ is a sum of identical functions of sums of distinct t_i, so it can be written as:

$$\begin{aligned}\mathfrak{D}(\vec{r}) = f_0 + &\sum_{i\in\{0,1,2,3\}} f_1(t_i) + \sum_{\substack{i,j\in\{0,1,2,3\}\\ i\neq j}} f_2(t_i+t_j) \\ &+ \sum_{\text{distinct } i,j,k\in\{0,1,2,3\}} f_3(t_i+t_j+t_k) + f_4(t_0+t_1+t_2+t_3)\end{aligned}. \tag{2.3.1}$$

Note the constraint $t_0 + t_1 + t_2 + t_3 = 1$ implies (by way of example) $t_0 + t_1 + t_2 = 1 - t_3$, so each sum of three t_i is a function of the remaining t_i. Also, the f_0 and $f_4(t_0 + t_1 + t_2 + t_3)$ are constants, so they can folded into f_1. Hence that definition is equivalent to requiring the form

$$\mathfrak{D}(\vec{r}) = \sum_{i\in\{0,1,2,3\}} f_1(t_i) + \sum_{\substack{i,j\in\{0,1,2,3\}\\ i\neq j}} f_2(t_i+t_j). \tag{2.3.2}$$

Note $t_0 + t_i = r_i$, so this is equivalent to requiring

$$\mathfrak{D}(\vec{r}) = \sum_{i\in\{0,1,2,3\}} f_1(t_i) + \sum_{i=1}^{3}(f_2(r_i) + f_2(1-r_i)). \tag{2.3.3}$$

Letting $E(t) = f_1(t)$ and $w(r) = f_2(r)+f_2(1-r)$ reaches the form in Equation (2.1.2). □

Remark 2.3.2. There are r-decouplings similar to Lemma 2.1.1 with respect to other barycentric planes, e.g.

$$\mathfrak{D}(r_1, r_2, r_3) = G^{\tau_1}(r_1) + G^{\tau_1}(1 - r_2) + G^{\tau_1}(1 - r_3),$$

where we define

$$G^{\tau_1}(r) := w(r) + E\left(r - \tau_1\right) + \frac{1}{3}E(\tau_1).$$

Remark 2.3.3. Lemma 2.1.1 emphasizes the r-decoupling, but we could equivalently create a t-decoupling, which holds on the plane $t_0 = \tau_0$ (i.e. $t_1 + t_2 + t_3 = 1 - \tau_0$), by

$$\mathfrak{D}(\vec{r}) = H^{\tau_0}(t_1) + H^{\tau_0}(t_2) + H^{\tau_0}(t_3),$$

where we define

$$H^{\tau_0}(t) := w(\tau_0 + t) + E\,(t) + \frac{1}{3}E(\tau_0).$$

Then the form for planes other than t_0 is a simple permutation, while Remark 2.3.2 had to perform a double-reflection of the arguments to G^{τ_1}. For example,

$$\mathfrak{D}(\vec{r}) = H^{\tau_1}(t_0) + H^{\tau_1}(t_2) + H^{\tau_1}(t_3),$$

where we define

$$H^{\tau_1}(t) := w(\tau_1 + t) + E\,(t) + \frac{1}{3}E(\tau_1).$$

3 Definition of h_c. Treatment of ν. Claim h_c is real analytic.

3.1 Preparation for defining h_c; the functions $z(\nu)$ and $\nu(z)$

Define

$$\nu(z) := \begin{cases} \dfrac{e^z - 1 - z}{z(e^z - 1)}, & z \neq 0 \\ \dfrac{1}{2}, & z = 0 \end{cases}.$$

Note $\nu(z) = \frac{1}{z} - \frac{1}{e^z - 1}$ for $z \neq 0$.

The function $\nu(z)$ is plotted in Figure 3.1, and its inverse function $z(v)$ (which we will show to be well-defined in the following lemma) is plotted in Figure 3.2.

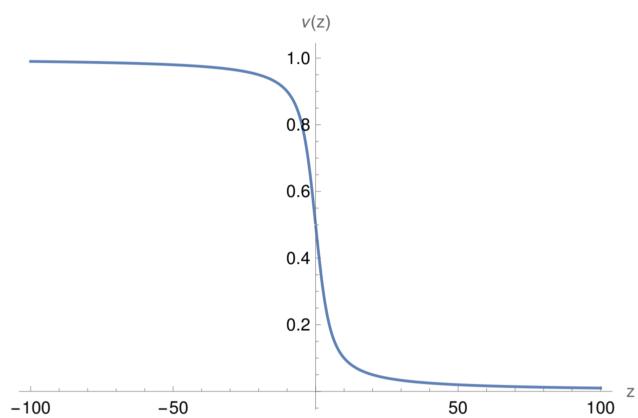

Figure 3.1: $\nu(z)$

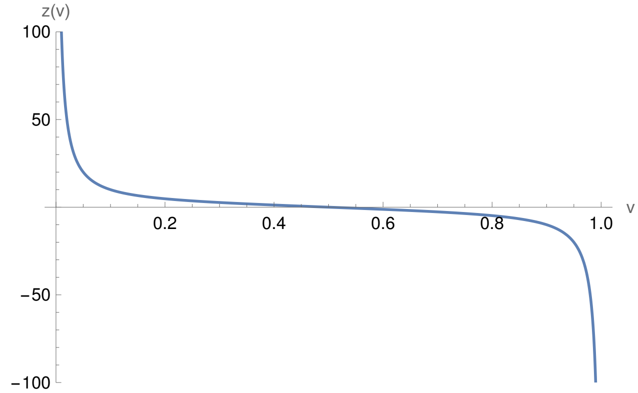

Figure 3.2: $z(v)$

Lemma 3.1.1. *We discuss some properties of* ν *and its inverse* $z(v)$*:*

(a) ν *is analytic on a strip containing the entire real axis. It has the symmetry* $\nu(-z)+\nu(z)=1$ *for all* z*. Also,* ν *has specific values*

$$\lim_{z\to 0}\nu(z)=\nu(0)=\frac{1}{2},\quad \nu'(0)=-\frac{1}{12},\quad \lim_{z\to+\infty}\nu(z)=0,\quad \lim_{z\to-\infty}\nu(z)=1$$

(b) ν *is strictly decreasing for all* $z\in\mathbb{R}$*. Consequently, it has an inverse function* $z\colon(0,1)\to\mathbb{R}$ *with analytic extension in some neighborhood of* $(0,1)$*.*

(c) $z(v)$ *is a decreasing function* $z\colon(0,1)\to\mathbb{R}$ *with* $z\left(\frac{1}{2}\right)=0$*.*
$z(v)$ *is an odd function about* $v=\frac{1}{2}$*, i.e.* $z(v)=-z(1-v)$ *for all* $v\in(0,1)$*.*

Proof (a). The numerator and denominator of ν are analytic on the entire complex plane. The denominator of ν has a zero of order 2 at $z=0$. However, the numerator has power series $\frac{1}{2}z^2+\frac{1}{3!}z^3+\frac{1}{4!}z^4+\ldots$ around $z=0$, hence it has a zero of order 2 at $z=0$, verifying that ν is analytic near 0.

The only other possible locations for poles are when the denominator is zero, but these are all pure imaginary, lying at $z=2\pi ik$ for $k\in\mathbb{Z}$. This proves the strip analyticity claim.

Simple algebra yields the limit evaluations and symmetry $\nu(-z)+\nu(z)=1$.

Proof (b). $\nu(z)$ is strictly monotonic decreasing for $z\in\mathbb{R}$.
For $z\neq 0$, calculate

$$\nu'(z)=\frac{e^z}{(e^z-1)^2}-\frac{1}{z^2}=\frac{1}{4\sinh(z/2)^2}-\frac{1}{z^2} \tag{3.1.1}$$

$$4\nu'(2x)=\frac{1}{\sinh(x)^2}-\frac{1}{x^2}. \tag{3.1.2}$$

For $x>0$, we have $\sinh(x)>x$. Hence $\nu'(z)<0$ for $z>0$. The reflection formula $\nu(z)+\nu(-z)=1$ implies $\nu'(-z)=\nu'(z)$, so $\nu'(z)<0$ for $z<0$. Using $\nu'(0)=-\frac{1}{12}$, we conclude $\nu'(z)<0$ for all $z\in\mathbb{R}$. Thus $\nu(z)$ is strictly decreasing for all $z\in\mathbb{R}$.

Since ν is analytic in a strip containing the real axis and $\nu'(z)\neq 0$ for all real $z\in\mathbb{R}$, the Analytic Inverse Function Theorem (Chapter 1.7 of [FG02]) implies there is an open neighborhood of $(0,1)$ in which an analytic function z exists with $\nu(z(v))=v$ for all $v\in(0,1)$.

Proof (c).
The properties of $z(v)$ claimed in the lemma follow immediately from the properties of ν established in part (a) since the function $z(v)$ is the inverse of $\nu(z)$. □

3.2 Definition of parallelogram $\mathcal{P}_c$ and polytope $\mathcal{U}_c$

For $c > 2$, define the open parallelogram $\mathcal{P}_c \subseteq \mathbb{R}^2$ and polytope $\mathcal{U}_c \subseteq \mathbb{R}^6$ by

$$\mathcal{P}_c := \left\{(r, \alpha) \in (0,1)^2 \mid \alpha < \frac{c}{2}r,\ 1 - \alpha < \frac{c}{2}(1-r)\right\} \tag{3.2.1}$$

$$\mathcal{U}_c := \{(r_1, r_2, r_3, \alpha_1, \alpha_2, \alpha_3) \mid (r_1, r_2, r_3) \in \mathcal{T}, (r_1, \alpha_1) \in \mathcal{P}_c, (r_2, \alpha_2) \in \mathcal{P}_c, (r_3, \alpha_3) \in \mathcal{P}_c\}. \tag{3.2.2}$$

Note $\mathcal{P}_c$ is open in $\mathbb{R}^2$, while the tetrahedron $\mathcal{T}$ is closed in $\mathbb{R}^3$. Hence $\mathcal{U}_c$ is neither open nor closed in $\mathbb{R}^6$. We impose $c > 2$ since $\mathcal{P}_c$ is empty for $c \le 2$.

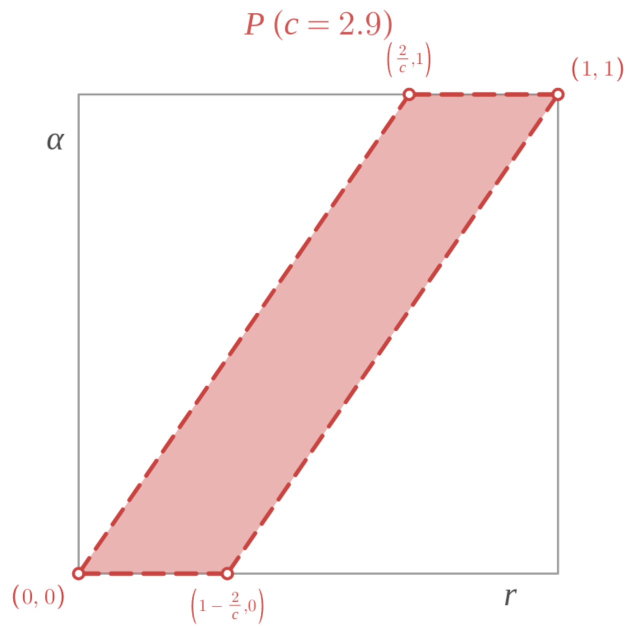

Figure 3.3: $\mathcal{P}_c$ at $c = 2.9$

3.3 Definition of h_c and $\overline{g}_c$

Define the **entropy function** H for one and four arguments as follows:

$$H(x) := -x\ln(x) - (1-x)\ln(1-x)$$
$$H(t_0, t_1, t_2, t_3) := -t_0\ln(t_0) - t_1\ln(t_1) - t_2\ln(t_2) - t_3\ln(t_3),$$

where we let $-0\ln(0) = 0$ by continuity.

For $c > 2$, define $h_c\colon \mathcal{U}_c \to \mathbb{R}$ via auxiliary functions $\breve{\kappa}_c, \tilde{w}_c\colon \mathcal{P}_c \to \mathbb{R}$ by

$$h_c(\vec{r}, \vec{\alpha}) := cH(t_0, t_1, t_2, t_3) + (c-3)\ln(2) + \tilde{w}_c(r_1, \alpha_1) + \tilde{w}_c(r_2, \alpha_2) + \tilde{w}_c(r_3, \alpha_3) \tag{3.3.1}$$

$$\tilde{w}_c(r, \alpha) := H(\alpha) - cH(r) + \breve{\kappa}_c(r, \alpha) + \breve{\kappa}_c(1-r, 1-\alpha) - \breve{\kappa}_c(1,1) \tag{3.3.2}$$

$$\breve{\kappa}_c(r, \alpha) := \alpha \ln(e^z - 1 - z) - cr\ln(z), \quad \text{with} \quad z := z(\alpha/(cr)) \tag{3.3.3}$$

$$z(v) := \nu^{-1}(v) = \text{inverse of } \nu(z) := \frac{e^z - 1 - z}{(e^z-1)z}, \tag{3.3.4}$$

For $c > 2$, define $\overline{g}_c\colon \mathcal{U}_c \to \mathbb{R}$ via auxiliary function $\widetilde{g}_c\colon \mathcal{P}_c \to \mathbb{R}$ by

$$\overline{g}_c(\vec{r}, \vec{\alpha}) = \widetilde{g}_c(r_1, \alpha_1)\widetilde{g}_c(r_2, \alpha_2)\widetilde{g}_c(r_3, \alpha_3)\frac{1}{\sqrt{t_0 t_1 t_2 t_3 (2\pi c)^3}} \tag{3.3.5}$$

$$\widetilde{g}_c(r, \alpha) := \sqrt{\frac{-z_0\nu'(z_0)}{z_1\nu'(z_1)z_2\nu'(z_2)}}\sqrt{\frac{1}{2c\pi r(1-r)}}, \tag{3.3.6}$$

where for $(r, \alpha) \in \mathcal{P}_c$, we define z_0, z_1, z_2 by

$$z_0 := z\left(\frac{1}{c}\right) \qquad z_1 := z\left(\frac{\alpha}{cr}\right) \qquad z_2 := z\left(\frac{1-\alpha}{c(1-r)}\right). \tag{3.3.7}$$

For the definitions of both h_c and $\overline{g}_c$ above, t_0, t_1, t_2, t_3 are given by Equation (2.1.1).

Remark 3.3.1. For $c > 2$ and $(r, \alpha) \in \mathcal{P}_c$, these (z_0, z_1, z_2) are well-defined, and

$$z_0, z_1, z_2 > 0. \tag{3.3.8}$$

Proof. The definition of $\mathcal{P}_c$ (Section 3.2) implies $\frac{\alpha}{cr} < \frac{1}{2}$ and $\frac{1-\alpha}{c(1-r)} < \frac{1}{2}$ for all $(r, \alpha) \in \mathcal{P}_c$. By Lemma 3.1.1, $z(v) > 0$ if $v < \frac{1}{2}$. □

4 Computing derivatives, values, the Hessian, and RHS = 1

The section does calculations needed in the rest of this thesis. Our list of derivatives etc. contain a bit more than is currently essential, so as to serve as a reference useful to future work.

4.1 Derivatives of $\tilde{w}_c$ and $\mathfrak{h}_c$

Next we shall give a list of first and second derivatives of $\tilde{w}_c$ and $\mathfrak{h}_c$, and after that prove the listed formulas.

4.1.1 List of derivatives

For $(r, \alpha) \in \mathcal{P}_c$, define

$$\tilde{q}(r, \alpha) := \frac{z_1(r, \alpha)(1-r)}{z_2(r, \alpha)r}. \tag{4.1.1}$$

The first partial derivatives of $\tilde{w}_c$ are:

$$\frac{\partial}{\partial r}\tilde{w}_c(r,\alpha) = -c\ln\left(\frac{(1-r)z_1}{rz_2}\right) = -c\ln(\tilde{q}(r,\alpha)) \tag{4.1.2}$$
$$\frac{\partial}{\partial \alpha}\tilde{w}_c(r,\alpha) = \ln\left(\frac{(1-r)(e^{z_1}-1)z_1}{r(e^{z_2}-1)z_2}\right) = \ln\left(\tilde{q}(r,\alpha)\frac{e^{z_1}-1}{e^{z_2}-1}\right) \tag{4.1.3}$$
$$\frac{\partial}{\partial c}\tilde{w}_c(r,\alpha) = \ln(z_0) - r\ln(z_1) - (1-r)\ln(z_2) - H(r). \tag{4.1.4}$$

There is a symmetry between the first partials of z_1 and of z_2 because $z_1(r,\alpha) = z_2(1-r, 1-\alpha)$:

$$\frac{\partial}{\partial r}z_1(r,\alpha) = -\frac{\alpha}{cr^2\nu'(z_1)} \qquad \frac{\partial}{\partial r}z_2(r,\alpha) = \frac{1-\alpha}{c(1-r)^2\nu'(z_2)} \tag{4.1.5}$$
$$\frac{\partial}{\partial r}z_1(r,\alpha) = -\frac{\nu(z_1)}{r\nu'(z_1)} \qquad \frac{\partial}{\partial r}z_2(r,\alpha) = \frac{\nu(z_2)}{(1-r)\nu'(z_2)} \tag{4.1.6}$$
$$\frac{\partial}{\partial \alpha}z_1(r,\alpha) = \frac{1}{cr\nu'(z_1)} \qquad \frac{\partial}{\partial \alpha}z_2(r,\alpha) = -\frac{1}{c(1-r)\nu'(z_2)} \tag{4.1.7}$$
$$\frac{\partial}{\partial c}z_1(r,\alpha) = -\frac{\alpha}{c^2r\nu'(z_1(r,\alpha))} \qquad \frac{\partial}{\partial c}z_2(r,\alpha) = -\frac{1-\alpha}{c^2(1-r)\nu'(z_2(r,\alpha))} \tag{4.1.8}$$
$$\frac{\partial}{\partial c}z_1(r,\alpha) = -\frac{\nu(z_1)}{c\nu'(z_1)} \qquad \frac{\partial}{\partial c}z_2(r,\alpha) = -\frac{\nu(z_2)}{c\nu'(z_2)}. \tag{4.1.9}$$

Substituting $r = \alpha = \frac{1}{2}$ into either z_1 or z_2 yields the first derivative of z_0:

$$\frac{\partial}{\partial c}z_0 = -\frac{\nu(z_0)}{c\nu'(z_0)}. \tag{4.1.10}$$

The second derivatives of $\tilde{w}_c$ follow directly from differentiating the first derivatives of $\tilde{w}_c$, and then substituting the first derivatives of z_1 and z_2. Here, we drop the c in the subscript for readability, so the subscripts represent partial derivatives:

$$\tilde{w}_{rr}(r,\alpha) := \frac{\partial^2}{\partial r^2}\tilde{w}_c(r,\alpha) = \frac{c}{r} + \frac{\alpha}{r^2z_1\nu'(z_1)} + \frac{c}{1-r} + \frac{1-\alpha}{(1-r)^2z_2\nu'(z_2)} \tag{4.1.11}$$
$$\tilde{w}_{rr}(r,\alpha) := \frac{\partial^2}{\partial r^2}\tilde{w}_c(r,\alpha) = c\left(\frac{1}{r} + \frac{\nu(z_1)}{rz_1\nu'(z_1)} + \frac{1}{1-r} + \frac{\nu(z_2)}{(1-r)z_2\nu'(z_2)}\right) \tag{4.1.12}$$
$$\tilde{w}_{r\alpha}(r,\alpha) := \frac{\partial^2}{\partial r\alpha}\tilde{w}_c(r,\alpha) = -\frac{1}{rz_1\nu'(z_1)} - \frac{1}{(1-r)z_2\nu'(z_2)} \tag{4.1.13}$$
$$\tilde{w}_{\alpha\alpha}(r,\alpha) := \frac{\partial^2}{\partial \alpha^2}\tilde{w}_c(r,\alpha) = \frac{1}{c}\left(\frac{\frac{1}{e^{z_1}-1} + \frac{1}{z_1} + 1}{r\nu'(z_1)} + \frac{\frac{1}{e^{z_2}-1} + \frac{1}{z_2} + 1}{(1-r)\nu'(z_2)}\right). \tag{4.1.14}$$

First derivatives of $\mathfrak{h}_c$ are

$$\frac{\partial}{\partial r_1}\mathfrak{h}_c(r_1,r_2,r_3) = -\frac{1}{2}c\left(\ln(t_0) + \ln(t_1) - \ln(t_2) - \ln(t_3)\right)$$
$$\frac{\partial}{\partial r_2}\mathfrak{h}_c(r_1,r_2,r_3) = -\frac{1}{2}c\left(\ln(t_0) - \ln(t_1) + \ln(t_2) - \ln(t_3)\right)$$
$$\frac{\partial}{\partial r_3}\mathfrak{h}_c(r_1,r_2,r_3) = -\frac{1}{2}c\left(\ln(t_0) - \ln(t_1) - \ln(t_2) + \ln(t_3)\right).$$

These formulas will be proved in the next few subsections. To prepare we recall from Section 3.3.

$$\tilde{w}_c(r,\alpha) = H(\alpha) - cH(r) + \breve{\kappa}_c(r,\alpha) + \breve{\kappa}_c(1-r,1-\alpha) - \breve{\kappa}_c(1,1) \tag{4.1.15}$$
$$\breve{\kappa}_c(r,\alpha) = \alpha\ln(e^z - 1 - z) - cr\ln(z), \quad z := z(\alpha/(cr)) \tag{4.1.16}$$
$$z(v) := \nu^{-1}(v) = \text{inverse of } \nu(z) := \frac{e^z-1-z}{(e^z-1)z}. \tag{4.1.17}$$

4.1.2 Proof: First derivatives of z_1, z_2 with respect to c, r, α

Recall $z(v) := \nu^{-1}(z)$. Note ν is monotone and continuously-differentiable (Lemma 3.1.1), so $z'(v) = \frac{1}{\nu'(z(v))}$. Since $z_1(r,\alpha) = z\left(\frac{\alpha}{cr}\right)$, it follows for $(r,\alpha) \in \mathcal{P}_c$ that

$$\frac{\partial}{\partial c}z_1(r,\alpha) = -\frac{\alpha}{c^2 r}z'\left(\frac{\alpha}{cr}\right) = -\frac{\alpha}{c^2 r\nu'(z_1(r,\alpha))}. \tag{4.1.18}$$

A similar approach works for the derivative of z_1 and z_2 with respect to α and r.

4.1.3 Proof: First derivatives of $\tilde{w}_c$

Since $\tilde{w}_c$ is constructed from $\breve{\kappa}_c$, we start by considering the derivatives of $\breve{\kappa}_c$:

$$\frac{\partial}{\partial r}\breve{\kappa}_c(r,\alpha) = -c\ln(z_1) + \frac{\partial z_1}{\partial r}\left(\alpha\frac{e^{z_1}-1}{e^{z_1}-1-z_1} - \frac{cr}{z_1}\right) \tag{4.1.19}$$
$$\frac{\partial}{\partial \alpha}\breve{\kappa}_c(r,\alpha) = \ln(e^{z_1}-1-z_1) + \frac{\partial z_1}{\partial \alpha}\left(\alpha\frac{e^{z_1}-1}{e^{z_1}-1-z_1} - \frac{cr}{z_1}\right) \tag{4.1.20}$$
$$\frac{\partial}{\partial c}\breve{\kappa}_c(r,\alpha) = -r\ln(z_1) + \frac{\partial z_1}{\partial c}\left(\alpha\frac{e^{z_1}-1}{e^{z_1}-1-z_1} - cr\frac{1}{z_1}\right) \tag{4.1.21}$$

By definition of z_1, we see $\nu(z_1) = \frac{\alpha}{cr}$, so

$$\frac{e^{z_1}-1}{e^{z_1}-1-z_1} = \frac{1}{z_1\nu(z_1)} = \frac{cr}{\alpha z_1}. \tag{4.1.22}$$

This simplifies all the above derivatives:

$$\frac{\partial}{\partial r}\breve{\kappa}_c(r,\alpha) = -c\ln(z_1) \tag{4.1.23}$$
$$\frac{\partial}{\partial \alpha}\breve{\kappa}_c(r,\alpha) = \ln(e^{z_1}-1-z_1) \tag{4.1.24}$$
$$\frac{\partial}{\partial c}\breve{\kappa}_c(r,\alpha) = -r\ln(z_1) \tag{4.1.25}$$

Using $H'(r) = \ln(1-r) - \ln(r)$ finishes the derivatives by definition of $\tilde{w}_c$:

$$\frac{\partial}{\partial r}\tilde{w}_c(r,\alpha) = -c(\ln(1-r) - \ln(r)) - c\ln(z_1) + c\ln(z_2) \tag{4.1.26}$$
$$= -c(\ln(1-r) - \ln(r) + \ln(z_1) - \ln(z_2)) \tag{4.1.27}$$
$$= -c\ln\left(\frac{z_1(1-r)}{rz_2}\right) \tag{4.1.28}$$

$$\frac{\partial}{\partial \alpha}\tilde{w}_c(r,\alpha) = \ln(e^{z_1} - 1 - z_1) - \ln(e^{z_2} - 1 - z_2) + \ln(1-\alpha) - \ln(\alpha) \tag{4.1.29}$$

$$= \ln\left(\frac{(1-\alpha)(e^{z_1} - 1 - z_1)}{\alpha(e^{z_2} - 1 - z_2)}\right) \tag{4.1.30}$$

$$= \ln\left(\frac{(1-r)(e^{z_1} - 1)z_1}{r(e^{z_2} - 1)z_2}\right) \tag{4.1.31}$$

$$\frac{\partial}{\partial c}\tilde{w}_c(r,\alpha) = \ln(z_0) - r\ln(z_1) - (1-r)\ln(z_2) - H(r). \tag{4.1.32}$$

The final simplification for $\frac{\partial}{\partial \alpha}\tilde{w}_c(r,\alpha)$ is by the definition of z_1, z_2.

4.2 Symmetry of $\tilde{w}_c$ and existence of maximizer $\hat{\alpha}(r)$

Define $\hat{\alpha}(r)$ as follows, well-defined by the following theorem.

$$\hat{\alpha}(r) \coloneqq \operatorname*{argmax}_{\{\alpha \ \mid \ (r,\alpha)\in\mathcal{P}_c\}} \tilde{w}_c(r,\alpha). \tag{4.2.1}$$

Theorem 4.2.1. *Take $2 < c < 3$ and fix $0 < r < 1$. Then $\tilde{w}_c$, defined on the parallelogram $\mathcal{P}_c$ in Section 3.3, satisfies:*

1. $\tilde{w}_c(r,\alpha) = \tilde{w}_c(1-r, 1-\alpha)$.
2. *$\tilde{w}_c$ is strictly concave in α.*
3. *For each r, $\tilde{w}_c$ attains its maximum at a unique $\hat{\alpha}(r)$ in $\mathcal{P}_c$.*
4. $\frac{\partial \tilde{w}_c}{\partial \alpha}(r, \hat{\alpha}(r)) = 0$.

In other words,

$$\{(r,\hat{\alpha}(r)) \mid 0 < r < 1\} = \{(r,\alpha) \in \mathcal{P}_c \mid \frac{\partial \tilde{w}_c}{\partial \alpha}(r,\alpha) = 0\}.$$

For each $0 < r < 1$, we have

$$\{\hat{\alpha}(r)\} = \{\alpha \in \mathcal{P}_c \mid \frac{\partial \tilde{w}_c}{\partial \alpha}(r,\alpha) = 0\}.$$

The next few subsubsections prove this.

4.2.1 $\tilde{w}_c(1-r, 1-\alpha) = \tilde{w}_c(r,\alpha)$

Item 1 of Theorem 4.2.1 follows directly from the definition of $\tilde{w}_c$,

$$\tilde{w}_c(r,\alpha) \coloneqq H(\alpha) - cH(r) + \breve{\kappa}_c(r,\alpha) + \breve{\kappa}_c(1-r, 1-\alpha) + \breve{\kappa}_c(1,1).$$

Remark 4.2.2. This symmetry of $\tilde{w}_c$ implies the following symmetries of h_c (defined in Section 3.3). Note these symmetries are analogous to the tetrahedral symmetries of barycentric-decoupled functions as described in Lemma 2.2.4, except these apply in six dimensions instead of three.

1. h_c is invariant under permutation $i \leftrightarrow j$ of pairs of (r_j, α_j).

$$h_c(r_1,r_2,r_3,\alpha_1,\alpha_2,\alpha_3) = h_c(r_1,r_3,r_2,\alpha_1,\alpha_3,\alpha_2) = h_c(r_2,r_1,r_3,\alpha_2,\alpha_1,\alpha_3)$$

2. h_c is invariant under reflections across two axes at a time:

$$h_c(r_1, 1-r_2, 1-r_3, \alpha_1, 1-\alpha_2, 1-\alpha_3) = h_c(r_1, r_2, r_3, \alpha_1, \alpha_2, \alpha_3)$$
$$h_c(1-r_1, r_2, 1-r_3, 1-\alpha_1, \alpha_2, 1-\alpha_3) = h_c(r_1, r_2, r_3, \alpha_1, \alpha_2, \alpha_3)$$
$$h_c(1-r_1, 1-r_2, r_3, 1-\alpha_1, 1-\alpha_2, \alpha_3) = h_c(r_1, r_2, r_3, \alpha_1, \alpha_2, \alpha_3).$$

Proof. These permutations permute (t_0, t_1, t_2, t_3), so $H(t_0, t_1, t_2, t_3)$ is constant under the symmetry.

For Item 1, the rest of the terms in the definition of h_c are merely permuted.

For Item 2, the rest of the terms are invariant because $\tilde{w}_c(r, \alpha) = \tilde{w}_c(1-r, 1-\alpha)$ (see Item 1 of Theorem 4.2.1). □

4.2.2 $\tilde{w}_c$ is strictly concave in α

From Section 4.1.1:

$$\tilde{w}_{\alpha\alpha}(r,\alpha) = \frac{\partial^2}{\partial\alpha^2}\tilde{w}_c(r,\alpha) = \frac{1}{c}\left(\frac{\frac{1}{e^{z_1}-1} + \frac{1}{z_1} + 1}{r\nu'(z_1)} + \frac{\frac{1}{e^{z_2}-1} + \frac{1}{z_2} + 1}{(1-r)\nu'(z_2)}\right).$$

From Lemma 3.1.1 we have $\nu'(z) < 0$ for all $z > 0$, and we have $z_1, z_2 > 0$. Together with $0 < r < 1$, this implies $\tilde{w}_{\alpha\alpha}(r,\alpha) < 0$ for all $(r,\alpha) \in \mathcal{P}_c$. Thus strict concavity of $\tilde{w}_c$ in α is established, proving Item 2 of Theorem 4.2.1. For fixed r, then $\tilde{w}_c(r,\alpha)$ has at most critical point in α since $\frac{\partial}{\partial\alpha}\tilde{w}_c$ is decreasing in α.

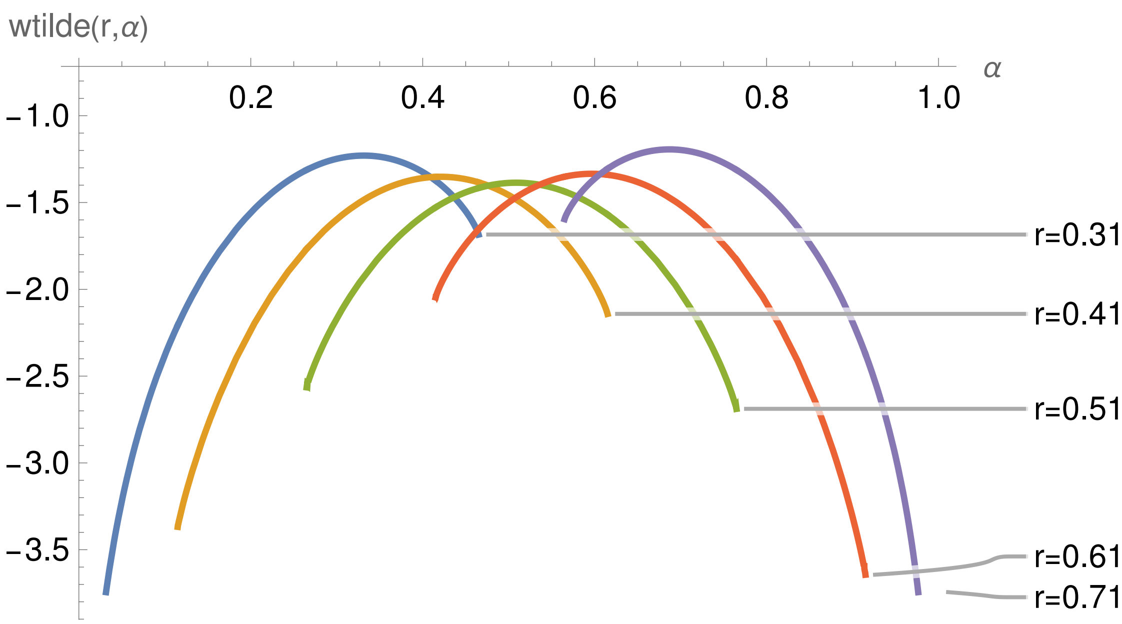

Figure 4.1: $\tilde{w}_c$ is strictly concave as α varies with c, r fixed. Here depicted for $c = 3$ and varying r. Note the plot is not defined everywhere due to the constraints on α imposed by $\mathcal{P}_c$.

4.2.3 $\tilde{w}_c$ attains its maximum for each $r \in (0,1)$; $\frac{\partial \tilde{w}_c}{\partial\alpha}(r,\alpha)$ has a zero

This subsection proves Item 3 of Theorem 4.2.1 (existence of the critical point $\hat{\alpha}(r)$), which by strict concavity must be the maximizer. Using z_1, z_2 from Equation (3.3.7), define

$$d(r,\alpha) := (1-r)(e^{z_1}-1)z_1 - r(e^{z_2}-1)z_2. \tag{4.2.2}$$

From Section 4.1.1, recall

$$\frac{\partial \tilde{w}_c}{\partial \alpha} = \ln\left(\frac{(1-r)(e^{z_1}-1)z_1}{r(e^{z_2}-1)z_2}\right),$$

so $\frac{\partial \tilde{w}_c}{\partial \alpha}(r,\alpha) = 0$ if and only if $d(r,\alpha) = 0$.

Fix $c > 2$ and any $0 < r < 1$. By the forthcoming Lemma 4.2.3, there exists α_1 with $(r,\alpha_1) \in \mathcal{P}_c$ and $d(r,\alpha_1) < 0$. By Lemma 4.2.3 again, there exists $\tilde{\alpha}_2$ with $(1-r,\tilde{\alpha}_2) \in \mathcal{P}_c$ and $d(1-r,\tilde{\alpha}_2) < 0$. Reflecting by the symmetry $d(r,\alpha) = -d(1-r,1-\alpha)$ gives $\alpha_2 = 1-\tilde{\alpha}_2$ such that $(r,\alpha_2) \in \mathcal{P}_c$ and $d(r,\alpha_2) > 0$.

By continuity of d, there exists some $\hat{\alpha}$ between α_1 and α_2 such that $d(r,\hat{\alpha}) = 0$. Note $(r,\hat{\alpha}) \in \mathcal{P}_c$ since $\mathcal{P}_c$ is convex. This proves Item 3 of Theorem 4.2.1.

Lemma 4.2.3. *For $c > 2$ and any $0 < r < 1$, there exists some α_1 such that $(r,\alpha_1) \in \mathcal{P}_c$ and $d(r,\alpha_1) < 0$.*

Proof. Fix $r \in (0,1)$. All limits in this proof are of sequences of α keeping $(r,\alpha) \in \mathcal{P}_c$.

The top boundary of $\mathcal{P}_c$ is given by $\alpha = \frac{c}{2}r$ for $0 < r \le \frac{2}{c}$ and $\alpha = 1$ for $\frac{2}{c} \le r < 1$. By casework below, we show d is negative as α converges to the top boundary of $\mathcal{P}_c$. Hence there exists α_1 with $(r,\alpha_1) \in \mathcal{P}_c$ and $d(r,\alpha_1) < 0$.

- Case 1: Suppose $0 < r < \frac{2}{c}$.

  By definition of z_1 and continuity of $z = \nu^{-1}$,

$$\lim_{\alpha\to\frac{c}{2}r} z_1 = \lim_{\alpha\to\frac{c}{2}r} z\left(\frac{\alpha}{cr}\right) = z\left(\frac{1}{2}\right) = 0. \tag{4.2.3}$$

  By definition of z_2,

$$\lim_{\alpha\to\frac{c}{2}r} \nu(z_2) = \lim_{\alpha\to\frac{c}{2}r} \frac{1-\alpha}{c(1-r)} = \frac{1-\frac{c}{2}r}{c(1-r)} < \frac{1}{c}. \tag{4.2.4}$$

  Thus since $z = \nu^{-1}$ is decreasing,

$$\lim_{\alpha\to\frac{c}{2}r} z_2 = \nu^{-1}\left(\frac{1-\frac{c}{2}r}{c(1-r)}\right) \ge \nu^{-1}\left(\frac{1}{c}\right) = z_0 > 0. \tag{4.2.5}$$

  Since d is continuous and $d(r,\alpha) < 0$ when $z_1 = 0$ and $z_2 > 0$, we see

$$\lim_{\alpha\to\frac{c}{2}r} d(r,\alpha) < 0. \tag{4.2.6}$$

- Case 2: Suppose $\frac{2}{c} \le r < 1$.

  As $\alpha \to 1$, we have $z_2 \to z(0) \to +\infty$ and $z_1 \to z(\frac{1}{cr})$, so z_1 converges to some finite number, and z_2 diverges to positive infinity. Hence $d(r,\alpha) \to -\infty$ as $\alpha \to 1$.

□

4.3 Preparation for applying Laplace Method: local behavior at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

Recall from Section 3.3,

$$h_c(\vec{r}, \vec{\alpha}) := cH(t_0, t_1, t_2, t_3) + (c-3)\ln(2) + \tilde{w}_c(r_1, \alpha_1) + \tilde{w}_c(r_2, \alpha_2) + \tilde{w}_c(r_3, \alpha_3)$$

Define $\mathfrak{h}_c$ as the terms other than $\tilde{w}_c$, so

$$\mathfrak{h}_c(\vec{r}) = cH(t_0, t_1, t_2, t_3) + (c-3)\ln(2) \tag{4.3.1}$$

$$h_c(\vec{r}, \vec{\alpha}) = \mathfrak{h}_c(\vec{r}) + \tilde{w}_c(r_1, \alpha_1) + \tilde{w}_c(r_2, \alpha_2) + \tilde{w}_c(r_3, \alpha_3) \tag{4.3.2}$$

Then $\mathfrak{h}_c$ accounts for the interaction between r_i and r_j for $i \neq j$, and the $\tilde{w}_c$ terms account for the interaction between r_i and α_i.

4.3.1 $h_c\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = 0$ is a critical point of h_c

Lemma 4.3.1. *For $0 < c < \infty$, a critical point for h_c is*

$$(r_1, r_2, r_3, \alpha_1, \alpha_2, \alpha_3) = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) \tag{4.3.3}$$

with the corresponding value of h_c being $h_c\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = 0$.

Proof. We begin by analyzing $\tilde{w}_c$.

Recall $z_2(r, \alpha) = z_1(1-r, 1-\alpha)$, so $z_2(\frac{1}{2}, \frac{1}{2}) = z_1(\frac{1}{2}, \frac{1}{2})$. Substituting these values, along with $\alpha = \frac{1}{2}$ and $r = \frac{1}{2}$ into derivative formulas from Section 4.1.1 yields $\frac{\partial \tilde{w}_c}{\partial r}(\frac{1}{2}, \frac{1}{2}) = 0$ and $\frac{\partial \tilde{w}_c}{\partial \alpha}(\frac{1}{2}, \frac{1}{2}) = 0$. Substitution gives $\tilde{w}_c(\frac{1}{2}, \frac{1}{2}) = -(c-1)\ln(2)$.

By substitution again,

$$\frac{\partial \mathfrak{h}_c}{\partial r_1}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \frac{\partial \mathfrak{h}_c}{\partial r_2}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \frac{\partial \mathfrak{h}_c}{\partial r_3}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = 0.$$

Substitution yields $\mathfrak{h}_c\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = 3(c-1)\ln(2)$. Addition via Equation (4.3.2) yields the result of the lemma. □

4.3.2 Hessian $h_c(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ is negative definite

Lemma 4.3.2. *The Hessian of h_c at $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ is negative definite for $c > 2$. Additionally, the determinant of the Hessian is*

$$\det\left(\mathcal{H}\{h_c\}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)\right) = \left(\frac{-16}{z_0 \nu'(z_0)}\right)^3. \tag{4.3.4}$$

Proof. Recall $\mathcal{H}\{f\}$ denotes the Hessian matrix of the function f with respect to variables $r_1, r_2, r_3, \alpha_1, \alpha_2, \alpha_3$. Then

$$\mathcal{H}\{h_c - \mathfrak{h}_c\} = \begin{bmatrix} \tilde{w}_{rr}(r_1,\alpha_1) & 0 & 0 & \tilde{w}_{r\alpha}(r_1,\alpha_1) & 0 & 0 \\ 0 & \tilde{w}_{rr}(r_2,\alpha_2) & 0 & 0 & \tilde{w}_{r\alpha}(r_2,\alpha_2) & 0 \\ 0 & 0 & \tilde{w}_{rr}(r_3,\alpha_3) & 0 & 0 & \tilde{w}_{r\alpha}(r_3,\alpha_3) \\ \tilde{w}_{r\alpha}(r_1,\alpha_1) & 0 & 0 & \tilde{w}_{\alpha\alpha}(r_1,\alpha_1) & 0 & 0 \\ 0 & \tilde{w}_{r\alpha}(r_2,\alpha_2) & 0 & 0 & \tilde{w}_{\alpha\alpha}(r_2,\alpha_2) & 0 \\ 0 & 0 & \tilde{w}_{r\alpha}(r_3,\alpha_3) & 0 & 0 & \tilde{w}_{\alpha\alpha}(r_3,\alpha_3) \end{bmatrix}.$$

$\mathcal{H}\{\mathfrak{h}_c\}$ has the form $\mathcal{H}\{\mathfrak{h}_c\} = \begin{bmatrix} \mathcal{H}_{\vec{r}}(\mathfrak{h}_c) & 0 \\ 0 & 0_{3\times 3} \end{bmatrix}$.

Letting $\otimes$ denote the Kronecker product, the Hessian of $\mathfrak{h}_c$ at $(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2})$ is

$$\begin{bmatrix} -4c & 0 \\ 0 & 0 \end{bmatrix} \otimes I_{3,3}.$$

The formulas for $\tilde{w}_c$ in Section 4.1.1 give the Hessian of h_c evaluated at $(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2})$:

$$\mathcal{H}\{h_c\}\left(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\right) =$$
$$[\mathcal{H}\{\mathfrak{h}_c\} + \mathcal{H}\{h_c - \mathfrak{h}_c\}]\left(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\right) =$$
$$\begin{bmatrix} -4c + 4\left(c + \frac{1}{z_0\nu'(z_0)}\right) & -\frac{4}{z_0\nu'(z_0)} \\ -\frac{4}{z_0\nu'(z_0)} & \frac{4}{c\nu'(z_0)}\left(1 + \frac{1}{z_0} + \frac{1}{e^{z_0}-1}\right) \end{bmatrix} \otimes I_{3,3},$$

The key 2×2 matrix is

$$M = \begin{bmatrix} \frac{4}{z_0\nu'(z_0)} & -\frac{4}{z_0\nu'(z_0)} \\ -\frac{4}{z_0\nu'(z_0)} & \frac{4}{c\nu'(z_0)}\left(1 + \frac{1}{z_0} + \frac{1}{e^{z_0}-1}\right) \end{bmatrix}$$
$$= \frac{4}{z_0\nu'(z_0)} \begin{bmatrix} 1 & -1 \\ -1 & \frac{z_0}{c}\left(1 + \frac{1}{z_0} + \frac{1}{e^{z_0}-1}\right) \end{bmatrix},$$

which has trace

$$\operatorname{tr}(M) = \frac{4}{\nu'(z_0)}\left(\frac{1}{z_0} + \frac{1}{c} + \frac{1}{cz_0} + \frac{1}{c(e^{z_0}-1)}\right).$$

Note $\nu'(z_0)$ is negative (Lemma 3.1.1), and the rest of the terms are positive, so $\operatorname{tr}(M) < 0$ for $c, z_0 > 0$. Next we will show the determinant of M is positive for $c > 2$. We directly compute $\det(M)$ to be

$$\det(M) = \left(\frac{4}{z_0\nu'(z_0)}\right)^2 \left(-1 + \frac{z_0}{c}\left(1 + \frac{1}{z_0} + \frac{1}{e^{z_0}-1}\right)\right).$$

The equation $\nu(z_0) = \frac{1}{z_0} - \frac{1}{e^{z_0}-1} = \frac{1}{c}$ defines z_0 and allows simplification:

$$\begin{aligned}
\det(M) &= \left(\frac{4}{z_0\nu'(z_0)}\right)^2 \left(-1 + z_0\nu(z_0)\left(1 + \frac{1}{z_0} + \frac{1}{e^{z_0}-1}\right)\right) \\
&= \left(\frac{4}{z_0\nu'(z_0)}\right)^2 \left(-1 + z_0\left(\frac{1}{z_0} - \frac{1}{e^{z_0}-1}\right)\left(1 + \frac{1}{z_0} + \frac{1}{e^{z_0}-1}\right)\right) \\
&= \left(\frac{4}{z_0\nu'(z_0)}\right)^2 \left(-1 + z_0\left(\frac{1}{z_0^2} - \frac{1}{(e^{z_0}-1)^2} + \frac{1}{z_0} - \frac{1}{e^{z_0}-1}\right)\right) \\
&= \left(\frac{4}{z_0\nu'(z_0)}\right)^2 \left(z_0\left(\frac{1}{z_0^2} - \frac{1}{(e^{z_0}-1)^2} - \frac{1}{e^{z_0}-1}\right)\right) \\
&= \left(\frac{4}{z_0\nu'(z_0)}\right)^2 \left(z_0\left(\frac{1}{z_0^2} - \frac{e^{z_0}}{(e^{z_0}-1)^2}\right)\right).
\end{aligned}$$

The derivative $\nu'(z) = \frac{e^z}{(e^z-1)^2} - \frac{1}{z^2}$ allows cancellation, concluding

$$\det(M) = \frac{-16}{z_0\nu'(z_0)}. \tag{4.3.5}$$

Hence, for $z_0 > 0$, we have $\operatorname{tr}(M) < 0$ and $\det(M) > 0$, so the eigenvalues of M must both be negative. Since $\mathcal{H}\{h_c\}(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) = M \otimes I_3$, all six eigenvalues of the Hessian of h_c must be negative at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ provided $z_0 > 0$. Recall $\nu(z_0) = \frac{1}{c}$, and $\nu(x) \geq \frac{1}{2}$ for $x \leq 0$ (Lemma 3.1.1). Hence for $c > 2$, we have $z_0 > 0$ and can conclude $\mathcal{H}\{h_c\}(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ is negative definite as desired.

Since $\mathcal{H}\{h_c\}(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) = M \otimes I_3$, we also have

$$\det\left(\mathcal{H}\{h_c\}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)\right) = (\det M)^3 = \left(\frac{-16}{z_0\nu'(z_0)}\right)^3.$$

thus proving the determinant part of the lemma. □

4.3.3 Evaluating the Laplace Method formula

When the Discrete Laplace Method is applied in Equation (1.2.3), it gives a formula for the asymptotic value we seek. This formula is rigorously evaluated in the following proposition.

Proposition 4.3.3. *Let* $\boldsymbol{x}_0 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. *For all* n *and* $c > 2$, *then*

$$\frac{c^3}{2}(2\pi)^3 \frac{\overline{g}_c(\boldsymbol{x}_0)}{\sqrt{\det(-\mathcal{H}\{h_c\}(\boldsymbol{x}_0))}} = 1. \tag{4.3.6}$$

Proof. From Section 3.3, $\overline{g}_c$ is defined as

$$\overline{g}_c(\vec{r}, \vec{\alpha}) = \widetilde{g}_c(r_1, \alpha_1)\widetilde{g}_c(r_2, \alpha_2)\widetilde{g}_c(r_3, \alpha_3)\frac{1}{\sqrt{t_0t_1t_2t_3(2\pi c)^3}}$$

$$\widetilde{g}_c(r, \alpha) := \sqrt{\frac{-z_0\nu'(z_0)}{z_1\nu'(z_1)z_2\nu'(z_2)}}\sqrt{\frac{1}{2c\pi r(1-r)}}.$$

Note $z_0 = z_1 = z_2 = \nu^{-1}\left(\frac{1}{c}\right)$ when $r = \alpha = \frac{1}{2}$, so at $\boldsymbol{x}_0 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, we have

$$\overline{g}_c(\boldsymbol{x}_0) = \widetilde{g}_c\left(\frac{1}{2}, \frac{1}{2}\right)^3 \frac{1}{\sqrt{(1/4)^4(2\pi c)^3}} = \widetilde{g}_c\left(\frac{1}{2}, \frac{1}{2}\right)^3 \sqrt{\frac{2^5}{(c\pi)^3}}$$

$$\widetilde{g}_c\left(\frac{1}{2}, \frac{1}{2}\right) = \sqrt{\frac{-1}{z_0\nu'(z_0)}}\sqrt{\frac{1}{2c\pi(1/2)^2}} = \sqrt{\frac{-2}{z_0\nu'(z_0)c\pi}}$$

$$\overline{g}_c(\boldsymbol{x}_0) = \sqrt{\frac{-2^8}{(z_0\nu'(z_0))^3(c\pi)^6}}.$$

From Section 4.3.2, we have

$$\det(\mathcal{H}\{h_c\}(\boldsymbol{x}_0)) = \left(\frac{-16}{z_0\nu'(z_0)}\right)^3$$

Note $h_c(\boldsymbol{x}_0) = 0$ by Lemma 4.3.1, so

$$\begin{aligned}
&\frac{c^3}{2}(2\pi)^3 \frac{\overline{g}_c(\boldsymbol{x}_0)}{\sqrt{\det(-\mathcal{H}\{h_c\}(\boldsymbol{x}_0))}} \\
&= 4(c\pi)^3 \overline{g}_c(\boldsymbol{x}_0) \sqrt{\det(\mathcal{H}\{h_c\}(\boldsymbol{x}_0))^{-1}} \\
&= 4(c\pi)^3 \sqrt{\frac{-2^8}{(z_0\nu'(z_0))^3(c\pi)^6}} \sqrt{\left(\frac{-16}{z_0\nu'(z_0)}\right)^{-3}} \\
&= 1.
\end{aligned}$$

□

5 Proving $h_c < 0$ on $\mathcal{U}_c \setminus \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ for $2 < c < 3$: reducing the 6-variable problem to maximizing a 3-variable function $\widehat{h}_c$.

The goal in this section is to present strong evidence that $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ is the global maximum of h_c on $\mathcal{U}_c$ whenever $2.5 \leq c < 3$. The derivations here, plus interval arithmetic, are used in [HH24] to prove this for all $c \in [2.5, 3)$.

5.1 An overview from coarse numerical evidence

Define

$$\widehat{h}_c(r_1, r_2, r_3) = \max_{\{(\alpha_1,\alpha_2,\alpha_3) \mid (r_i,\alpha_i)\in\mathcal{P}_c,\, i\in\{1,2,3\}\}} h_c(r_1, r_2, r_3, \alpha_1, \alpha_2, \alpha_3). \tag{5.1.1}$$

We saw that $\widehat{h}_c\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = 0$ is a local maximum in Lemma 4.3.1 and need to see for which values of c it is a global maximum over the tetrahedron $\mathcal{T}$.

The plot in Figure 5.1 illustrates the situation. It suggests that if other admissible maximizers exist, then the maximizers must be in a region around $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ or at one of 4 corners of the cube.

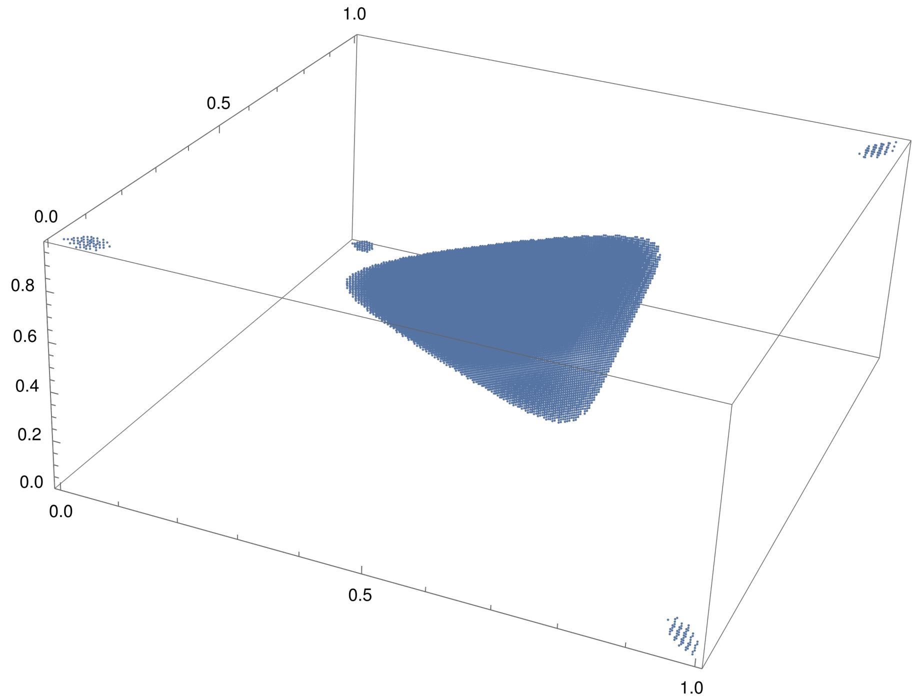

Figure 5.1: $c = 3$. All points (r_1, r_2, r_3) where $\widehat{h}_c(r_1, r_2, r_3) > -0.08$, on a 100^3-point grid. Note that besides the blob near $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, the only points are near the corners of the tetrahedron $\mathcal{T}$.

5.1.1 No more maxima near $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$

The plot Figure 5.2 illustrates that the Hessian of $\widehat{h}_c$ is negative definite on a region centered at $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$.

The plot shows that this region contains the cube $[\frac{1}{2} - 0.125, \frac{1}{2} + 0.125]^3$ Since $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ is a local maximum of $\widehat{h}_c$ with $\widehat{h}_c\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = 0$, this implies $\widehat{h}_c < 0$ in $[\frac{1}{2} - 0.125, \frac{1}{2} + 0.125]^3 \setminus \{\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)\}$. Hence $\widehat{h}_c$ has no global maxima in that cube near $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$.

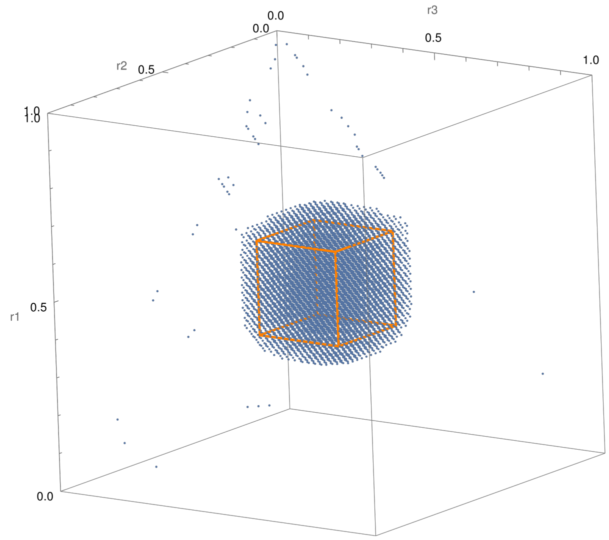

Figure 5.2: Plot for $c = 3$ where the Hessian of $\widehat{h}_c$ is negative definite, on a 50^3-point grid. The orange cube, provided for scale, is $\left[\frac{1}{2} - 0.125, \frac{1}{2} + 0.125\right]^3$. Thus $\widehat{h}_c$ is unimodal on this cube.

Next, we give a much more detailed argument which leads us in this thesis to convincing plots. The argument involves a fair amount of tricky calculation to produce formulas upon which interval arithmetic can apply to yield a proof. The interval arithmetic itself is a matter for a paper in preparation, [HH24].

5.2 Defining $\hat{\alpha}(r), w(r)$ and preparing $\widehat{h}_c$

Recall $\mathcal{P}_c \subseteq (0,1)^2$ is a parallelogram defined in Equation (3.2.1), and $\tilde{w}_c(r,\alpha)$ is defined for $(r,\alpha) \in \mathcal{P}_c$ in Section 3.3, relying on the tricky functions $z_1(r,\alpha)$ and $z_2(r,\alpha)$. Recall from Theorem 4.2.1 that for each $r \in (0,1)$,

$$\hat{\alpha}(r) := \underset{\{\alpha \mid (r,\alpha)\in\mathcal{P}_c\}}{\operatorname{argmax}} \tilde{w}_c(r,\alpha) \tag{5.2.1}$$

exists and is unique. Set $w(r) := \tilde{w}_c(r, \hat{\alpha}(r))$. Then

$$w(r) = \max_{\{\alpha \mid (r,\alpha)\in\mathcal{P}_c\}} \tilde{w}_c(r,\alpha). \tag{5.2.2}$$

For $c > 2$, this maximum is well defined due to Theorem 4.2.1. In Section 6, we will show that w can be extended to be continuous for $r \in [0,1]$ and real-analytic over $r \in (0,1)$.

5.2.1 Reflection of w

Lemma 5.2.1. *$w(r) = w(1-r)$ and $\hat{\alpha}(1-r) = 1 - \hat{\alpha}(r)$*

Proof. By definition, $\tilde{w}_c(r,\hat{\alpha}(r)) > \tilde{w}_c(r,\alpha)$ for all $\alpha \neq \hat{\alpha}(r)$.

By the symmetry $\tilde{w}_c(r,\alpha) = \tilde{w}_c(1-r, 1-\alpha)$ from Item 1,

$$\tilde{w}_c(1-r, 1-\hat{\alpha}(r)) = \tilde{w}_c(r,\hat{\alpha}(r)) > \tilde{w}_c(r,\alpha) = \tilde{w}_c(1-r, 1-\alpha).$$

Hence $\tilde{w}_c(1-r, 1-\hat{\alpha}(r)) > \tilde{w}_c(1-r, 1-\alpha)$ for all $1-\alpha \neq 1-\hat{\alpha}(r)$, so $\tilde{w}_c(1-r, 1-\hat{\alpha}(r)) > \tilde{w}_c(1-r, \alpha)$ for all $\alpha \neq 1-\hat{\alpha}(r)$. Hence $\hat{\alpha}(1-r) = 1-\hat{\alpha}(r)$, so

$$w(1-r) = \tilde{w}_c(1-r, \hat{\alpha}(1-r)) = \tilde{w}_c(1-r, 1-\hat{\alpha}(r)) = \tilde{w}_c(r, \hat{\alpha}(r)) = w(r).$$

□

5.2.2 $\widehat{h}_c$ in barycentic-decoupled form

By definition of $\widehat{h}_c$ earlier,

$$\widehat{h}_c(r_1, r_2, r_3) = \max_{\{(\alpha_1,\alpha_2,\alpha_3) \mid (r_i,\alpha_i)\in\mathcal{P}_c,\, i\in\{1,2,3\}\}} h_c(r_1, r_2, r_3, \alpha_1, \alpha_2, \alpha_3). \tag{5.2.3}$$

The only terms depending on the α_i are the $\tilde{w}_c(r_i, \alpha_i)$, which are maximized at $\alpha_i = \hat{\alpha}(r_i)$ by $w(r_i) = \max_{\alpha_i} \tilde{w}_c(r_i, \alpha_i)$. Thus by definition of h_c in Section 3.3,

$$\widehat{h}_c(r_1, r_2, r_3) = \mathfrak{h}_c(r_1, r_2, r_3) + w(r_1) + w(r_2) + w(r_3) \tag{5.2.4}$$

$$\mathfrak{h}_c(r_1, r_2, r_3) = cH(t_0, t_1, t_2, t_3) + (c-3)\ln(2). \tag{5.2.5}$$

Let $E(x) = -cx\ln(x)$. Then $\widehat{h}_c$ can be written in barycentric-decoupled form as

$$\widehat{h}_c(r_1, r_2, r_3) = E(t_0) + E(t_1) + E(t_2) + E(t_3) + w(r_1) + w(r_2) + w(r_3) + (c-3)\ln(2). \tag{5.2.6}$$

Note $w(r) = w(1-r)$ by Lemma 5.2.1. Define $w(0) = w(1) = 0$ by continuity (see the forthcoming Proposition 6.6.2). Likewise, define $E(0) = E(1) = 0$ by continuity.

5.3 Applying the 4 lines theorem to $\widehat{h}_c$

Now we reduce the global max problem for $\widehat{h}_c$ (for fixed c) from maximization over a 3-dimensional volume $\mathcal{T}$ to five 1-dimensional problems.

As in Lemma 2.1.1, define

$$G^{\tau_0}(r) := w(r) + E(r - \tau_0) + \frac{1}{3}E(\tau_0).$$

so that

$$\widehat{h}_c(r_1, r_2, r_3) = G^{\tau_0}(r_1) + G^{\tau_0}(r_2) + G^{\tau_0}(r_3).$$

We wish to apply Corollary 2.2.2. To invoke it, we must check that $\frac{dG^{\tau_0}(r)}{dr} = y$ has at most two solutions for each y.

If this succeeds, then the corollary says we can check $\widehat{h}_c$ restricted to each of the 4 line segments:

1. Diagonal: (r, r, r) for $r \in \left(\frac{1}{3}, 1\right)$.
2. Central vertical segment: $\left(\frac{1}{2}, \frac{1}{2}, r\right)$ for $r \in \left(0, \frac{1}{2}\right)$.
3. Centerline of face: $(r, r, 1-2r)$ for $r \in \left(0, \frac{1}{2}\right)$.
4. Edge of tetrahedron: $(r, r, 1)$ for $r \in \left[0, \frac{1}{2}\right]$.

If we show $\widehat{h}_c < 0$ on all of those segments except for at $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$, then that would imply $\widehat{h}_c < 0$ on $\mathcal{T} \setminus \{\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)\}$. Equivalently, $h_c < 0$ on $\mathcal{U}_c \setminus \{\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)\}$ as follows:

- If $\vec{r} \neq \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$, then $h_c(\vec{r}, \vec{\alpha}) \leq \widehat{h}_c(\vec{r}) < 0$
- If $\vec{r} = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ and $\vec{\alpha} \neq \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$, then $h_c(\vec{r}, \vec{\alpha}) < \widehat{h}_c(\vec{r}) = 0$.

We shall not prove this rigorously in this thesis, since our proof involves a heavy use of interval arithmetic, to appear in [HH24]. However, we next show convincing plots for three values of c including $c = 3$.

5.3.1 Derivative calculations: derivative of G^{τ_0} wrt r.

To apply Corollary 2.2.2, recall we need to verify that $\frac{dG^{\tau_0}(r)}{dr} = y$ has at most two solutions for each y.

Recall $G^{\tau_0}(r) := w(r) + E\left(r - \tau_0\right) + \frac{1}{3}E(\tau_0)$, where $E(x) = -cx\ln(x)$. Note $E'(x) = -c(1 + \ln(x))$. Then since $w(r) = \tilde{w}_c(r, \hat{\alpha}(r))$,

$$\frac{\mathrm{d}G^{\tau_0}}{\mathrm{d}r} = \frac{\partial \tilde{w}_c}{\partial r}(r, \hat{\alpha}(r)) + \frac{\partial \tilde{w}_c}{\partial \alpha}(r, \hat{\alpha}(r))\frac{\mathrm{d}\hat{\alpha}(r)}{\mathrm{d}r} + cE'(r - \tau_0).$$

Note $\frac{\partial \tilde{w}_c}{\partial \alpha}(r, \hat{\alpha}(r)) = 0$ by definition of $\hat{\alpha}$ as the maximizer of $\tilde{w}_c$ for fixed r, so by Section 4.1.1 we find

$$\begin{aligned}\frac{\mathrm{d}G^{\tau_0}}{\mathrm{d}r} &= \frac{\partial \tilde{w}_c}{\partial r}(r, \hat{\alpha}(r)) + cE'(r - \tau_0)\\ &= -c\ln(\tilde{q}(r, \hat{\alpha}(r))) - c(1 + \ln(r - \tau_0)).\end{aligned}$$

5.3.2 Plot suggesting $\frac{dG^{\tau_0}(r)}{dr}$ is at-most 2-to-1

To show $\frac{dG^{\tau_0}(r)}{dr} = y$ has at most two solutions for each y, it will suffice to show $\frac{dG^{\tau_0}(r)}{dr}$ is convex (resp. concave) or even a weaker concept which we nickname "**bi-monotone**." A function f is **bi-monotone** if there exists x_0 where $f(x)$ is strictly decreasing (resp.increasing) for $x < x_0$ and strictly increasing (resp. decreasing) for $x > x_0$. If f is concave on $[a, b] \subset (0, 1)$, increasing on $(0, a]$, and decreasing on $[b, 1)$, then f is bi-monotone on $(0, 1)$. This will have the advantage of only requiring first-derivative checks near the boundary $r \approx 0$ and $r \approx 1$, where the function may have an asymptote.

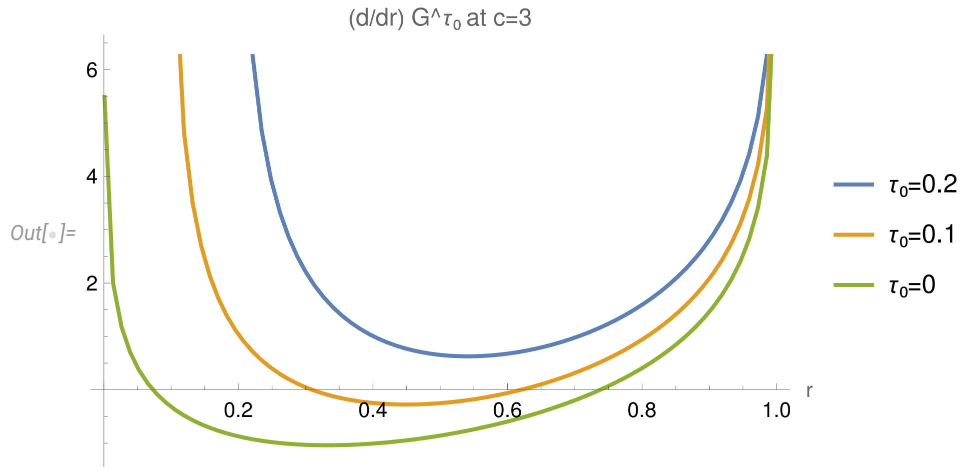

Figure 5.3: Plot of $\frac{dG^{\tau_0}(r)}{dr}$ for $c = 3$ and three values of τ_0

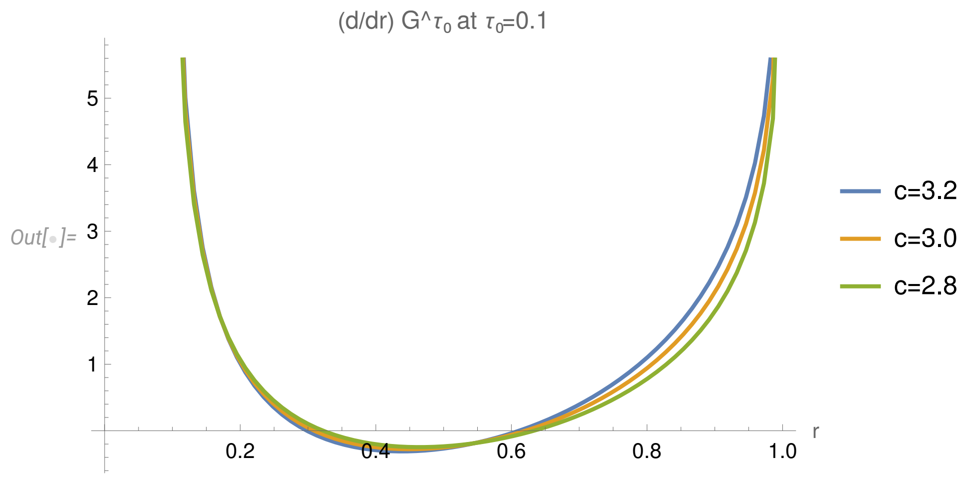

Figure 5.4: Plot of $\frac{dG^{\tau_0}(r)}{dr}$ for $\tau_0 = 0.1$ and three values of c.

5.3.3 Plots suggesting $\widehat{h}_c < 0$ along the four segments, except $\widehat{h}_c(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) = 0$.

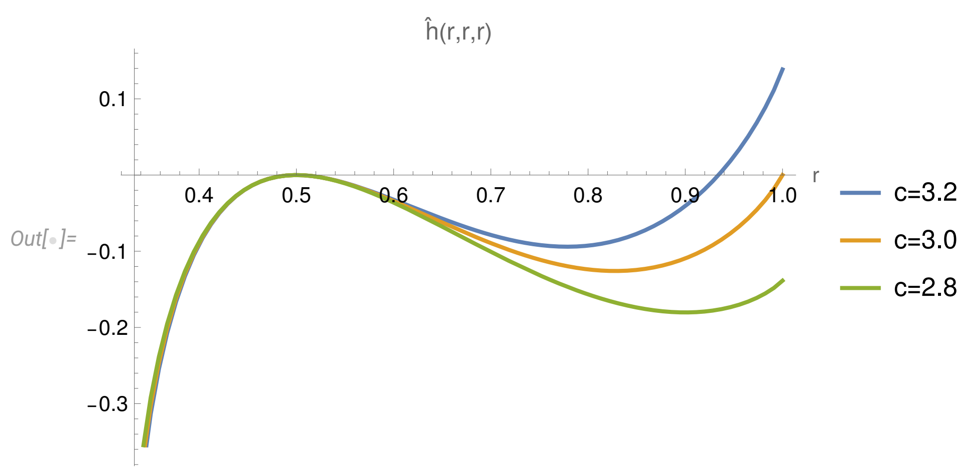

Figure 5.5: Diagonal: Plot of $\widehat{h}_c(r, r, r)$ for three values of c.

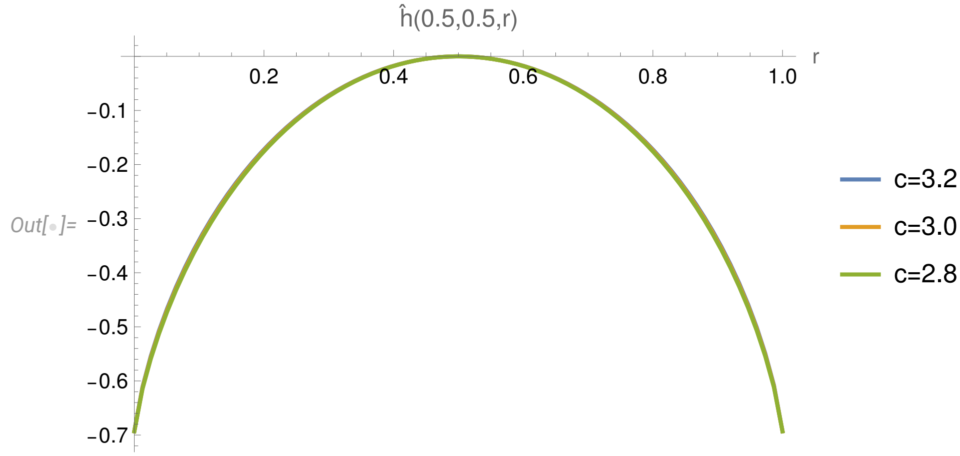

Figure 5.6: Vertical: Plot of $\widehat{h}_c\left(\frac{1}{2},\frac{1}{2},r\right)$ for three values of c.

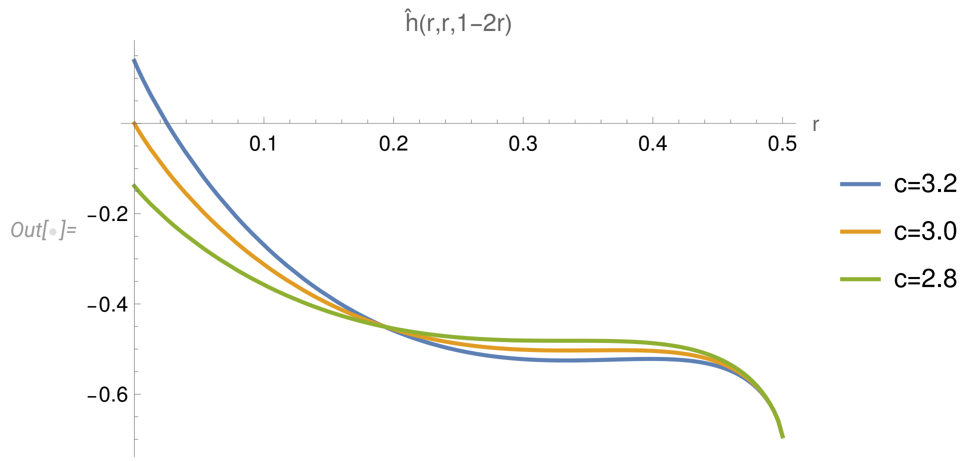

Figure 5.7: Centerline of face: Plot of $\widehat{h}_c\left(r,r,1-2r\right)$ for three values of c.

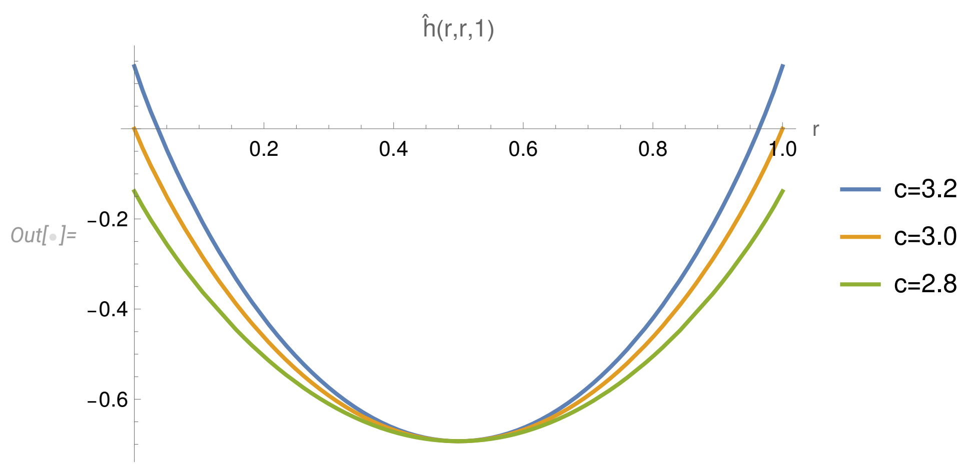

Figure 5.8: Edge: Plot of $\widehat{h}_c\left(r,r,1\right)$ for three values of c.

5.4 The 1-D results using interval arithmetic

Computing with interval arithmetic allows many types of bounds to be obtained rigorously with a computer. We have successfully applied this to the 5 one-dimensional calculations required for the application of Corollary 2.2.2 for all c in the interval $[2.5, 3)$ and plan to put this in an article [HH24], now in preparation. This discussion is involved, so we do not attempt to include it here since it takes much exposition and Mathematica code to perform the calculation.

6 Analytic behavior of w

6.1 Definitions: $\gamma_1, \gamma_2, \eta, F_{S,T}$

For $0 < r < 1$, define $\gamma_1(r)$ and $\gamma_2(r)$ based on $\hat{\alpha}$ (Equation (4.2.1)) and ν (Section 3.1) as follows, plotted in Figure 6.1, Figure 6.2, and Figure 6.3:

$$\gamma_1(r) = \frac{1}{\sqrt{r}}\nu^{-1}\left(\frac{\hat{\alpha}(r)}{cr}\right), \qquad \gamma_2(r) = \frac{1}{\sqrt{1-r}}\nu^{-1}\left(\frac{1-\hat{\alpha}(r)}{c(1-r)}\right). \tag{6.1.1}$$

In Lemma 6.3.1, we will show (for $j = 1$ and $j = 2$), γ_j has a finite limit as $r \to 0$ and $r \to 1$, then define $\gamma_j(0)$ and $\gamma_j(1)$ as this limit.

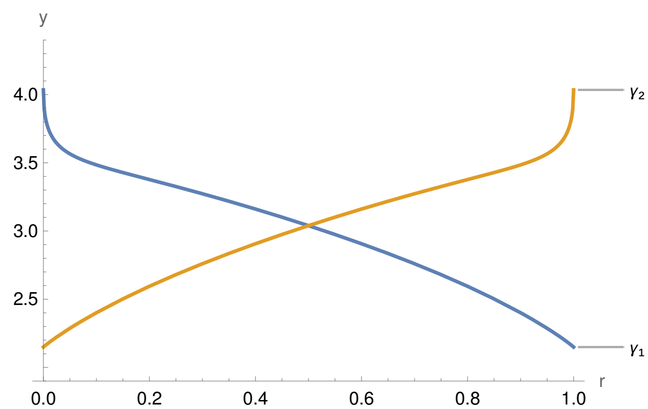

Figure 6.1: $\gamma_1(r)$ and $\gamma_2(r)$ plotted for $c = 3$.

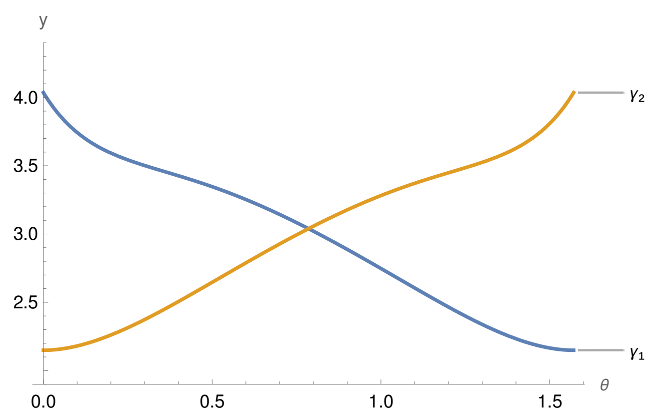

Figure 6.2: $\gamma_1(r)$ and $\gamma_2(r)$ plotted for $c = 3$ under the change of variables $r = \sin^2\theta$, so $(S, T) = (\sin\theta, \cos\theta)$ uniformly parameterizes the arc $\mathfrak{a}$ defined in the forthcoming Equation (6.1.2).

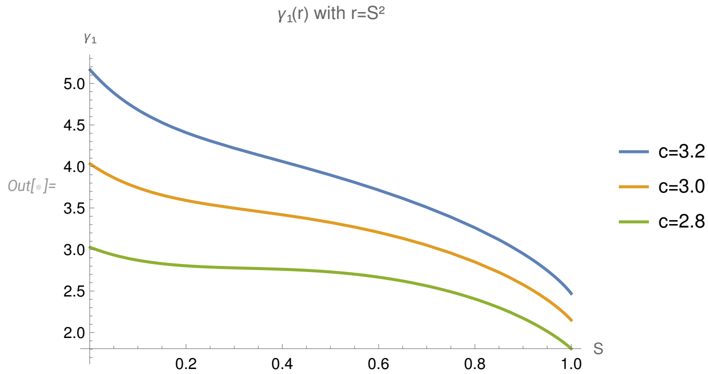

Figure 6.3: $\gamma_1(r)$ plotted for different values of c under the change of variables $r = S^2$.

Define the entire function η by

$$\eta(z) := \begin{cases} \dfrac{e^z - 1}{z}, & z \neq 0 \\ 1, & z = 0 \end{cases}.$$

Let $\mathfrak{a}$ be the quarter-circle arc

$$\mathfrak{a} := \{(S, T) \in \mathbb{R}^2 \mid S^2 + T^2 = 1, S \geq 0, T \geq 0\} \subseteq \mathbb{R}^2 \subseteq \mathbb{C}^2. \tag{6.1.2}$$

Define $F_{S,T}$ for $(S, T) \in \mathfrak{a}$ and $(y_1, y_2) \in \mathbb{R}^2$ as

$$F_{S,T}(y_1, y_2) := \begin{pmatrix} y_2^2\eta(Ty_2) - y_1^2\eta(Sy_1) \\ T^2\nu(Ty_2) + S^2\nu(Sy_1) - 1/c \end{pmatrix}. \tag{6.1.3}$$

6.2 (γ_1, γ_2) are the unique solutions to $F_{S,T} = 0$

Lemma 6.2.1. *Take $0 < r < 1$ given, and let $S = \sqrt{r}$, $T = \sqrt{1 - r}$. Then for $y_1, y_2 > 0$,*

$$F_{S,T}(y_1, y_2) = \vec{0} \iff (y_1, y_2) = (\gamma_1(r), \gamma_2(r)). \tag{6.2.1}$$

Proof. Take $0 < r < 1$ given.
Backwards direction: Assume $y_1 = \gamma_1(r)$ and $y_2 = \gamma_2(r)$, so by definition (Equation (6.1.1)),

$$y_1 = \gamma_1(r) = \frac{1}{S}\nu^{-1}\left(\frac{\hat{\alpha}(r)}{cr}\right), \qquad y_2 = \gamma_2(r) = \frac{1}{T}\nu^{-1}\left(\frac{1 - \hat{\alpha}(r)}{c(1 - r)}\right). \tag{6.2.2}$$

By Theorem 4.2.1, $\frac{\partial \tilde{w}_c}{\partial \alpha}(r, \hat{\alpha}(r)) = 0$, so Equation (4.1.2) applies:

$$0 = \frac{\partial \tilde{w}_c}{\partial \alpha}(r, \hat{\alpha}(r)) = \ln\left(\frac{(1 - r)\left(e^{z_1} - 1\right) z_1}{r\left(e^{z_2} - 1\right) z_2}\right)$$

where $z_1 = \nu^{-1}\left(\frac{\hat{\alpha}(r)}{cr}\right) = Sy_1 > 0$ and $z_2 = \nu^{-1}\left(\frac{1-\hat{\alpha}(r)}{c(1-r)}\right) = Ty_2 > 0$. Hence

$$(1 - r)\left(e^{z_1} - 1\right) z_1 - r\left(e^{z_2} - 1\right) z_2 = 0 \tag{6.2.3}$$
$$T^2 z_1^2 \eta(z_1) - S^2 z_2^2 \eta(z_2) = 0 \tag{6.2.4}$$
$$y_1^2 \eta(Sy_1) - y_2^2 \eta(Ty_2) = 0. \tag{6.2.5}$$

Since ν is the inverse of $z = \nu^{-1}$, we also have:

$$\nu(Sy_1) = \frac{\hat{\alpha}(r)}{cr}, \qquad \nu(Ty_2) = \frac{1 - \hat{\alpha}(r)}{c(1-r)}.$$

By algebra,

$$r\nu(Sy_1) + (1-r)\nu(Ty_2) = \frac{\hat{\alpha}(r)}{c} + \frac{1 - \hat{\alpha}(r)}{c} = \frac{1}{c}.$$

Hence, as desired:

$$\vec{0} = F_{S,T}(y_1, y_2) = \begin{pmatrix} y_2^2\eta(Ty_2) - y_1^2\eta(Sy_1) \\ T^2\nu(Ty_2) + S^2\nu(Sy_1) - 1/c \end{pmatrix}.$$

Forwards direction: Assume $y_1, y_2 > 0$, and $F_{S,T}(y_1, y_2) = \vec{0}$, so

$$y_2^2\eta(Ty_2) = y_1^2\eta(Sy_1) \tag{6.2.6}$$

$$c(1-r)\nu(Ty_2) + cr\nu(Sy_1) = 1. \tag{6.2.7}$$

Let $\alpha = cr\nu(Sy_1)$. Then Equation (6.2.7) implies $1 - \alpha = c(1-r)\nu(Ty_2)$. By rearranging, this gives

$$y_1 = \frac{1}{T}\nu^{-1}\left(\frac{\alpha}{cr}\right), \quad y_2 = \frac{1}{T}\nu^{-1}\left(\frac{1-\alpha}{c(1-r)}\right). \tag{6.2.8}$$

It remains to show $\alpha = \hat{\alpha}(r)$. Since $S, y_1 > 0$, we have $0 < \nu(Sy_1) < \frac{1}{2}$. Then $0 < \alpha < \frac{1}{2}cr$. Likewise, $T, y_2 > 0$ implies $0 < 1 - \alpha < \frac{1}{2}c(1-r)$. Thus $(r, \alpha) \in \mathcal{P}_c$. Equation (4.1.2) together with Equation (6.2.6) implies $\frac{\partial \tilde{w}_c}{\partial \alpha}(r, \alpha) = 0$. For fixed r, by Theorem 4.2.1, $\hat{\alpha}(r)$ is the unique solution to $\frac{\partial \tilde{w}_c}{\partial \alpha}(r, \alpha) = 0$, so indeed $\alpha = \hat{\alpha}(r)$. Hence by comparing Equation (6.2.8) and the definition of γ_1, γ_2 in Equation (6.1.1), we see $y_1 = \gamma_1(r)$ and $y_2 = \gamma_2(r)$. □

6.3 γ_j is continuous on $[0, 1]$

Lemma 6.3.1. *The following limits exist*

$$\gamma_2(0) = \lim_{r \to 0} \gamma_2(r) = \nu^{-1}\left(\frac{1}{c}\right) > 0, \qquad \gamma_1(0) = \lim_{r \to 0} \gamma_1(r) = \gamma_2(0)\sqrt{\gamma_2(0)} > 0. \tag{6.3.1}$$

Henceforth use these values to define $\gamma_j(0)$. Since $\gamma_1(r) = \gamma_2(1-r)$, the limits hold likewise to define $\gamma_j(1)$:

$$\gamma_1(1) = \gamma_2(0), \qquad \gamma_2(1) = \gamma_1(0) \tag{6.3.2}$$

Hence γ_1, γ_2 are continuous functions on $r \in [0, 1]$ with $\gamma_1(r), \gamma_2(r) > 0$ for all r.

Corollary 6.3.2. *Fix $c > 2$. Then there exists constants $0 < a < b$ such that*

$$\gamma_1(r), \gamma_2(r) \in [a, b]$$

for all $r \in [0, 1]$. Existence of these bounds follows from γ_j being continuous on the compact set $[0, 1]$. The lower bound is positive because $\gamma_1(r), \gamma_2(r)$ are positive for all $r \in [0, 1]$. Henceforth we will define the closed square Q_c to be

$$Q_c \coloneqq \{(y_1, y_2) \mid y_1, y_2 \in [a, b]\}, \tag{6.3.3}$$

so Q_c includes all possible pairs $(\gamma_1(r), \gamma_2(r))$.

Proof. By Lemma 6.2.1, for all $0 < r < 1$,

$$T^2\nu(T\gamma_2(r)) + S^2\nu(S\gamma_1(r)) = \frac{1}{c}$$

where $S = \sqrt{r}$ and $T = \sqrt{1-r}$. Since $0 < \nu < 1$ (from Lemma 3.1.1), we have $S^2\nu(S\gamma_2(r)) \to 0$ as $S^2 = r \to 0$. Hence

$$\lim_{r\to 0} T^2\nu(T\gamma_2(r)) = \frac{1}{c}.$$

By continuity, since $T = \sqrt{1-r} \to 1$ as $r \to 0$,

$$\lim_{r\to 0} \gamma_2(r) = \nu^{-1}\left(\frac{1}{c}\right).$$

This proves the first limit formula.

To prove the second formula, we shall begin by showing that γ_1 is bounded. By Lemma 6.2.1, for all $0 < r < 1$,

$$\gamma_1(r)^2\eta(S\gamma_1(r)) = \gamma_2(r)^2\eta(T\gamma_2(r)).$$

Note $\eta(x) \geq 1$ for all $x \geq 0$, so

$$\gamma_1(r)^2 \leq \gamma_1(r)^2\eta(S\gamma_1(r)),$$

hence

$$\gamma_1(r)^2 \leq \gamma_2(r)^2\eta(T\gamma_2(r)).$$

The right-hand-side limits to a positive finite constant as $r \to 0$, so $\gamma_1(r)^2$ is bounded as $r \to 0$. Hence $S\gamma_1(r) \to 0$ as $S^2 = r \to 0$. Note η is continuous with $\eta(0) = 1$, so

$$\lim_{r\to 0} \gamma_1(r)^2 = \lim_{r\to 0} \gamma_1(r)^2\eta(0) = \lim_{r\to 0} \gamma_2(r)^2\eta(T\gamma_2(r)) = \gamma_2(0)^2\eta(\gamma_2(0)).$$

Finally, rearrangement concludes:

$$\lim_{r\to 0} \gamma_1(r) = \gamma_2(0)\sqrt{\eta(\gamma_2(0))}.$$

□

6.4 $F_{S,T}$ is real-analytic

Lemma 6.4.1. *$F_{S,T}$ is real analytic on $\mathfrak{a} \times \mathbb{R}^2$. Equivalently: There exists a neighborhood $\mathcal{N}$ with $\mathfrak{a} \subseteq \mathcal{N} \subseteq \mathbb{C}^2$, and a neighborhood $\mathcal{Y}$ with $\mathbb{R}^2 \subseteq \mathcal{Y} \subseteq \mathbb{C}^2$, such that $F_{S,T}$ is analytic for $(S, T, y_1, y_2) \in \mathcal{N} \times \mathcal{Y}$.*

Proof. Note $\eta(x) = \frac{e^x-1}{x}$ with $\eta(0) = 1$ is entire. Additionally, $\nu(x)$ is real-analytic on $\mathbb{R}$ by Lemma 3.1.1. $F_{S,T}$ is a sum/difference/product of a composition of real-analytic functions, so it is real-analytic. □

6.5 $\gamma_1(S,T), \gamma_2(S,T)$ are real-analytic on $\mathfrak{a}$

For $(S,T) \in \mathfrak{a}$ and $j = 1, 2$, define $\gamma_j(S,T)$ in terms of $\gamma_j(r)$ by

$$\gamma_j(S,T) \coloneqq \gamma_j(S^2) = \gamma_j(1 - T^2),$$

where $\gamma_j(r)$ with one-argument is defined as in Equation (6.1.1) for $r \in [0, 1]$.

We make this change of variables because $\gamma_j(r)$ on its own behaves poorly towards the endpoints. For example, $\gamma_1'(r)$ looks like $\frac{1}{\sqrt{r}}$ times a bounded function, so $\gamma_1'(r)$ blows up as $r \to 0$. On the other hand, $\gamma_j(S,T)$ is well-behaved for all $(S,T) \in \mathfrak{a}$, as we shall show in this section.

To prepare for this proof, we must prove invertability of the Jacobian of $F_{S,T}$ in order to apply the Implicit Function Theorem.

6.5.1 Jacobian of $F_{S,T}$

Lemma 6.5.1. *Denote the Jacobian of $F_{S,T}$ (with respect to y_1, y_2) by:*

$$J_{F,S,T,y_1,y_2} \coloneqq J_{(y_1,y_2)}\{F_{S,T}\}(y_1, y_2)$$

and let $Q_c \subseteq \mathbb{R}^2_{>0}$ be the compact region as defined in Corollary 6.3.2.

Then the Jacobian of $F_{S,T}$ and its inverse are real analytic on $\mathfrak{a} \times Q_c$. In addition, for all $(S, T, y_1, y_2) \in \mathfrak{a} \times Q_c$,

$$\det(J_{F,S,T,y_1,y_2}) > 0.$$

Let $\beta(x) = (e^x - 1)x$, so $\beta'(x) = e^x(x + 1) - 1$. The Jacobian is explicitly given by

$$J_{F,S,T,y_1,y_2} = \begin{bmatrix} -\frac{\beta'(Sy_1)}{S} & \frac{\beta'(Ty_2)}{T} \\ S^3\nu'(Sy_1) & T^3\nu'(Ty_2) \end{bmatrix}.$$

Its inverse is

$$J^{-1}_{F,S,T,y_1,y_2} = \frac{1}{\det(J_{F,S,T,y_1,y_2})} \begin{bmatrix} T^3\nu'(Ty_2) & -\frac{\beta'(Ty_2)}{T} \\ -S^3\nu'(Sy_1) & -\frac{\beta'(Sy_1)}{S} \end{bmatrix}.$$

Proof. Computing the derivatives of $F_{S,T}$ for use in the Jacobian J_{F,S,T,y_1,y_2} is straightforward by differentiation rules. Since $F_{S,T}$ is real analytic on $\mathfrak{a} \times Q_c$, its Jacobian is as well. Next we analyse its determinant:

$$\det(J_{F,S,T,y_1,y_2}) = -T^3 y_1 \frac{\beta'(Sy_1)}{Sy_1}\nu'(Ty_2) - S^3 y_2 \frac{\beta'(Ty_2)}{Ty_2}\nu'(Sy_1).$$

Case: $0 < S$ and $0 < T$:

Note $\frac{\beta'(x)}{x} \geq 2$ for all $x > 0$, and $\nu'(x) < 0$ for all $x \in \mathbb{R}$. All the other quantities are clearly positive for $y_1, y_2 > 0$, so for $0 < S$ and $0 < T$:

$$\det(J_{F,S,T,y_1,y_2}) > 0.$$

Case: $(S,T) = (1,0)$ or $(S,T) = (0,1)$:

The above conclusion $\det(J_{F,S,T,y_1,y_2}) > 0$ applies to the quarter circle $\mathfrak{a}$ without its endpoints. Now we extend it to the endpoints $(0, 1)$ and $(1, 0)$. Since Q_c is compact, y_1 and y_2 are bounded, so as $(S,T) \to (0,1)$, we have $Sy_1 \to 0$ and $Ty_2 \to y_2 > 0$. Also, note $\frac{\beta'(x)}{x} \to 2$ as $x \to 0$, so $\frac{\beta'(Sy_1)}{Sy_1} \to 2$. Hence as $(S,T) \to (0,1)$:

$$\det(J_{F,S,T,y_1,y_2}) \sim -2T^3 y_1 \nu'(Ty_2) \to -2y_1\nu'(y_2) > 0. \tag{6.5.1}$$

Similarly, as $(S,T) \to (1,0)$:

$$\det(J_{F,S,T,y_1,y_2}) \sim -2S^3 y_2 \nu'(Sy_1) \to -2y_2\nu'(y_1) > 0. \tag{6.5.2}$$

These last two displays imply $\det(J_{F,S,T,y_1,y_2}) > 0$ at the endpoints of $\mathfrak{a}$, namely at the points $(S,T) = (1,0)$ and $(S,T) = (0,1)$. Thus for $(S,T) \in \mathfrak{a}$ and $(y_1,y_2) \in Q_c$, we have

$$\det(J_{F,S,T,y_1,y_2}) > 0.$$

□

6.5.2 Proof that $\gamma_1(S,T), \gamma_2(S,T)$ are real-analytic

Lemma 6.5.2. *Consider γ_1 and γ_2 from Section 6.1. Then $\gamma_1(S,T), \gamma_2(S,T)$ are real analytic on $\mathfrak{a}$ and $2 < c < 4$. Note $\mathfrak{a}$ includes its endpoints $(S,T) = (1,0)$ and $(S,T) = (0,1)$),*

Proof. Let $Q_c \subseteq \mathbb{R}^2_{>0}$ be the compact region as defined in Corollary 6.3.2.

From Lemma 6.4.1, $F_{S,T}$ is real analytic in $\mathfrak{a} \times Q_c$. Hence there exists some open sets $\mathfrak{a} \subseteq \mathcal{N}_1 \subseteq \mathbb{C}^2$, $Q_c \subseteq \mathcal{Y}_1 \subseteq \mathbb{C}^2$ such that $F_{S,T}$ is analytic in $\mathcal{N}_1 \times \mathcal{Y}_1$.

From Lemma 6.5.1, $\det(J_{F,S,T,y_1,y_2}) > 0$ on $\mathfrak{a} \times Q_c$. By continuity, there exist open sets $\mathfrak{a} \subseteq \mathcal{N}_2 \subseteq \mathbb{C}^2$, $Q_c \subseteq \mathcal{Y}_2 \subseteq \mathbb{C}^2$ such that $\det(J_{F,S,T,y_1,y_2}) > 0$ on $\mathcal{N}_2 \times \mathcal{Y}_2$.

Let $\mathcal{N} = \mathcal{N}_1 \cap \mathcal{N}_2$ and $\mathcal{Y} = \mathcal{Y}_1 \cap \mathcal{Y}_2$. Then

1. $\mathfrak{a} \times Q_c \subseteq \mathcal{N} \times \mathcal{Y}$
2. $F_{S,T}$ is analytic in $\mathcal{N} \times \mathcal{Y}$
3. $\det(J_{F,S,T,y_1,y_2}) > 0$ in $\mathcal{N} \times \mathcal{Y}$.

Consider some $(S_0,T_0) \in \mathfrak{a}$. By Corollary 6.3.2, $(\gamma_1(S_0,T_0), \gamma_2(S_0,T_0)) \in Q_c \subseteq \mathcal{Y}$. Hence $(S_0, T_0, \gamma_1(S_0,T_0), \gamma_2(S_0,T_0)) \in \mathcal{N} \times \mathcal{Y}$, so

$$\det(J_{F,S,T,y_1,y_2}(S_0, T_0, \gamma_1(S_0,T_0), \gamma_2(S_0,T_0))) > 0.$$

Then Theorem 7.6 of [FG02], the Analytic Implicit Function Theorem, implies $\gamma_1(S,T)$, $\gamma_2(S,T)$ (the solutions (y_1,y_2) to $F_{S,T}(S,T,y_1,y_2) = \vec{0}$) are analytic functions in a neighborhood of (S_0,T_0). Since $(S_0,T_0) \in \mathfrak{a}$ is arbitrary, we thus have γ_1, γ_2 are real analytic on $\mathfrak{a}$.

Note we have treated c as constant in the above discussion, but (γ_1,γ_2) being real analytic in c follows similarly since $F_{S,T}$ is real analytic in c. Apply the Analytic Implicit Function Theorem by introducing $c \in (2,4)$ analogous to the way we considered $(S,T) \in \mathfrak{a}$. □

6.6 w in terms of γ and r

For later use, we write a formula for w in terms of γ_1, γ_2, so it does not involve functions such as $\hat{\alpha}(r)$ which are defined by maximizing another function. Hence w can be evaluated directly by solving $F_{S,T} = 0$ for (γ_1, γ_2) without needing a maximization routine.

In Proposition 6.6.2, we will also use this to show $w(r)$ is real-analytic on $(0, 1)$.

Lemma 6.6.1. *Suppose $r \in (0, 1)$. Let $S = \sqrt{r}$ and $T = \sqrt{1-r}$, and γ_1, γ_2 be as in Equation (6.1.1). Then w can be expressed in the equivalent forms:*

$$\begin{aligned} w(r) &= -\frac{1}{2}cH(r) + r\ln\big(\eta(S\gamma_1)\gamma_1^2\big) + (1-r)\ln\big(\eta(T\gamma_2)\gamma_2^2\big) \\ &\quad - \ln(c) - cr\ln(\gamma_1) - c(1-r)\ln(\gamma_2) - \breve{\kappa}_c(1,1) \\ &= -\frac{1}{2}cH(r) + \ln\big(\eta(S\gamma_1)\gamma_1^2\big) - \ln(c) - cr\ln(\gamma_1) - c(1-r)\ln(\gamma_2) - \breve{\kappa}_c(1,1) \\ &= -\frac{1}{2}cH(r) + \ln\big(\eta(T\gamma_2)\gamma_2^2\big) - \ln(c) - cr\ln(\gamma_1) - c(1-r)\ln(\gamma_2) - \breve{\kappa}_c(1,1), \end{aligned}$$

where we note $\breve{\kappa}_c(1, 1)$ is a constant (function of c only) and recall:

$$H(r) := -r\ln(r) - (1-r)\ln(1-r), \qquad \eta(z) := \frac{e^z - 1}{z}.$$

Proof. By definitions from Section 3.3,

$$\tilde{w}_c(r,\alpha) = H(\alpha) - cH(r) + \breve{\kappa}_c(r,\alpha) + \breve{\kappa}_c(1-r, 1-\alpha) - \breve{\kappa}_c(1,1) \tag{6.6.1}$$

$$\breve{\kappa}_c(r,\alpha) = \alpha\ln(e^z - 1 - z) - cr\ln(z), \quad \text{with} \quad z := z(\alpha/(cr)) \tag{6.6.2}$$

$$z(v) := \nu^{-1}(v) = \text{inverse of } \nu(z) := \frac{e^z - 1 - z}{(e^z - 1)z}. \tag{6.6.3}$$

By definition, $w_c(r) = \tilde{w}_c(r, \hat{\alpha}(r))$, so by defining $\widehat{\kappa}_c(r) = \breve{\kappa}_c(r, \hat{\alpha}(r))$, we see

$$w_c(r) = H(\hat{\alpha}(r)) - cH(r) + \widehat{\kappa}_c(r) + \widehat{\kappa}_c(1-r) - \breve{\kappa}_c(1,1) \tag{6.6.4}$$

$$\widehat{\kappa}_c(r) = \hat{\alpha}(r)\ln(e^z - 1 - z) - cr\ln(z), \quad \text{with} \quad z := z(\hat{\alpha}(r)/(cr)). \tag{6.6.5}$$

For further simplification, we define $\widehat{\kappa}_c^*$

$$\widehat{\kappa}_c^*(r) := \hat{\alpha}(r)\ln\left(\frac{e^z - 1 - z}{\hat{\alpha}(r)}\right) - cr\ln\left(\frac{z}{\sqrt{r}}\right), \quad \text{with} \quad z := z(\hat{\alpha}(r)/(cr)). \tag{6.6.6}$$

This allows writing w_c in terms of $\widehat{\kappa}_c^*(r)$, and $\widehat{\kappa}_c^*(r)$ can be simplified by using $\hat{\alpha}(r) = cr\nu(z)$ with $\nu(z) = \frac{e^z - 1 - z}{(e^z - 1)z}$, so

$$w_c(r) = -\frac{1}{2}cH(r) + \widehat{\kappa}_c^*(r) + \widehat{\kappa}_c^*(1-r) - \breve{\kappa}_c(1,1) \tag{6.6.7}$$

$$\widehat{\kappa}_c^*(r) = \hat{\alpha}(r)\ln\left(\frac{(e^z - 1)z}{cr}\right) - cr\ln\left(\frac{z}{\sqrt{r}}\right), \quad \text{with} \quad z := z(\hat{\alpha}(r)/(cr)) \tag{6.6.8}$$

$$\widehat{\kappa}_c^*(r) = \hat{\alpha}(r)\ln\left(\eta(z)\frac{z^2}{cr}\right) - cr\ln\left(\frac{z}{\sqrt{r}}\right), \quad \text{with} \quad z := z(\hat{\alpha}(r)/(cr)). \tag{6.6.9}$$

Passing to γ_1, γ_2 by their definitions, we see

$$\widehat{\kappa}_c^*(r) = cr\nu(S\gamma_1)\ln\left(\eta(S\gamma_1)\frac{\gamma_1^2}{c}\right) - cr\ln(\gamma_1) \tag{6.6.10}$$

$$\widehat{\kappa}_c^*(1-r) = c(1-r)\nu(T\gamma_2)\ln\left(\eta(T\gamma_2)\frac{\gamma_2^2}{c}\right) - c(1-r)\ln(\gamma_2). \tag{6.6.11}$$

By Lemma 6.2.1,

$$\gamma_2^2\eta(T\gamma_2) = \gamma_1^2\eta(S\gamma_1) \tag{6.6.12}$$

$$(1-r)\nu(T\gamma_2) + r\nu(S\gamma_1) = \frac{1}{c}. \tag{6.6.13}$$

Hence

$$\begin{aligned}
&cr\nu(S\gamma_1)\ln\left(\eta(S\gamma_1)\frac{\gamma_1^2}{c}\right) + c(1-r)\nu(T\gamma_2))\ln\left(\eta(T\gamma_2)\frac{\gamma_2^2}{c}\right)\\
&= c(r\nu(S\gamma_1) + (1-r)\nu(T\gamma_2))\ln\left(\eta(S\gamma_1)\frac{\gamma_1^2}{c}\right)\\
&= \ln\left(\eta(S\gamma_1)\frac{\gamma_1^2}{c}\right).
\end{aligned}$$

That is a nice simplification which yields

$$w_c(r) = -\frac{1}{2}cH(r) + \ln\big(\eta(S\gamma_1)\gamma_1^2\big) - \ln(c) - cr\ln(\gamma_1) - c(1-r)\ln(\gamma_2) - \breve{\kappa}_c(1,1). \tag{6.6.14}$$

□

Due to the $H(r) = -r\ln(r) - (1-r)\ln(1-r)$ term, w is not real-analytic for $r \in [0,1]$. However, we can show it is real-analytic for $r \in (0,1)$.

Proposition 6.6.2. *The function w is a real-analytic function of $r \in (0,1)$ and extends continuously on $[0,1]$ with $w(0) = w(1) = 0$.*

Proof. Since γ_1, γ_2 are real-analytic functions under the change of variables with $(S,T) \in \mathfrak{a}$, we see γ_1, γ_2 are real-analytic functions of $r \in (0,1)$. Also, γ_1, γ_2 are continuous on $[0,1]$. Likewise, $\sqrt{r}$, $\sqrt{1-r}$, and $H(r)$ are real-analytic functions of $r \in (0,1)$ and continuous for $r \in [0,1]$.

Hence the formula in Lemma 6.6.1 writes w as a sum and product of compositions of real-analytic functions over appropriate domains. Hence w is real-analytic for $r \in (0,1)$. □

7 Combinatorics (bounds on c for two-cores): The big sum

We are now finished discussing the behavior of h_c and $\overline{g}_c$, so we proceed to proving the combinatorics and asymptotics that lead to h_c and $\overline{g}_c$ appearing in the first palce.

We begin by proving the main result of this thesis (Conjecture 1.2.1) along the lines indicated. The approach is based on analyzing the moment ratio

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2}.$$

and its asymptotics. This section devoted to deriving formulas for this ratio. Then later sections give asymptotic bounds.

In the first subsection, we derive a simple formula for $\mathbb{E}(N)$ which holds for general distributions of matrices. Formulas for the variance $\mathbb{E}(N^2)$ are harder to derive and much more complicated. We do this for the uniform distribution over the set $\Psi_{m,3n}$ of two-core 3-XOR-games as defined in Section 1.1.1, and we devote most of the section to these formulas and their properties.

7.1 First moment: $\mathbb{E}(N)$ and proof that $2 < c \leq 3$

Let $\#S = |S|$ denote the size of the set S. We will use $|S|$ usually except for the size of a set comprehension like

$$\#\{(\Gamma, z) \in \Psi_{m,3n} \times \mathbb{Z}_2^{3n} \mid \Gamma z = 0\},$$

where the $|\{\cdots\}|$ is less readable.

Lemma 7.1.1. *Let $G_{m,3n} \subseteq \mathbb{Z}_2^{m\times 3n}$ be a set of $m \times 3n$ binary matrices, and $\Theta_{m,3n} := G_{m,3n} \times \mathbb{Z}_2^m$.*

Suppose a random equation $\Gamma x = s$ is constructed by picking a pair (Γ, s) uniformly from $\Theta_{m,3n}$. Let the random variable $N = N(\Gamma, s)$ denote the number of binary solutions x to this equation. Then

$$\mathbb{E}(N) = 2^{3n-m}.$$

Proof.

$$\begin{aligned}
\mathbb{E}(N) &= |\Theta_{m,3n}|^{-1} \sum_{(\Gamma,s)\in\Theta_{m,3n}} N(\Gamma, s) && (7.1.1)\\
&= \frac{\sum_{(\Gamma,s)\in\Theta_{m,3n}} \#\{x \in \mathbb{Z}_2^{3n} \mid \Gamma x = s\}}{|\Theta_{m,3n}|} && (7.1.2)\\
&= \frac{\#\{(\Gamma, s, x) \in \Theta_{m,3n} \times \mathbb{Z}_2^{3n} \mid \Gamma x = s\}}{|\Theta_{m,3n}|} && (7.1.3)\\
&= \frac{\#\{(\Gamma, s, x) \in G_{m,3n} \times \mathbb{Z}_2^{m} \times \mathbb{Z}_2^{3n} \mid \Gamma x = s\}}{|G_{m,3n} \times \mathbb{Z}_2^m|} && (7.1.4)\\
&= \frac{\#\{(\Gamma, x) \in G_{m,3n} \times \mathbb{Z}_2^{3n}\}}{|G_{m,3n} \times \mathbb{Z}_2^m|} && (7.1.5)\\
&= \frac{|G_{m,3n} \times \mathbb{Z}_2^{3n}|}{|G_{m,3n} \times \mathbb{Z}_2^m|} = \frac{|G_{m,3n}| \cdot |\mathbb{Z}_2^{3n}|}{|G_{m,3n}| \cdot |\mathbb{Z}_2^m|} && (7.1.6)\\
&= \frac{2^{3n}}{2^m} = 2^{3n-m}. && (7.1.7)
\end{aligned}$$

This argument is effectively the same as a standard argument, see e.g. Remark 3 of Pittel-Sorkin ([PS16],[PS14]). □

7.1.1 Unsatisfiability with high probability when $c > 3$

Corollary 7.1.2. *Suppose $c > 3$. With the setup as in Lemma 7.1.1 the probability of there being a solution, $\Pr(N \geq 1)$, goes to 0 as $n \to \infty$ with $m = n(c + o(1))$. Hence any critical threshold must be at most 3.*

Proof. The first moment inequality says

$$\Pr(N \geq 1) \leq \mathbb{E}(N) = 2^{3n-m} = 2^{(3-c-o(1))n}.$$

If $c > 3$, then as $n \to \infty$, this yields $\mathbb{E}(N) \to 0$ and hence $\Pr(N \geq 1) \to 0$, i.e. there are no solutions. □

Note the above lemma and corollary does not require a 2–core structure or even a 3-XOR-game structure, but it does require the assignment vector (s in (Γ, s)) to be uniformly-distributed on $\mathbb{Z}_2^m$.

7.2 Second moment of the probability of a solution existing in terms of counting $\Gamma z = 0$

Lemma 7.2.1. *We assume the same setup as Lemma 7.1.1. Then*

$$\mathbb{E}(N^2) = 2^{3n} |\Theta_{m,3n}|^{-1} \ \#\{(\Gamma, z) \in G_{m,3n} \times \mathbb{Z}_2^{3n} \ \mid \ \Gamma z = 0\}.$$

Proof.

$$\begin{aligned}
\mathbb{E}(N^2) &= |\Theta_{m,3n}|^{-1} \sum_{(\Gamma,s)\in\Theta_{m,3n}} (N(\Gamma, s))^2 \\
&= |\Theta_{m,3n}|^{-1} \sum_{(\Gamma,s)\in\Theta_{m,3n}} \left(\#\{x \in \mathbb{Z}_2^{3n} \ \mid \ \Gamma x = s\}\right)^2 \\
&= |\Theta_{m,3n}|^{-1} \sum_{(\Gamma,s)\in\Theta_{m,3n}} \# \left(\{x \in \mathbb{Z}_2^{3n} \ \mid \ \Gamma x = s\} \times \{y \in \mathbb{Z}_2^{3n} \mid \ \Gamma y = s\}\right) \\
&= |\Theta_{m,3n}|^{-1} \sum_{(\Gamma,s)\in\Theta_{m,3n}} \#\{(x, y) \in \mathbb{Z}_2^{3n} \times \mathbb{Z}_2^{3n} \ \mid \ \Gamma x = s \text{ and } \Gamma y = s\} \\
&= |\Theta_{m,3n}|^{-1} \ \#\{(\Gamma, s, x, y) \in \Theta_{m,3n} \times \mathbb{Z}_2^{3n} \times \mathbb{Z}_2^{3n} \mid \ \Gamma x = s \text{ and } \Gamma y = s\} \\
&= |\Theta_{m,3n}|^{-1} \ \#\{(\Gamma, x, y) \in G_{m,3n} \times \mathbb{Z}_2^{3n} \times \mathbb{Z}_2^{3n} \ \mid \ \Gamma x = \Gamma y\} \\
&= |\Theta_{m,3n}|^{-1} \ \#\{(\Gamma, x, y) \in G_{m,3n} \times \mathbb{Z}_2^{3n} \times \mathbb{Z}_2^{3n} \ \mid \ \Gamma(x - y) = 0\} \\
&= |\Theta_{m,3n}|^{-1} \ \#\{(\Gamma, z, y) \in G_{m,3n} \times \mathbb{Z}_2^{3n} \times \mathbb{Z}_2^{3n} \ \mid \ \Gamma(x - y) = 0, x = y + z\} \\
&= 2^{3n} |\Theta_{m,3n}|^{-1} \ \#\{(\Gamma, z) \in G_{m,3n} \times \mathbb{Z}_2^{3n} \ \mid \ \Gamma z = 0\}
\end{aligned}$$

where we remind the addition and subtraction in $\mathbb{Z}_2^{3n}$ is modulo 2. □

Note the above lemma does not require a 2–core structure or even a 3-XOR-game structure.

7.3 Definition of 3-XOR-game and two-cores (most of this repeats intro)

Since we are now getting back to our game equations we recall basic definitions from the introduction, Section 1.1.1.

A **3-XOR-game matrix** is a matrix $\Gamma = (A\ B\ C) \in \mathbb{Z}_2^{m\times 3n}$, where $A, B, C \in \mathbb{Z}_2^{m\times n}$ are blocks with 1 one in each row (the rest of the entries being zero). Define a **two-core matrix** to be a matrix where each column has at least 2 ones. In particular, a **two-core 3-XOR-game matrix** Γ is a matrix in $\mathbb{Z}_2^{m\times 3n}$ satisfying the block structure $\Gamma = (A\ B\ C)$, such that each column has at least 2 ones.

Recall $\Psi_{m,3n}$ is the set of **two-core 3-XOR-games**, i.e. the set of pairs (Γ, s) such that Γ is a two-core 3-XOR-game matrix and $s \in \mathbb{Z}_2^m$. To ensure $\Psi_{m,3n}$ is nonempty, $m \geq 2n$ must hold by the following argument. The matrix Γ has m rows each with 3 ones, so it has exactly $3m$ ones total in the matrix. At the same time, each of the n columns must have at least 2 ones, so it must have at least $6n$ ones total. Hence $3m \geq 6n$, so $m \geq 2n$. Elsewhere in the thesis, this is realized as $c > 2$, which ensures $\mathcal{P}_c$ is nonempty.

7.4 Big nested sum for $\mathbb{E}(N^2)$ for a 2-core

Now we take up counting. Let $S_2(p, q)$ be the 2-associated Stirling numbers of the second kind (the Ward numbers), the number of ways to partition a set of size p into q subsets of size at least 2. For $m, n \in \mathbb{Z}_{\geq 1}$ and $u_0, u_1, u_2, u_3 \in \mathbb{Z}_{\geq 1}$ satisfying $m = u_0 + u_1 + u_2 + u_3$, and $a, b, c \in \{0, 1, 2, \ldots, n\}$, define:

$$\begin{aligned}\widehat{\mathsf{S}}_{m,n}(u_0, u_1, u_2, u_3, a, b, c) := \frac{m!}{u_0!u_1!u_2!u_3!} \times \\ S_2(u_0 + u_1, a)S_2(u_2 + u_3, n - a)\times \\ S_2(u_0 + u_2, b)S_2(u_1 + u_3, n - b)\times \\ S_2(u_0 + u_3, c)S_2(u_2 + u_3, n - c).\end{aligned}$$

Proposition 7.4.1. *If N is a random variable denoting the number of solutions to a random 3-XOR-game problem in $\Psi_{m,3n}$ (2-cores), then*

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} = S_2(m, n)^{-3} 2^{m-3n} \sum_{\substack{u_0+u_1+u_2+u_3=m \\ u_0,u_1,u_2,u_3\geq 0}} \sum_{a=0}^{n}\sum_{b=0}^{n}\sum_{c=0}^{n} \widehat{\mathsf{S}}_{m,n}(u_0, u_1, u_2, u_3, a, b, c).$$

Proof. Use Lemma 7.2.1 applied to $\Theta_{m,3n} = \Psi_{m,3n}$ to get:

$$\mathbb{E}(N^2) = 2^{3n}|\Psi_{m,3n}|^{-1}\ \#\{(\Gamma, z) \in \Psi_{m,3n} \times \mathbb{Z}_2^{3n} \mid \Gamma z = 0\}.$$

Then Lemma 7.4.2 and Lemma 7.4.3 finish the calculation of $\mathbb{E}(N^2)$.

Lemma 7.1.1 states $\mathbb{E}(N) = 2^{3n-m}$, finishing the calculation of $\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2}$. □

Lemma 7.4.2. $|\Psi_{m,3n}| = S_2(m, n)^3 n!^3 2^m$

Proof. In this proposition, Γ has the two-core 3-XOR-game structure $\Gamma = (A\ B\ C)$. For the A block:

1. Partition the m rows into n subsets of size at least 2: $S_2(m, n)$ ways

2. Order the subsets to get an assignment of 1s to columns: $n!$ ways

Hence there are $S_2(m,n)n!$ for the A block. The B and C blocks have the same choices independently, so there are $S_2(m,n)^3 n!^3$ choices for the two-core Γ matrix. Independent of the rest of the choices, there are 2^m possible s vectors, completing the count. □

Lemma 7.4.3.

$$\#\{(\Gamma, z) \in \Psi_{m,3n} \times \mathbb{Z}_2^{3n} \mid \Gamma z = 0\} = \\ n!^3 \sum_{\substack{u_0+u_1+u_2+u_3=m \\ u_0,u_1,u_2,u_3 \geq 0}} \sum_{a=0}^{n} \sum_{b=0}^{n} \sum_{c=0}^{n} \widehat{\mathsf{S}}_{m,n}(u_0, u_1, u_2, u_3, a, b, c).$$

Proof. Given a vector $z \in \mathbb{Z}_2^{3n}$, let $I(z)$ denote the set of indices i where $z_i = 1$, so $|I(z)|$ is the number of ones in z. For any vector $z \in \mathbb{Z}_2^{3n}$, split it into three blocks of size n, denoted by $z = (z_A \; z_B \; z_C)$ corresponding to the game structure of Γ. Let $a = |I(z_A)|$, $b = |I(z_B)|$, and $c = |I(z_C)|$, so $a, b, c \in \{0, 1, 2, \ldots, n\}$ are the number of ones in each block of the vector z.

Define Γ_z to be the submatrix of Γ obtained by selecting its columns given by $I(z)$ (so Γ_z are precisely those columns multiplied by 1 when computing Γz, while the rest of the columns are multiplied by 0). Partition Γ_z into blocks as $\Gamma_z =: (A_z \; B_z \; C_z)$ based on which block in $\Gamma = (A \; B \; C)$ each column came from. Then A_z has a columns, B_z has b columns, and C_z has c columns.

Let Γ_z^j be the jth row of the matrix Γ_z. Suppose $(\Gamma, z) \in \Psi_{m,3n} \times \mathbb{Z}_2^{3n}$ is a 3XOR game matrix. Then $\Gamma z = 0$ iff each row of Γ_z has one of the following four forms (with respect to the $\Gamma_z := (A_z \; B_z \; C_z)$ block partitioning):

(I) $\Gamma_z^j = (0 \; 0 \; 0)$.

(II) $\Gamma_z^j = (0 \; e_1 \; e_1)$.

(III) $\Gamma_z^j = (e_1 \; 0 \; e_1)$.

(IV) $\Gamma_z^j = (e_1 \; e_1 \; 0)$.

where each e_1 stands for a block row vector with exactly one 1 (with potentially different sizes depending on a, b, c), and the 0 is a zero block row vector.

Let u_0, u_1, u_2, u_3 respectively count the number of rows Γ^j where the sum is satisfied in each of these four forms. Since $\Gamma^j z = 0$ holds for each of the m rows of Γ, and the four forms ((I), (II), (III), (IV)) are mutually exclusive, we have

$$u_0 + u_1 + u_2 + u_3 = m.$$

Hence every (Γ, z) pair with $\Gamma z = 0$ has corresponding $a, b, c \in \{0, 1, 2, \ldots, n\}$ and $u_0, u_1, u_2, u_3 \geq 0$ with $u_0 + u_1 + u_2 + u_3 = m$.

We count the number of possible pairs (Γ, z) with $\Gamma z = 0$ given (a, b, c) and (u_0, u_1, u_2, u_3) satisfying these constraints by a procedure constructing all such (Γ, z). Here is an overview of the construction:

1. Pick $z \in \mathbb{Z}_2^{3n}$.

2. Pick which rows of Γ_z are of each form (I), (II), (III), (IV). For each row of each block A, B, C, this fixes whether the 1 is in the submatrix Γ_z (the columns corresponding to the 1s of z), or the 1 is the in the submatrix $\Gamma_{\overline{z}}$ (the columns corresponding to the 0s of z).

3. Based on z and the row selection, now we build the matrix $\Gamma = (A\ B\ C)$ satisfying all necessary constraints.

The number of ways to pick such (Γ, z) is then the product of the number of choices in each step, since the counts in the steps only depend on (a, b, c) and (u_0, u_1, u_2, u_3), not the particular choices in the earlier steps.

The detailed procedure follows:

1. Pick $z \in \mathbb{Z}_2^{3n}$ by picking which entries of z are 1 (the rest being 0):

   (a) choose a entries of z_A to be 1: $\binom{n}{a}$ ways,

   (b) choose b entries of z_B to be 1: $\binom{n}{b}$ ways,

   (c) choose c entries of z_C to be 1: $\binom{n}{c}$ ways.

   Hence there are a total of $\binom{n}{a}\binom{n}{b}\binom{n}{c}$ ways to pick z.

2. We will build the two-core 3-XOR-Game matrix $\Gamma \in \mathbb{Z}_2^{m\times 3n}$ by building two submatrices

$$\Gamma_z = (A_z, B_z, C_z) \in \mathbb{Z}_2^{m\times(a+b+c)}, \quad \Gamma_{\overline{z}} = (A_{\overline{z}}, B_{\overline{z}}, C_{\overline{z}}) \in \mathbb{Z}_2^{m\times((n-a)+(n-b)+(n-c))},$$

   and threading them back together. The submatrix Γ_z consists of the columns of Γ corresponding to 0 entries of z, and the submatrix $\Gamma_{\overline{z}}$ consists of the columns of Γ corresponding to 1 entries of z.

3. Pick which rows of Γ_z are going to be of each form (I), (II), (III), (IV) subject to the constraint that u_0 rows are of form (I), u_1 rows are of form (II), u_2 rows are of form (III), and u_3 rows are of form (IV). There are $\dfrac{m!}{u_0!u_1!u_2!u_3!}$ ways to do this.

4. Consider the jth row of A. It has exactly one 1 by virtue of being a block of a 3-XOR-game matrix. If the 1 is in a column contained in A_z, then row j of Γ_z must be of the form $(e_1\ 0\ e_1)$ (III) or $(e_1\ e_1\ 0)$ (IV). Otherwise, the 1 is in a column contained in $A_{\overline{z}}$, and row j of Γ_z is of the form $(0\ 0\ 0)$ (I) or $(0\ e_1\ e_1)$ (II).

   There are $u_0 + u_1$ rows of the form (I) or (II), and $n - a$ columns in $A_{\overline{z}}$. Each column needs at least 2 ones, so there are $S_2(u_0 + u_1, n - a)\,(n - a)!$ ways to place the 1s into $A_{\overline{z}}$.

   There are $u_2 + u_3$ rows of the form (III) or (IV), and a columns in A_z. Thus there are $S_2(u_2 + u_3, a)\,a!$ ways to place the 1s into A_z

   Since these counts are independent, there are

$$S_2(u_0 + u_1, n - a)\,(n - a)!\,S_2(u_2 + u_3, a)\,a!$$

   ways to pick the block A.

5. By the same logic, there are $S_2(u_0+u_2, n-b)\,(n-b)!\,S_2(u_1+u_3, b)\,b!$ ways to pick the block B.

6. By the same logic, there are $S_2(u_0+u_3, n-c)\,(n-c)!\,S_2(u_1+u_2, c)\,c!$ ways to pick the block C.

All of these counts are independent, so they can be multiplied to give the total count for each (a,b,c) and (u_0,u_1,u_2,u_3). Then summing over the possible (a,b,c) and (u_0,u_1,u_2,u_3) gives the total number of pairs (Γ, z) with $\Gamma z = 0$:

$$\begin{aligned}
\#\{(\Gamma, z) \in \Psi_{m,3n} \times \mathbb{Z}_2^{3n} \mid \Gamma z = 0\} = \\
\sum_{\substack{u_0+u_1+u_2+u_3=m \\ u_0,u_1,u_2,u_3 \geq 0}} \sum_{a=0}^{n}\sum_{b=0}^{n}\sum_{c=0}^{n} \binom{n}{a}\binom{n}{b}\binom{n}{b} \frac{m!}{u_0!u_1!u_2!u_3!} \times \\
S_2(u_0+u_1, n-a)\,(n-a)!\,S_2(u_2+u_3, a)\,a! \times \\
S_2(u_0+u_2, n-b)\,(n-b)!\,S_2(u_1+u_3, b)\,b! \times \\
S_2(u_0+u_3, n-c)\,(n-c)!\,S_2(u_2+u_3, c)\,c!.
\end{aligned}$$

To align with convention from [DM02a], we interchange the roles of a and $n-a$ (respectively b and $n-b$, resp. c and $n-c$).

$$\begin{aligned}
\#\{(\Gamma, z) \in \Psi_{m,3n} \times \mathbb{Z}_2^{3n} \mid \Gamma z = 0\} = \\
\sum_{\substack{u_0+u_1+u_2+u_3=m \\ u_0,u_1,u_2,u_3 \geq 0}} \sum_{a=0}^{n}\sum_{b=0}^{n}\sum_{c=0}^{n} \binom{n}{a}\binom{n}{b}\binom{n}{b} \frac{m!}{u_0!u_1!u_2!u_3!} \times \\
S_2(u_0+u_1, a)\,a!\,S_2(u_2+u_3, n-a)\,(n-a)! \times \\
S_2(u_0+u_2, b)\,b!\,S_2(u_1+u_3, n-b)\,(n-b)! \times \\
S_2(u_0+u_3, c)\,c!\,S_2(u_2+u_3, n-c)\,(n-c)!.
\end{aligned}$$

Simplifying $\binom{n}{a}a!(n-a)! = n!$ (and likewise for b, c) yields the result (Lemma 7.4.3). □

7.5 Reparameterizing the Big Sum

Define $\mathcal{I}_m = \{0, \frac{1}{m}, \frac{2}{m}, \ldots, 1\}$ and $\mathcal{I}_n = \{0, \frac{1}{n}, \frac{2}{n}, \ldots, 1\}$. In notation that will be motivated in the proof of Proposition 7.5.1, we define the summand $\mathscr{S}_{m,n}$ on vectors of rational numbers $\vec{r} := (r_1, r_2, r_3) \in \mathcal{I}_m^3 \cap \mathcal{T}$ and $\vec{\alpha} := (\alpha_1, \alpha_2, \alpha_3) \in \mathcal{I}_n^3$ as:

$$\begin{aligned}
\mathscr{S}_{m,n}(\vec{r}, \vec{\alpha}) := \mathscr{S}_{m,n}(r_1, r_2, r_3, \alpha_1, \alpha_2, \alpha_3) := \mathrm{mc}(r_1, r_2, r_3) \times \\
S_2(mr_1, n\alpha_1) S_2(m(1-r_1), n(1-\alpha_1)) \times \\
S_2(mr_2, n\alpha_2) S_2(m(1-r_2), n(1-\alpha_2)) \times \\
S_2(mr_3, n\alpha_3) S_2(m(1-r_3), n(1-\alpha_3))
\end{aligned}$$

where

$$\mathrm{mc}(r_1, r_2, r_3) := \frac{m!}{u_0!u_1!u_2!u_3!} \qquad \text{with}$$

$$\begin{aligned}
u_0 &= mt_0 = m(r_1+r_2+r_3-1)/2 \qquad & u_1 &= mt_1 = m(r_1-r_2-r_3+1)/2 \\
u_2 &= mt_2 = m(-r_1+r_2-r_3+1)/2 \qquad & u_3 &= mt_3 = m(-r_1-r_2+r_3+1)/2.
\end{aligned}$$

Define the matrix A_c as follows:

$$A_c \coloneqq \begin{bmatrix} 1/c & 1/c & 0 & & & \\ 1/c & 0 & 1/c & & & \\ 0 & -1/c & -1/c & & & \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & 1 \end{bmatrix}. \tag{7.5.1}$$

Define the lattice $\mathscr{L}_{m,n}$ by the following, where $c = m/n$,

$$\mathscr{L}_{m,n} \coloneqq \frac{1}{n} A_c \mathbb{Z}^6 + \left[0, 0, 1, 0, 0, 0\right]^\top. \tag{7.5.2}$$

As a remark, $\mathscr{L}_{m,n}$ is a subset of an axis-aligned lattice:

$$\mathscr{L}_{m,n} = \left\{ (\vec{r}, \vec{\alpha}) \in \frac{1}{m}\mathbb{Z}^3 \times \frac{1}{n}\mathbb{Z}^3 \mid m(r_1 + r_2 + r_3) \text{ even} \right\}. \tag{7.5.3}$$

Proposition 7.5.1. *If N is a random variable denoting the number of solutions to a random problem $(\Gamma, s) \in \Psi_{m,3n}$ (two-core 3-XOR-games), then*

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} = S_2(m,n)^{-3} 2^{m-3n} \sum_{(\vec{r},\vec{\alpha}) \in \mathscr{L}_{m,n} \cap (\mathcal{T} \times [0,1]^3)} \mathscr{S}_{m,n}(\vec{r}, \vec{\alpha}). \tag{7.5.4}$$

Proof. Start from Proposition 7.4.1:

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} = S_2(m,n)^{-3} 2^{m-3n} \sum_{\substack{u_0+u_1+u_2+u_3=m \\ u_0,u_1,u_2,u_3 \geq 0}} \sum_{a=0}^{n} \sum_{b=0}^{n} \sum_{c=0}^{n} \widehat{\mathsf{S}}_{m,n}(u_0, u_1, u_2, u_3, a, b, c).$$

Using integers (a, b, c) made the combinatorics clear, but it is more convenient to normalize the values to $[0, 1]$. Define $\alpha_1, \alpha_2, \alpha_3$ as

$$\vec{\alpha} \coloneqq (\alpha_1, \alpha_2, \alpha_3) \coloneqq (a, b, c)/n.$$

Applying this substitution yields

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} = S_2(m,n)^{-3} 2^{m-3n} \sum_{\substack{u_0+u_1+u_2+u_3=m \\ u_0,u_1,u_2,u_3 \geq 0}} \sum_{(\alpha_1,\alpha_2,\alpha_3) \in \mathcal{I}_n^3} \widehat{\mathsf{S}}_{m,n}(u_0, u_1, u_2, u_3, n\alpha_1, n\alpha_2, n\alpha_3).$$

The S_2 terms in $\widehat{\mathsf{S}}_{m,n}$ involve arguments such as $u_0 + u_1$ and $u_0 + u_2$, so we will reparameterize to $r_i \in [0, 1]$ given by:

$$\begin{aligned} r_1 &= \frac{1}{m}(u_0 + u_1) \\ r_2 &= \frac{1}{m}(u_0 + u_2) \\ r_3 &= \frac{1}{m}(u_0 + u_3) = 1 - \frac{1}{m}(u_1 + u_2). \end{aligned}$$

Hence we have the relationship

$$\begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} = \begin{bmatrix} 1/m & 1/m & 0 \\ 1/m & 0 & 1/m \\ 0 & -1/m & -1/m \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}.$$

The overall change of variables is the following, where $c = m/n$,

$$\begin{bmatrix} r_0 \\ r_1 \\ r_2 \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} = \frac{1}{n} A_c \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ a \\ b \\ c \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

Since $0 \leq u_0 + u_1 + u_2 \leq m = cn$ and $0 \leq a, b, c \leq n$, we have $(r_0, r_1, r_2) \in \mathcal{T}$ and $(\alpha_1, \alpha_2, \alpha_3) \in [0,1]^3$. Hence the summation terms are given by precisely $\mathscr{L}_{m,n} \cap (\mathcal{T} \times [0,1]^3)$, yielding

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} = S_2(m,n)^{-3} 2^{m-3n} \sum_{(\vec{r},\vec{\alpha}) \in \mathscr{L}_{m,n} \cap (\mathcal{T} \times [0,1]^3)} \mathscr{S}_{m,n}(\vec{r}, \vec{\alpha}). \tag{7.5.5}$$

□

7.6 Introducing parallelogram $\mathcal{P}_c^{0,1}$ and polytope $\mathcal{U}_c^{01}$

Proposition 7.5.1 introduced the parameters $\vec{r}$ and $\vec{\alpha}$ by a change of variables. Recall $\vec{r}$ must lie within the tetrahedron $\mathcal{T}$ defined in Equation (2.1.1), and $\vec{\alpha}$ lies arbitrarily within the cube $[0,1]^3$. However, we will see that the summand $\breve{\mathscr{S}}_{m,n}$ is identically zero except on a certain region. For approximation purposes, it will be useful to constrain $\vec{\alpha}$ to lie in the region in which $\breve{\mathscr{S}}_{m,n}$ can be nonzero.

We begin this topic by defining an essential parallelogram. For each real $c > 2$, define the parallelogram $\mathcal{P}_c^{0,1}$, depicted in Figure 7.1 as

$$\mathcal{P}_c^{0,1} := \{(r,\alpha) \in (0,1)^2 \mid \alpha \leq \frac{c}{2} r,\ 1 - \alpha \leq \frac{c}{2}(1-r)\} \cup \{(0,0),(1,1)\}. \tag{7.6.1}$$

Note the parallelogram $\mathcal{P}_c$ from Section 3.2 is the interior of $\mathcal{P}_c^{0,1}$.

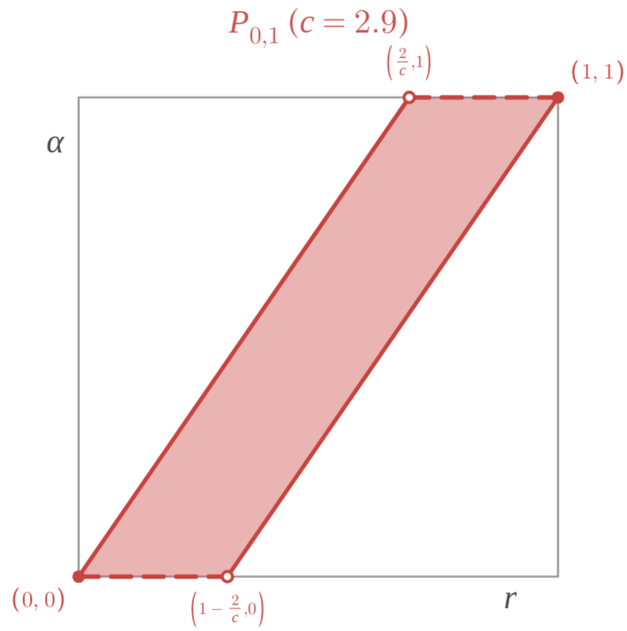

Figure 7.1: $\mathcal{P}_c^{0,1}$ at $c = 2.9$

Lemma 7.6.1. *If* $(r, \alpha) \notin \mathcal{P}_c^{0,1}$ *and* $c = m/n$*, then* $S_2(mr, n\alpha)\, S_2(m(1-r), n(1-\alpha)) = 0$.

Corollary 7.6.2. *Suppose* $(r_1, r_2, r_3, \alpha_1, \alpha_2, \alpha_3) \in [0, 1]^6$*. If* $(r_j, \alpha_j) \notin \mathcal{P}_c^{0,1}$ *for some* $j \in \{1, 2, 3\}$*, then* $\breve{\mathscr{S}}_{m,n}(r_1, r_2, r_3, \alpha_1, \alpha_2, \alpha_3) = 0$.

Proof. For $p, q \geq 0$ integers, if $p < 2q$, then $S_2(p, q) = 0$ since a set with less than $2q$ elements cannot be partitioned into q parts of size at least 2. If $\alpha > \frac{c}{2}r$ or $1 - \alpha > \frac{c}{2}(1 - r)$, then cross-multiplying gives $mr < 2n\alpha$ or $m(1 - r) < 2n(1 - \alpha)$. Thus in these cases,

$$S_2(mr, n\alpha)\, S_2(m(1 - r), n(1 - \alpha)) = 0.$$

For $p, q \geq 0$ integers, if $q = 0$ and $p > 0$, then $S_2(p, q) = 0$ by definition since a set with $p > 0$ elements cannot be partitioned into 0 parts. Hence, if ($\alpha = 0$ and $r > 0$) or ($\alpha = 1$ and $r < 1$), then

$$S_2(mr, n\alpha)\, S_2(m(1 - r), n(1 - \alpha)) = 0.$$

This finishes the proof, since $\mathcal{P}_c^{0,1}$ as defined above is also given by

$$\begin{aligned} \mathcal{P}_c^{0,1} &:= ([0, 1] \times [0, 1]) \setminus \mathcal{Q}_c, \qquad \text{where} \\ \mathcal{Q}_c &:= \{(r, \alpha) \mid \alpha > \frac{c}{2}r\} \,\cup\, \{(r, \alpha) \mid 1 - \alpha_j > \frac{c}{2}(1 - r_j)\} \\ &\quad \cup \{(r, 0) \mid r > 0\} \,\cup\, \{(r, 1) \mid r < 1\} \end{aligned}$$

where we just showed that if $(r, \alpha) \in \mathcal{Q}_c$, then

$$S_2(mr, n\alpha)\, S_2(m(1 - r), n(1 - \alpha)) = 0.$$

The corollary follows from $\breve{\mathscr{S}}_{m,n}(\vec{r}, \vec{\alpha})$ being a product of terms including

$$S_2(mr_j, n\alpha_j)\, S_2(m(1 - r_j), n(1 - \alpha_j)) = 0.$$

If any term is zero, then the product is zero, so if $(r_j, \alpha_j) \in \mathcal{Q}_c$ for some $j \in \{1, 2, 3\}$, then $\breve{\mathscr{S}}_{m,n}(\vec{r}, \vec{\alpha}) = 0$. □

Define the convex 6-polytope $\mathcal{U}_c^{01}$:

$$\mathcal{U}_c^{01} = \{(r_1, r_2, r_3, \alpha_1, \alpha_2, \alpha_3) \in \mathcal{T} \times [0, 1]^3 \mid (r_1, \alpha_1) \in \mathcal{P}_c^{0,1}, (r_2, \alpha_2) \in \mathcal{P}_c^{0,1}, (r_3, \alpha_3) \in \mathcal{P}_c^{0,1}\}.. \tag{7.6.2}$$

When working with the discrete grid, we will use

$$\mathcal{U}_{m,n}^{01} := \mathcal{U}_c^{01} \cap \mathscr{L}_{m,n} \tag{7.6.3}$$

where $\mathscr{L}_{m,n}$ is defined in Equation (7.5.2).

Lemma 7.6.3.

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} = S_2(m, n)^{-3} 2^{m-3n} \sum_{(\vec{r},\vec{\alpha}) \in \mathcal{U}_{m,n}^{01}} \mathscr{S}_{m,n}(\vec{r}, \vec{\alpha}).$$

Proof. Start from Proposition 7.5.1, which states

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} = S_2(m, n)^{-3} 2^{m-3n} \sum_{(\vec{r},\vec{\alpha}) \in \mathscr{L}_{m,n} \cap (\mathcal{T} \times [0,1]^3)} \mathscr{S}_{m,n}(\vec{r}, \vec{\alpha}). \tag{7.6.4}$$

Then Lemma 7.6.1 states $\mathscr{S}_{m,n}(\vec{r}, \vec{\alpha}) = 0$ if $(r_j, \alpha_j) \notin \mathcal{P}_c^{0,1}$ for some $j = 1, 2, 3$. This finishes the proof by definition of $\mathcal{U}_c^{01}$ since both sums add the same nonzero terms. □

Corollary 7.6.4. *To simplify notation for later, we introduce the full summand:*

$$\breve{\mathscr{S}}_{m,n}(\vec{r}, \vec{\alpha}) := S_2(m, n)^{-3} 2^{m-3n} \mathscr{S}_{m,n}(\vec{r}, \vec{\alpha}).$$

Hence

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} = \sum_{(\vec{r},\vec{\alpha}) \in \mathcal{U}_{m,n}^{01}} \breve{\mathscr{S}}_{m,n}(\vec{r}, \vec{\alpha}).$$

8 Stirling/Binomial approximations approximations to the summand ($\breve{\mathscr{S}}_{m,n}$)

In this section, we give ultimately give asymptotic approximations to the summand $\breve{\mathscr{S}}_{m,n}$ from Corollary 7.6.4, as $n \to \infty$ with $m = cn$ for fixed $c > 2$. En route, we describe the asymptotics of various functions which are factors of $\breve{\mathscr{S}}_{m,n}$, namely, the multichoose function, S_2, and products of these.

The discussion is complicated by issues of uniformity of convergence of the asymptotic expansion of S_2 which we use from the literature. We issue a warning that while pointwise convergence is proved (we checked the proof) and uniform convergence is asserted we did not extract a careful proof from the literature. Next, we give a description of these convergence issues.

Suppose a positive-valued function $f(n, \alpha)$ is defined for all positive integers n and α in some set. There are many ways in which another function $g(n, \alpha)$ can be an approximation to $f(n, \alpha)$, and we consider a few. Let $\sigma(n, \alpha) = \frac{g(n,\alpha)}{f(n,\alpha)}$ be the approximation ratio.

1. **Pointwise convergent**: For fixed α, then $\sigma \to 1$ as $n \to \infty$
2. **Uniformly bounded error**: There exists upper and lower bounds $0 < L < U < \infty$ such that $L \leq \sigma \leq U$ for all n, α.
3. **Uniformly convergent in** α: There exists upper and lower bounds $0 < L(n) < U(n) < \infty$ such that $L(n) \leq \sigma \leq U(n)$ for all n, α; and $L(n) \to 1$ and $U(n) \to 1$ as $n \to \infty$.

Note "Uniformly convergent in α" implies the other two, but neither "Pointwise convergent" nor "Uniformly-bounded error' implies the others.

This section begins with subsections which provide the asymptotics for basic factors of $\breve{\mathscr{S}}_{m,n}$. Then Proposition 8.3.1 combines these.

8.1 Stirling-type approximation to multinomial coefficients

We give a Stirling asymptotic the multinomial coefficient, together with lower and upper bounds. This Stirling-type approximation relies on the **entropy function** H, recalled from Section 3.3:

$$H(t_0, t_1, t_2, t_3) := -t_0 \ln(t_0) - t_1 \ln(t_1) - t_2 \ln(t_2) - t_3 \ln(t_3) \tag{8.1.1}$$

$$H(x) := -x \ln(x) - (1-x) \ln(1-x) \tag{8.1.2}$$

where we define (by continuity) $-x\ln(x) = 0$ at $x = 0$. Define the **shrunk tetrahedron** in barycentric coordinates by

$$\mathcal{T}_{\text{bary}}^{1/12} := \{(t_0, t_1, t_2, t_3) \mid t_0 + t_1 + t_2 + t_3 = 1,\ t_i > \frac{1}{12},\ i \in \{0, 1, 2, 3\}\}. \tag{8.1.3}$$

The motivation of introducing $\mathcal{T}_{\text{bary}}^{1/12}$ is to have a region upon which the asymptotics are uniformly convergent. It could be replaced with any compact subset of $\mathcal{T}$, for example, but we stick with $\mathcal{T}_{\text{bary}}^{1/12}$ for concreteness.

For later usage, we define $\mathcal{T}^{1/12}$ in non-barycentric coordinates by way of the coordinates introduced in Equation (2.1.1) as

$$\mathcal{T}^{1/12} := \{\vec{r} \in \mathcal{T} \mid (t_0(\vec{r}), t_1(\vec{r}), t_2(\vec{r}), t_3(\vec{r})) \in \mathcal{T}_{\text{bary}}^{1/12}\}. \tag{8.1.4}$$

Proposition 8.1.1. *Fix positive rationals t_0, t_1, t_2, t_3 satisfying $t_0 + t_1 + t_2 + t_3 = 1$. As $m \to \infty$ such that $m, t_0 m, t_1 m, t_2 m, t_3 m$ are positive integers, we have*

$$\binom{m}{t_0 m, t_1 m, t_2 m, t_3 m} \sim e^{H(t_0,t_1,t_2,t_3)m} \sqrt{\frac{1}{t_0 t_1 t_2 t_3 (2\pi m)^3}}. \tag{8.1.5}$$

Furthermore, the asymptotic approximation in Equation (8.1.5) *is uniformly convergent over $\mathcal{T}_{bary}^{1/12}$ as $m \to \infty$. The approximation also has uniformly bounded error for all m, t_0, t_1, t_2, t_3 satisfying the hypothesis.*

Proof. We omit the proof because it is the same as for the following Lemma 8.1.2, but with more factorials multiplied.

The shrunk tetrahedron $\mathcal{T}_{\text{bary}}^{1/12}$ comes into play because the error bound comes from the factorial error bounds. By imposing $t_i > \frac{1}{12}$, we get $mt_i > \frac{1}{12}m$, so the Stirling approximation for $(mt_i)!$ is uniformly convergent as $m \to \infty$. □

The following lemma gives bounds on the approximation which are a bit looser than those in Theorem 2.6 [Stă01]. Our proof is simpler, so we include it; also being self-contained is a convenience.

Lemma 8.1.2. *Fix rational $t \in (0,1)$. As $m \to \infty$ such that $m, mt, m(1-t)$ are positive integers, we have*

$$\binom{m}{tm} \sim e^{H(t)m} \sqrt{\frac{1}{t(1-t)(2\pi m)}}. \tag{8.1.6}$$

Furthermore, the asymptotic approximation in Equation (8.1.6) is uniformly convergent over $t \in \left(\frac{1}{12}, \frac{11}{12}\right)$ as $m \to \infty$. The approximation also has uniformly bounded error for all m, t satisfying the hypothesis.

Proof. Define $\sigma^!_n$ as the approximation ratio of the Stirling factorial approximation:

$$n! = \sqrt{2\pi n}\left(\frac{n}{e}\right)^n \sigma^!_n. \tag{8.1.7}$$

Robbins[Rob55] bounds this ratio by

$$\frac{1}{12n+1} < \ln\left(\sigma^!_n\right) < \frac{1}{12n}.$$

For $n \geq 1$, we have $1 \leq e^{1/(12n+1)}$, so

$$\sigma^!_n \in \left(1, e^{1/(12n)}\right).$$

Hence

$$\begin{aligned}
\binom{m}{tm} &= \frac{m!}{(tm)!((1-t)m)!} \\
&= \frac{\sigma^!_m}{\sigma^!_{tm}\sigma^!_{(1-t)m}} \frac{\sqrt{2\pi m}(m/e)^m}{\sqrt{2\pi tm}(tm/e)^{tm}\sqrt{2\pi(1-t)m}((1-t)m/e)^{(1-t)m}} \\
&= \sigma_{t,m}\frac{1}{\sqrt{2\pi mt(1-t)}}\frac{1}{t^{tm}(1-t)^{(1-t)m}} \\
&= \sigma_{t,m}\frac{1}{\sqrt{2\pi mt(1-t)}}e^{H(t)m}
\end{aligned}$$

where we let

$$\sigma_{t,m} = \frac{\sigma^!_m}{\sigma^!_{tm}\sigma^!_{(1-t)m}} \in \left(\frac{1}{e^{1/(12mt)}e^{1/(12m(1-t))}}, e^{1/(12m)}\right).$$

In particular, for $t \in \left(\frac{1}{12}, \frac{11}{12}\right)$, we have $12t, 12(1-t) \geq 1$, so

$$\ln(\sigma_{t,m}) \in \left(-\frac{2}{m}, \ \frac{1}{12m}\right).$$

Hence as $m \to \infty$, then $\sigma_{t,m} \to 1$ uniformly for $t \in \left(\frac{1}{12}, \frac{11}{12}\right)$.

For all m, t satisfying the hypothesis, $m, mt, m(1-t) \geq 1$, so

$$\sigma^!_m, \sigma^!_{tm}, \sigma^!_{(1-t)m} \in \left(1, e^{1/12}\right)$$

which yields a uniform bound given by

$$\sigma_{t,m} \in \left(e^{-1/6}, e^{1/12}\right).$$

Hence the approximation Equation (8.1.6) has uniformly bounded error for all m, t satisfying the hypothesis. □

The next lemma treats a ratio of binomial coefficients which appears in the big summand $\breve{\mathscr{S}}_{m,n}$. To state it, let $\mathcal{P}_c^{1/12} \subseteq \mathcal{P}_c$ be the shrunk parallelogram, given by

$$\mathcal{P}_c^{1/12} := \left\{ (r,\alpha) \in \mathcal{P}_c \mid r, \alpha \in \left(\frac{1}{12}, \frac{11}{12}\right), \frac{cr-2\alpha}{c-2} \in \left(\frac{1}{12}, \frac{11}{12}\right) \right\}.$$

As with $\mathcal{T}_{\text{bary}}^{1/12}$, this is introduced to provide a concrete region upon which convergence is uniform for upcoming approximations.

In the upcoming proofs, it is useful to factor $\widetilde{g}_c$ as

$$\widetilde{g}_c(r,\alpha) = \widetilde{g}_c^{main}(r,\alpha) \frac{\underline{\breve{g}}_c(r,\alpha)\underline{\breve{g}}_c(1-r,1-\alpha)}{\underline{\breve{g}}_c(1,1)}, \quad \text{where we define} \tag{8.1.8}$$

$$\underline{\breve{g}}_c(r,\alpha) := \frac{1}{cr}\sqrt{\frac{\alpha(cr-2\alpha)}{-z\nu'(z)}} \text{ with } z = z(\alpha/(cr)) \tag{8.1.9}$$

$$\widetilde{g}_c^{main}(r,\alpha) = \frac{1}{\sqrt{2\pi}} \frac{\sqrt{cr(1-r)}}{\sqrt{\alpha(1-\alpha)}\sqrt{(cr-2\alpha)(1-\frac{cr-2\alpha}{c-2})}}. \tag{8.1.10}$$

Simplification verifies this as equivalent to the previous definition of $\widetilde{g}_c$ in Equation (3.3.6):

$$\begin{aligned}
\widetilde{g}_c(r,\alpha) &= \frac{1}{\sqrt{2\pi n}} \frac{\sqrt{cr(1-r)}}{\sqrt{\alpha(1-\alpha)}\sqrt{(cr-2\alpha)(1-\frac{cr-2\alpha}{c-2})}} \frac{\underline{\breve{g}}_c(r,\alpha)\underline{\breve{g}}_c(1-r,1-\alpha)}{\underline{\breve{g}}_c(1,1)} \\
&= \frac{1}{\sqrt{2\pi n}} \frac{\sqrt{cr(1-r)}}{\sqrt{\alpha(1-\alpha)}\sqrt{(cr-2\alpha)(1-\frac{cr-2\alpha}{c-2})}} \frac{\frac{1}{cr}\sqrt{\frac{\alpha(cr-2\alpha)}{-z_1\nu'(z_1)}}\frac{1}{c(1-r)}\sqrt{\frac{(1-\alpha)(c(1-r)-2(1-\alpha))}{-z_2\nu'(z_2)}}}{\frac{1}{c}\sqrt{\frac{c-2}{-z_0\nu'(z_0)}}} \\
&= \frac{1}{\sqrt{2\pi n}} \frac{1}{\sqrt{(1-\frac{cr-2\alpha}{c-2})}} \frac{\frac{1}{\sqrt{cr(1-r)}}\sqrt{\frac{1}{-z_1\nu'(z_1)}}\sqrt{\frac{(c(1-r)-2(1-\alpha))}{-z_2\nu'(z_2)}}}{\sqrt{\frac{c-2}{-z_0\nu'(z_0)}}} \\
\widetilde{g}_c(r,\alpha) &= \sqrt{\frac{-z_0\nu'(z_0)}{z_1\nu'(z_1)z_2\nu'(z_2)}}\sqrt{\frac{1}{2c\pi nr(1-r)}}.
\end{aligned}$$

Lemma 8.1.3. *Fix rational $c > 2$ and let $(r,\alpha) \in \mathcal{P}_c$. As $n \to \infty$ such that $n, cn, cnr, cn(1-r), cn\alpha, cn(1-\alpha)$ are positive integers, we have*

$$\binom{cn}{cnr}^{-1}\binom{n}{n\alpha}\binom{(c-2)n}{(cr-2\alpha)n} \sim \frac{1}{\sqrt{n}}\widetilde{g}_c^{main}(r,\alpha)\exp\left(n\left(H(\alpha) - cH(r) + (c-2)H\left(\frac{cr-2\alpha}{c-2}\right)\right)\right). \tag{8.1.11}$$

Furthermore, this asymptotic approximation in Equation (8.1.11) *is uniformly convergent over* $(r,\alpha) \in \mathcal{P}_c^{1/12}$ *as* $n \to \infty$. *The approximation also has uniformly bounded error for all* n, r, α *satisfying the hypothesis.*

Proof. We apply Lemma 8.1.2 three times:

1. On $\binom{n}{n\alpha}$, so $(t,m) = (\alpha, n)$. Let $\sigma_\alpha \coloneqq \sigma_{\alpha,n}$ be the approximation ratio here.
2. On $\binom{cn}{cnr}$, so $(t,m) = (r, cn)$. Let $\sigma_r \coloneqq \sigma_{r,cn}$.
3. On $\binom{(c-2)n}{(cr-2\alpha)n}$, so $(t,m) = \left(\frac{cr-2}{c-2}, (c-2)n\right)$. Let $\sigma_\div \coloneqq \sigma_{\frac{cr-2}{c-2},(c-2)n}$.

Then:

$$\begin{aligned}
&\binom{cn}{cnr}^{-1}\binom{n}{n\alpha}\binom{(c-2)n}{(cr-2\alpha)n} \\
&= \frac{\sigma_\alpha\sigma_\div}{\sigma_r}\frac{\sqrt{2\pi cnr(1-r)}}{\sqrt{2\pi n\alpha(1-\alpha)}\sqrt{2\pi(c-2)n\left(\frac{cr-2\alpha}{c-2}\right)\left(1-\frac{cr-2\alpha}{c-2}\right)}}\times \\
&\quad \exp\left(n\left(H(\alpha) - cH(r) + (c-2)H\left(\frac{cr-2\alpha}{c-2}\right)\right)\right) \\
&= \sigma\frac{1}{\sqrt{2\pi n}}\frac{\sqrt{cr(1-r)}}{\sqrt{\alpha(1-\alpha)}\sqrt{(cr-2\alpha)(1-\frac{cr-2\alpha}{c-2})}}\times \\
&\quad \exp\left(n\left(H(\alpha) - cH(r) + (c-2)H\left(\frac{cr-2\alpha}{c-2}\right)\right)\right) \\
&= \sigma\frac{1}{\sqrt{n}}\widetilde{g}_c^{main}(r,\alpha)\exp\left(n\left(H(\alpha) - cH(r) + (c-2)H\left(\frac{cr-2\alpha}{c-2}\right)\right)\right)
\end{aligned}$$

where we find $\sigma = \frac{\sigma_\alpha\sigma_\div}{\sigma_r}$ is the approximation ratio.

For $(r,\alpha) \in \mathcal{P}_c^{1/12}$, we have $r, \alpha, \frac{cr-2\alpha}{c-2} \in \left(\frac{1}{12}, \frac{11}{12}\right)$. Hence the uniform part of Lemma 8.1.2 applies to imply each binomial approximation is uniformly convergent for $(r,\alpha) \in \mathcal{P}_c^{1/12}$. Since the quantity is a product of such binomials (which are bounded for each n), the approximation Equation (8.1.11) is uniformly convergent as $n \to \infty$ over $(r,\alpha) \in \mathcal{P}_c^{1/12}$.

Additionally, Lemma 8.1.2 implies the errors $\sigma_\alpha, \sigma_r, \sigma_\div$ of each binomial approximation are uniformly bounded, so the asymptotic Equation (8.1.11) has uniformly bounded error as well. □

8.2 Approximating S_2 asymptotically

8.2.1 S_2 Asymptotics from [Hen94]

Temme [Tem92] (see also Chapter 34 of his book [Tem14]) derived a Stirling-like asymptotic formula for Stirling numbers of the second kind. Hennecart [Hen94] used this method on more general problems, in particular associated Stirling numbers of the second kind. Recall $S_2(p,q)$ is the 2-associated Stirling numbers of the second kind (the Ward numbers), the number of ways to partition a set of size p into q subsets of size at least 2. For these, he obtained the following lemma.

Lemma 8.2.1. *For any integers $p \geq 1$ and $0 \leq q \leq p/2$, let*

$$\Phi(z) = -p\ln(z) + q\ln(e^z - 1 - z)$$

and let z_0 (as a function of p, q) be the unique positive root of $\Phi'(z_0) = 0$. Then the approximation

$$S_2(p,q) \sim \frac{p!}{q!(p-2q)!}\left(\frac{p-2q}{e}\right)^{p-2q}\frac{(e^{z_0}-1-z_0)^q}{z_0^{p+1}}\sqrt{\frac{p-2q}{\Phi''(z_0)}}. \tag{8.2.1}$$

is uniformly convergent over integers $q \in [0, p/2]$ as $p \to \infty$. We shall use the following algebraically-equivalent form, noting z_0 is the unique root of $\nu(z_0) = q/p$:

$$S_2(p,q) \sim \left(\frac{p!}{q!(p-2q)!}\right)\left(\frac{1}{p}\sqrt{\frac{q(p-2q)}{-z_0\nu'(z_0)}}\right)\left(\left(\frac{p-2q}{e}\right)^{p-2q}\frac{(e^{z_0}-1-z_0)^q}{z_0^p}\right). \tag{8.2.2}$$

As a cultural note, we mention that this lemma is used and cited in Theorem 3.4 in [DM02a].

Proof (Lemma 8.2.1). Directly from Equation 4.9 in [Hen94], with Hennecart's r set to 2, we find the asymptotic behavior for S_2 written in Lemma 8.2.1.

Hennecart's assertion of uniformity occurs after equation (4.9) [Hen94]. Hennecart states "Several computations with different values of n and r was done, and showed the uniform character of (4.9) with respect to k." (where Equation 4.9 is the approximation $S_2(n,k) \sim ...$).

To obtain the algebraically-equivalent formula, we begin with a preliminary calculation

$$\Phi'(z) = -\frac{p}{z} + \frac{q(e^z-1)}{e^z-1-z} \tag{8.2.3}$$

$$z\Phi'(z) = -p + \frac{q}{\nu(z)} \tag{8.2.4}$$

$$\nu(z_0) = \frac{q}{p} \tag{8.2.5}$$

$$\Phi''(z_0) = \frac{q}{z_0}\frac{\partial}{\partial z}(1/\nu(z)) = -\frac{q}{z_0}\frac{\nu'(z_0)}{\nu(z_0)^2} = -\frac{p^2}{q}\frac{\nu'(z_0)}{z_0} \tag{8.2.6}$$

and substitute to obtain

$$S_2(p,q) \sim \frac{p!}{q!(p-2q)!}\left(\frac{p-2q}{e}\right)^{p-2q}\frac{(e^{z_0}-1-z_0)^q}{z_0^{p+1}}\sqrt{\frac{p-2q}{-\frac{p^2}{q}\frac{\nu'(z_0)}{z_0}}} \tag{8.2.7}$$

$$S_2(p,q) \sim \frac{p!}{q!(p-2q)!}\frac{1}{p}\left(\frac{p-2q}{e}\right)^{p-2q}\frac{(e^{z_0}-1-z_0)^q}{z_0^p}\sqrt{\frac{q(p-2q)}{-z_0\nu'(z_0)}} \tag{8.2.8}$$

$$S_2(p,q) \sim \left(\frac{p!}{q!(p-2q)!}\right)\left(\frac{1}{p}\sqrt{\frac{q(p-2q)}{-z_0\nu'(z_0)}}\right)\left(\left(\frac{p-2q}{e}\right)^{p-2q}\frac{(e^{z_0}-1-z_0)^q}{z_0^p}\right). \tag{8.2.9}$$

□

8.2.2 Asymptotics of the ratio of S_2s

Lemma 8.2.2. *Fix $c > 2$ and let $(r, \alpha) \in \mathcal{P}_c$. As $m, n \to \infty$ satisfying $m/n = c > 2$ such that $mr, m(1-r), n\alpha, n(1-\alpha)$ are positive integers, we have*

$$\frac{S_2(mr, n\alpha)S_2(m(1-r), n(1-\alpha))}{S_2(m,n)} \sim \frac{1}{\sqrt{n}}\widetilde{g}_c(r,\alpha)\exp(\tilde{w}_c(r,\alpha)n). \tag{8.2.10}$$

where we repeat the definitions of $\widetilde{g}_c$ and $\tilde{w}_c$ from Section 3.3:

$$\begin{aligned}
\widetilde{g}_c(r,\alpha) &:= \sqrt{\frac{-z_0\nu'(z_0)}{z_1\nu'(z_1)z_2\nu'(z_2)}}\sqrt{\frac{1}{2c\pi r(1-r)}} \\
\tilde{w}_c(r,\alpha) &:= H(\alpha) - cH(r) + \breve{\kappa}_c(r,\alpha) + \breve{\kappa}_c(1-r, 1-\alpha) - \breve{\kappa}_c(1,1) \\
\breve{\kappa}_c(r,\alpha) &:= \alpha\ln(e^z - 1 - z) - cr\ln(z) \quad \text{with } z = \nu^{-1}(\alpha/(cr)).
\end{aligned}$$

Furthermore, the asymptotic approximation in Equation (8.2.10) is uniformly convergent over $(r,\alpha) \in \mathcal{P}_c^{1/12}$ as $m, n \to \infty$. The approximation also has uniformly bounded error for all m, n, r, α satisfying the hypothesis.

Proof. From Lemma 8.2.1, the following asymptotic approximation is uniformly convergent in q as $p \to \infty$:

$$S_2(p,q) \sim \left(\frac{p!}{q!(p-2q)!}\right)\left(\frac{1}{p}\sqrt{\frac{q(p-2q)}{-z_0\nu'(z_0)}}\right)\left(\left(\frac{p-2q}{e}\right)^{p-2q}\frac{(e^{z_0}-1-z_0)^q}{z_0^p}\right).$$

We evaluate several S_2s of the same form, so we simplify that now by substituting $p = cnr$ and $q = n\alpha$, to get an asymptotic approximation that is uniformly convergent in n, α as $mr = cnr \to \infty$:

$$\begin{aligned}
&S_2(cnr, n\alpha) && (8.2.11)\\
&\sim \left(\frac{(cnr)!}{(n\alpha)!((cr-2\alpha)n)!}\right)\left(\frac{1}{cr}\sqrt{\frac{\alpha(cr-2\alpha)}{-z\nu'(z)}}\right)\times && (8.2.12)\\
&\quad n^{(cr-2\alpha)n}\left(\left(\frac{cr-2\alpha}{e}\right)^{(cr-2\alpha)n}\frac{(e^z-1-z)^{n\alpha}}{z^{cnr}}\right) && (8.2.13)\\
&= \left(\frac{(cnr)!}{(n\alpha)!((cr-2\alpha)n)!}\right)n^{(cr-2\alpha)n}\left(\frac{1}{cr}\sqrt{\frac{\alpha(cr-2\alpha)}{-z\nu'(z)}}\right)\times && (8.2.14)\\
&\quad \exp\left(n\ln\left(\left(\frac{cr-2\alpha}{e}\right)^{cr-2\alpha}\frac{(e^z-1-z)^{\alpha}}{z^{cr}}\right)\right) && (8.2.15)\\
&= \left(\frac{(cnr)!}{(n\alpha)!((cr-2\alpha)n)!}\right)n^{(cr-2\alpha)n}\breve{\underline{g}}_c(r,\alpha)\exp(n\breve{\kappa}_c^{\text{new}}(r,\alpha)) && (8.2.16)
\end{aligned}$$

where $\breve{\underline{g}}_c(r,\alpha)$ is defined in Equation (8.1.9), and we define $\breve{\kappa}_c^{\text{new}}$ as:

$$\begin{aligned}
\breve{\kappa}_c^{\text{new}}(r,\alpha) &:= \alpha\ln(e^z-1-z) - cr\ln(z) + (cr-2\alpha)(\ln(cr-2\alpha)-1) \\
&= \breve{\kappa}_c(r,\alpha) + (cr-2\alpha)(\ln(cr-2\alpha)-1).
\end{aligned}$$

Multiplying and dividing approximations of the form in Equation (8.2.16) yields the following approximation, which is uniformly convergent in n, α as $m, mr, m(1-r) \to \infty$ with $m = cn$ for $c > 2$.

$$\frac{S_2(cnr, n\alpha)S_2(cn(1-r), n(1-\alpha))}{S_2(cn, n)} \tag{8.2.17}$$

$$= \binom{cn}{cnr}^{-1}\binom{n}{n\alpha}\binom{(c-2)n}{(cr-2\alpha)n}\frac{\breve{g}_c(r,\alpha)\breve{g}_c(1-r,1-\alpha)}{\breve{g}_c(1,1)}\times \tag{8.2.18}$$

$$\exp\left(n\left[\breve{\kappa}_c^{\text{new}}(r,\alpha) + \breve{\kappa}_c^{\text{new}}(1-r,1-\alpha) - \breve{\kappa}_c^{\text{new}}(1,1)\right]\right).. \tag{8.2.19}$$

With $m = cn$, substituting Lemma 8.1.3 (which is uniformly convergent for $(r, \alpha) \in \mathcal{P}_c^{1/12}$) to approximate the binomial coefficients in Equation (8.2.19) yields

$$\frac{S_2(mr, n\alpha)S_2(m(1-r), n(1-\alpha))}{S_2(m, n)}$$
$$\sim \frac{1}{\sqrt{n}}\widetilde{g}_c^{main}(r,\alpha)\frac{\breve{g}_c(r,\alpha)\breve{g}_c(1-r,1-\alpha)}{\breve{g}_c(1,1)}\times$$
$$\exp\Bigg(n\Big[H(\alpha) - cH(r) +$$
$$(c-2)H\left(\frac{cr-2\alpha}{c-2}\right) + \breve{\kappa}_c^{\text{new}}(r,\alpha) + \breve{\kappa}_c^{\text{new}}(1-r,1-\alpha) - \breve{\kappa}_c^{\text{new}}(1,1)\Big]\Bigg).$$

By algebraic manipulation, we have

$$(c-2)H\left(\frac{cr-2\alpha}{c-2}\right) + \breve{\kappa}_c^{\text{new}}(r,\alpha) + \breve{\kappa}_c^{\text{new}}(1-r,1-\alpha) - \breve{\kappa}_c^{\text{new}}(1,1)$$
$$= \breve{\kappa}_c(r,\alpha) + \breve{\kappa}_c(1-r,1-\alpha) - \breve{\kappa}_c(1,1),$$

The factoring of $\widetilde{g}_c$ in Equation (8.1.8) and definition of $\tilde{w}_c$ finally yields

$$\frac{S_2(mr, n\alpha)S_2(m(1-r), n(1-\alpha))}{S_2(m, n)} \sim \frac{1}{\sqrt{n}}\widetilde{g}_c(r,\alpha)\exp(n\tilde{w}_c(r,\alpha))$$

is uniformly convergent over $(r, \alpha) \in \mathcal{P}_c^{1/12}$ as $m, mr, m(1-r) \to \infty$. Note since $r \in \left(\frac{1}{12}, \frac{11}{12}\right)$, then $mr, m(1-r) \to \infty$ when $m \to \infty$.

This finishes the derivation of the main formula of Lemma 8.2.2. Since the approximations applied (Lemma 8.2.1 and Lemma 8.1.3) have uniformly bounded error, the result has uniformly bounded error as well. □

8.3 The asymptotic approximation to the big sum's summand

Using the definition of $\mathcal{T}^{1/12}$ from Equation (8.1.4), define for $c = m/n$,

$$\mathcal{U}_c^{\text{Int}} := \text{Int}\,\mathcal{U}_c = \mathcal{U}_c^{01} \cap \{0 < r_i < 1, 0 < \alpha_i < 1, 0 < t_i\} \tag{8.3.1}$$

$$\mathcal{U}_{m,n}^{\text{Int}} := \mathcal{U}_c^{\text{Int}} \cap \mathscr{L}_{m,n} = \mathcal{U}_{m,n}^{01} \cap \{0 < r_i < 1, 0 < \alpha_i < 1, 0 < t_i\} \tag{8.3.2}$$

$$\mathcal{U}_{m,n}^{\partial} := \mathcal{U}_{m,n}^{01} \setminus \mathcal{U}_{m,n}^{\text{Int}} \tag{8.3.3}$$

$$\mathcal{U}_c^{1/12} := \{(\vec{r}, \vec{\alpha}) \mid \vec{r} \in \mathcal{T}^{1/12}, (r_i, \alpha_i) \in \mathcal{P}_c^{1/12}, i = 1, 2, 3\} \subseteq \mathcal{U}_c^{\text{Int}}. \tag{8.3.4}$$

As motivation, recall from Corollary 7.6.4 that the big sum we care about is

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} = \sum_{(\vec{r},\vec{\alpha})\in\mathcal{U}^{01}_{m,n}} \breve{\mathscr{S}}_{m,n}(\vec{r},\vec{\alpha}).$$

We will approximate $\breve{\mathscr{S}}_{m,n}(\vec{r},\vec{\alpha})$ well on $\mathcal{U}^{\mathrm{Int}}_{m,n}$, so $\mathcal{U}^{\partial}_{m,n}$ provides the terms of the sum where the approximation does not hold.

Proposition 8.3.1. *Fix $c > 2$ and let $(\vec{r},\vec{\alpha}) \in \mathcal{U}_c$. As $m,n \to \infty$ with $m/n = c > 2$ such that $mr_i, m(1-r_i), n\alpha_i, n(1-\alpha_i)$ are positive integers for $i = 1,2,3$, we have*

$$\breve{\mathscr{S}}_{m,n}(\vec{r},\vec{\alpha}) \sim n^{-3}\overline{g}_c(\vec{r},\vec{\alpha})e^{nh_c(\vec{r},\vec{\alpha})} \tag{8.3.5}$$

where $\overline{g}_c$ and h_c are defined in Section 3.3.

Furthermore, the asymptotic approximation in Equation (8.3.5) *is uniformly convergent over $(\vec{r},\vec{\alpha}) \in \mathcal{U}^{1/12}_c$ as $m,n \to \infty$. The approximation also has uniformly bounded error for all $(\vec{r},\vec{\alpha}) \in \mathcal{U}^{\mathrm{Int}}_{m,n}$ and $m,n \geq 1$ satisfying the hypothesis.*

Proof. Expanding definitions, we have

$$\begin{aligned}\breve{\mathscr{S}}_{m,n}(\vec{r},\vec{\alpha}) = 2^{m-3n}\,&\mathrm{mc}(r_1,r_2,r_3)\times\\ &S_2(mr_1,n\alpha_1)S_2(m(1-r_1),n(1-\alpha_1))/S_2(m,n)\times\\ &S_2(mr_2,n\alpha_2)S_2(m(1-r_2),n(1-\alpha_2))/S_2(m,n)\times\\ &S_2(mr_3,n\alpha_3)S_2(m(1-r_3),n(1-\alpha_3))/S_2(m,n).\end{aligned}$$

This 6 dimensional sum has three groups of terms:

1. $2^{m-3n} = \exp(n((c-3)\ln 2))$
2. Multichoose $\mathrm{mc}(r_1,r_2,r_3) = \binom{cn}{cnt_0,cnt_1,cnt_2,cnt_3}$
3. Three copies of S_2 ratio.

Since the definition of $\mathcal{U}^{\mathrm{Int}}_{m,n}$ implies mt_0, mt_1, mt_2, mt_3 are positive integers, then by Proposition 8.1.1, the multichoose term is asymptotically:

$$\mathrm{mc}(r_1,r_2,r_3) = \binom{cn}{cnt_0,cnt_1,cnt_2,cnt_3} \sim \frac{1}{\sqrt{(2\pi cn)^3 t_0t_1t_2t_3}}\exp(nH(t_0,t_1,t_2,t_3)). \tag{8.3.6}$$

Note $\vec{r} \in \mathcal{T}^{1/12}$ implies $t_0,t_1,t_2,t_3 > \frac{1}{12}$, so the uniform part of Proposition 8.1.1 can apply. Hence, this asymptotic expansion Equation (8.3.6) is uniformly convergent for $\vec{r} \in \mathcal{T}^{1/12}$ as $cn \to \infty$. Also, the expansion has uniformly bounded error for $\vec{r}$ in the interior of $\mathcal{T}$.

From Lemma 8.2.2, each S_2 ratio is asymptotically

$$\frac{S_2(mr,n\alpha)S_2(m(1-r),n(1-\alpha))}{S_2(m,n)} \sim \frac{1}{\sqrt{n}}\widetilde{g}_c(r,\alpha)\exp(n\cdot\tilde{w}_c(r,\alpha)). \tag{8.3.7}$$

Equation (8.3.7) holds uniformly over $(r,\alpha) \in \mathcal{P}^{1/12}_c$ as $m,n \to \infty$ with $m/n = c > 2$. Also, Equation (8.3.7) has uniformly bounded error for $(r,\alpha) \in \mathcal{P}_c$.

Since $\breve{\mathscr{S}}_{m,n}(\vec{r},\vec{\alpha})$ is a product of the above terms, the result follows. ☐

9 Discrete Laplace method

9.1 Laplace's Asymptotic Formula, background

The Discrete Laplace Method is used in applied mathematics, though often without thorough justification, with the classical threshold paper [DM02a] being an example. To explain the situation we start with the classical continuous Laplace method, which the discrete Laplace method imitates.

Let $\mathcal{W}$ be open and bounded. We say a pair of functions $g, h \colon \mathcal{W} \to \mathbb{R}$ "**satisfies Laplace assumptions**" with maximizer $\boldsymbol{x}_0$ when:

1. $g \geq 0$ is continuous and Riemann-integrable on $\mathcal{W}$.
2. $h \leq 0$ is twice continuously-differentiable, and $h(\boldsymbol{x}_0) = 0$ is its unique global maximizer (so $h(\boldsymbol{x}_0) = 0$, and $h(\boldsymbol{x}) < 0$ for $\boldsymbol{x} \neq \boldsymbol{x}_0$).
3. $\mathcal{H}\{h\}(\boldsymbol{x}_0)$ (the Hessian of h at $\boldsymbol{x}_0$) is negative definite.
4. $\liminf_{\boldsymbol{x} \to w} h(\boldsymbol{x}) < 0$ for all $w \in \partial\mathcal{W}$.

Lemma 9.1.1 (Laplace's Method (continuous))**.** *Let $\mathcal{W} \subseteq \mathbb{R}^d$ be open and bounded, and suppose g, h satisfies Laplace assumptions with maximizer $x_0 \in \mathcal{W}$. Then as $n \to \infty$,*

$$\int_{x \in \mathcal{W}} g(\boldsymbol{x}) e^{nh(\boldsymbol{x})} d\boldsymbol{x} \sim \left(\frac{2\pi}{n}\right)^{d/2} \frac{g(\boldsymbol{x}_0)}{\sqrt{\det\left(-\mathcal{H}\{h\}(\boldsymbol{x}_0)\right)}}. \tag{9.1.1}$$

Proof. This is a slight variation of the statement of Theorem 15.2.2 from [Sim15]. For further terms of the expansion, see Theorem 15.2.5, which relies on g, h being infinitely differentiable.

□

The basic problem the Discrete Laplace Method addresses is:

Define an invertible square matrix A and vector v to determine a sequence of lattices $\Lambda_n := \frac{1}{n} A\mathbb{Z}^d + v$. Given a domain $D \subseteq \mathbb{R}^d$, suppose $\mathscr{S}_n \colon D \cap \Lambda_n \to \mathbb{R}$ is sequence of non-negative functions. We want to see how

$$\sum_{x \in D \cap \Lambda_n} \mathscr{S}_n(x) \tag{9.1.2}$$

behaves asymptotically as $n \to \infty$.

If we are in a case where the sum behaves like a Riemann sum and $\mathscr{S}_n$ has an asymptotic approximation $\mathscr{S}_n(x) \sim g(x) e^{nh(x)}$, then optimistically

$$\sum_{x \in D \cap \Lambda_n} \mathscr{S}_n(x) \sim \frac{n^d}{|\det(A)|} \int_D g e^{nh} d\boldsymbol{x}. \tag{9.1.3}$$

If we are in a nice enough situation, this integral succumbs to the Laplace Integral Method, which would yield

$$\sum_{x \in D \cap \Lambda_n} \mathscr{S}_n(x) \sim \frac{(2\pi n)^{d/2}}{|\det(A)|} \frac{g(\boldsymbol{x}_0) e^{nh(\boldsymbol{x}_0)}}{\sqrt{\det(-\mathcal{H}\{h\}(\boldsymbol{x}_0))}}. \tag{9.1.4}$$

□

9.2 Critical Threshold Situations

The classic Dubois-Mandler paper [DM02b], when they face this issue in their simpler situation, assert without much discussion that the Discrete Laplace Method works: "The proof is broadly similar to the ordinary Laplace approximation ... except that instead of working directly on the integral, one has to highlight a Riemann sum." While situation in [DM02b] is simpler than ours, it still has complications (which they do not mention) which are similar to the three listed below which are a problem for us.

We are in the process of trying to rigorously prove this in our situation to obtain the main formula Equation (1.2.3): If $m = cn$, then

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} \sim n^{-3}\frac{c^3}{2}(2\pi n)^3 \frac{\overline{g}_c(\boldsymbol{x}_0)}{\sqrt{\det(-\mathcal{H}\{h_c\}(\boldsymbol{x}_0))}}$$

where $\mathcal{H}\{h_c\}(\boldsymbol{x}_0)$ denotes the Hessian of h_c evaluated at $\boldsymbol{x}_0$, and $\boldsymbol{x}_0 = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ is the global maximizer of h_c on $\mathcal{U}_c$.

9.2.1 Impediments to Rigor

The main troubles in proving this rigorously come from three sources:

1. $\overline{g}_c e^{nh_c}$ is not defined on the boundary $\mathcal{U}^{\partial}_{m,n}$ of the summation region (this comes from expressions like $\frac{1}{t_0}$ which are ill-defined on the boundary of $\mathcal{T}$ where $t_0 = 0$, as well as $(0,0) \in \mathcal{P}_c^{0,1}$ being excluded from $\mathcal{P}_c$).

   This can be addressed by combinatorial arguments (not Stirling-type approximations) that carefully handle the growth rate of the summand $\breve{\mathscr{S}}_{m,n}$ near the boundary $\mathcal{U}^{\partial}_{m,n}$, and leverage the fact that the boundary $\mathcal{U}^{\partial}_{m,n}$ is "lower-dimensional" (has on order $1/n$ of the total points) compared to the full $\mathcal{U}^{01}_{m,n}$.

   This claim is formally stated in Conjecture 9.3.1.

2. $\overline{g}_c e^{nh}$ is not uniformly convergent to $\breve{\mathscr{S}}_{m,n}$ on the entire summation region (this arises from $q!$ being poorly-approximated by Stirling at $q = 1$, and such a term appears regardless of n).

   This can be approached by noting the error $\frac{\breve{\mathscr{S}}_{m,n}}{n^{-3}\overline{g}_c e^{nh}}$ is uniformly bounded on the whole summation region except the boundary $(\mathcal{U}^{01}_{m,n} \setminus \mathcal{U}^{\partial}_{m,n})$. Hence the exponential factor e^{nh} takes the summands to 0 faster than the summands can grow as $n \to \infty$. This argument is carried out in Corollary 9.2.3.

   Also needed for this argument is that $\overline{g}_c$ is integrable, which we proved with algebra and interval arithmetic and are preparing for [HH24].

3. We have a sequence of functions $\mathscr{S}_n$ that vary at the same time the grid $D \cap \Lambda_n$ varies, so the situation is not a Riemann sum of a single function

   The evaluation near $\boldsymbol{x}_0 = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ can be addressed by leveraging the particular behavior of $\overline{g}_c e^{nh}$. This satisfies the assumptions for Laplace method, so the function value falls off quickly away from $\boldsymbol{x}_0$. A shrinking ball (such as $|\boldsymbol{x} - \boldsymbol{x}_0| < \frac{1}{n}$) intersected with the summation region would contain most of the non-negligible function values, but without a rapidly-growing number of points.

9.2.2 Conjectures about the Discrete Laplace Method (DLM)

Next we give some general conjectures about the DLM which apply to our particular problem.

Lemma 9.2.1 (Intersecting with a lattice)**.** *Fix a dimension $d \geq 1$, vector $v \in \mathbb{R}^d$, and invertible linear transformation $A\colon \mathbb{R}^d \to \mathbb{R}^d$. This determines a sequence of lattices*

$$\Lambda_n := \frac{1}{n} A\mathbb{Z}^d + v. \tag{9.2.1}$$

Let $\mathcal{W} \subseteq \mathbb{R}^d$ be open and bounded, and fix some continuous, Riemann-integrable function $g\colon \mathcal{W} \to \mathbb{R}$. Then as $n \to \infty$, we have:

$$\sum_{\boldsymbol{x} \in \mathcal{W} \cap \Lambda_n} g(\boldsymbol{x}) d\boldsymbol{x} \sim \frac{n^d}{|\det(A)|} \int_{\mathcal{W}} g(\boldsymbol{x}) d\boldsymbol{x}. \tag{9.2.2}$$

Moreover, by letting $g = 1$, if $\mathcal{W}$ has finite volume, then

$$|\mathcal{W} \cap \Lambda_n| \sim \frac{n^d}{|\det(A)|} \operatorname{Volume}(\mathcal{W}) \tag{9.2.3}$$

Proof. The sum is a Riemann sum for the displayed Riemann integral. □

Lemma 9.2.2 (Discrete Laplace sum: outside part goes to 0)**.** *Let $A, \mathcal{W}, \Lambda_n$ be as in Lemma 9.2.1. Suppose $g, h\colon \mathcal{W} \to \mathbb{R}$ satisfies Laplace assumptions with maximizer $\boldsymbol{x}_0$. Let B be a ball around $\boldsymbol{x}_0$ with $\overline{B} \subseteq \mathcal{W}$. Then as $n \to \infty$,*

$$\sum_{\boldsymbol{x} \in (\mathcal{W} \setminus B) \cap \Lambda_n} g(\boldsymbol{x}) e^{nh(\boldsymbol{x})} \to 0. \tag{9.2.4}$$

Proof. Item 2 and continuity of h implies $\limsup_{\boldsymbol{x} \to \partial B} h(\boldsymbol{x}) < 0$. Since $\partial(\mathcal{W} \setminus B) \subseteq \partial \mathcal{W} \cup \partial B$, together with Item 4, we get

$$\limsup_{\boldsymbol{x} \to \partial(\mathcal{W} \setminus B)} h(\boldsymbol{x}) < 0.$$

Since $\overline{\mathcal{W}}$ is compact and $h < 0$ on $\mathcal{W} \setminus B$ by Item 2, we thus have

$$\sup_{\boldsymbol{x} \in \mathcal{W} \setminus B} h(\boldsymbol{x}) < 0.$$

Thus there exists $s > 0$ such that $h(\boldsymbol{x}) < -s$ for all $\boldsymbol{x} \in \mathcal{W} \setminus B$.

$$\begin{aligned}
\sum_{\boldsymbol{x} \in (\mathcal{W} \setminus B) \cap \Lambda_n} g(\boldsymbol{x}) e^{nh(\boldsymbol{x})} &\leq \left(\sum_{\boldsymbol{x} \in (\mathcal{W} \setminus B) \cap \Lambda_n} g(\boldsymbol{x}) \right) \sup_{\boldsymbol{x} \in \mathcal{W} \setminus B} e^{nh(\boldsymbol{x})} && (9.2.5) \\
&\leq e^{-ns} \left(\sum_{\boldsymbol{x} \in (\mathcal{W} \setminus B) \cap \Lambda_n} g(\boldsymbol{x}) \right) && (9.2.6) \\
&\sim e^{-ns} \frac{n^d}{\det(A)} \int_{\mathcal{W} \setminus B} g(\boldsymbol{x}) d\boldsymbol{x} && (9.2.7) \\
&\to 0 && (9.2.8)
\end{aligned}$$

where the final step follows from $\det(A)$ and $\int_{\mathcal{W} \setminus B} g(\boldsymbol{x}) d\boldsymbol{x}$ being constant. □

Corollary 9.2.3. *Let* $A, \Lambda_n, \mathcal{W}$ *be as in Lemma 9.2.1 and* $g, h\colon \mathcal{W} \to \mathbb{R}$ *satisfies Laplace assumptions with maximizer* $\boldsymbol{x}_0$*. Let* $B \subseteq \mathcal{W}$ *be a fixed ball containing* $\boldsymbol{x}_0$*. Suppose* $\mathscr{S}_n\colon \mathcal{W} \cap \Lambda_n \to \mathbb{R}$ *has asymptotic approximation* $\mathscr{S}_n(\boldsymbol{x}) \sim g(\boldsymbol{x})e^{nh(\boldsymbol{x})}$ *with uniformly bounded error in* $\mathcal{W} \setminus B$*, precisely:*

> *There exists fixed* $k_{\text{upper}} > 0$ *such that for all* $\boldsymbol{x} \in (\mathcal{W} \setminus B) \cap \Lambda_n$ *and all* $n \geq 1$*, we have*
>
> $$0 \leq \mathscr{S}_n(\boldsymbol{x}) \leq k_{\text{upper}} g(\boldsymbol{x}) e^{nh(\boldsymbol{x})}. \tag{9.2.9}$$

Then as $n \to \infty$*,*

$$\sum_{\boldsymbol{x} \in (\mathcal{W} \setminus B) \cap \Lambda_n} \mathscr{S}_n(\boldsymbol{x}) \to 0.. \tag{9.2.10}$$

Proof.

$$\sum_{\boldsymbol{x} \in (\mathcal{W} \setminus B) \cap \Lambda_n} \mathscr{S}_n(\boldsymbol{x}) \leq k_{\text{upper}} \sum_{\boldsymbol{x} \in (\mathcal{W} \setminus B) \cap \Lambda_n} g(\boldsymbol{x}) e^{nh(\boldsymbol{x})} \to 0.$$

□

Conjecture 9.2.4 (Discrete Laplace sum: inside)**.** *Let* $A, \mathcal{W}, \Lambda_n$ *be as in Lemma 9.2.1. Suppose* $g, h\colon \mathcal{W} \to \mathbb{R}$ *satisfies Laplace assumptions with maximizer* $\boldsymbol{x}_0$*. Let* B *be a ball around* $\boldsymbol{x}_0$ *with* $\overline{B} \subseteq \mathcal{W}$*. Then as* $n \to \infty$*,*

$$\sum_{\boldsymbol{x} \in B \cap \Lambda_n} g(\boldsymbol{x}) e^{nh(\boldsymbol{x})} \sim \frac{(2\pi n)^{d/2}}{|\det(A)|} \frac{g(\boldsymbol{x}_0) e^{nh(\boldsymbol{x}_0)}}{\sqrt{\det(-\mathcal{H}\{h\}(\boldsymbol{x}_0))}}. \tag{9.2.11}$$

Proof idea: There is a convergence problem with naively applying the continuous Laplace method (Lemma 9.1.1) and the integral convergence from Lemma 9.2.1.

The integral of a Gaussian is

$$\int_{\mathbb{R}^d} \exp\left(-\frac{1}{2}\boldsymbol{x}^\top H \boldsymbol{x}\right) d\boldsymbol{x} = \frac{(2\pi)^{d/2}}{\sqrt{\det(H)}} \tag{9.2.12}$$

We do not have time to fix this carefully, but we expect that the following sketch can be filled-in to work out. Let $H = \mathcal{H}\{h\}(\boldsymbol{x}_0)$. Leveraging the Taylor expansion

$h(\boldsymbol{x}) \sim h(\boldsymbol{x}_0) + (x - \boldsymbol{x}_0)^\top H(x - \boldsymbol{x}_0)$, we see

$$\sum_{\boldsymbol{x} \in B \cap \Lambda_n} g(\boldsymbol{x}) e^{nh(\boldsymbol{x})} \sim \frac{n^d}{|\det(A)|} \int_B g(\boldsymbol{x}) e^{nh(\boldsymbol{x})} d\boldsymbol{x} \tag{9.2.13}$$

$$\int_B g(\boldsymbol{x}) e^{nh(\boldsymbol{x})} d\boldsymbol{x} \sim g(\boldsymbol{x}_0) \int_B e^{nh(\boldsymbol{x})} d\boldsymbol{x} \tag{9.2.14}$$

$$\int_B e^{nh(\boldsymbol{x})} d\boldsymbol{x} \sim \int_B e^{\frac{1}{2} n (\boldsymbol{x}-\boldsymbol{x}_0)^\top H (\boldsymbol{x}-\boldsymbol{x}_0)} d\boldsymbol{x} \tag{9.2.15}$$

$$\sim \int_{B-\boldsymbol{x}_0} e^{\frac{1}{2} n \boldsymbol{x}^\top H \boldsymbol{x}} d\boldsymbol{x} \tag{9.2.16}$$

$$\sim \frac{1}{n^d} \int_{n(B-\boldsymbol{x}_0)} e^{\frac{1}{2} \boldsymbol{x}^\top H \boldsymbol{x}} d\boldsymbol{x} \tag{9.2.17}$$

$$\sim \frac{1}{n^d} \int_{\mathbb{R}^n} e^{\frac{1}{2} \boldsymbol{x}^\top H \boldsymbol{x}} d\boldsymbol{x} \tag{9.2.18}$$

$$\sim \frac{1}{n^d} \frac{(2\pi)^{d/2}}{\sqrt{\det(-\mathcal{H}\{h\}\boldsymbol{x}_0)}} \tag{9.2.19}$$

$$\sim \left(\frac{2\pi}{n}\right)^{d/2} \frac{e^{nh(\boldsymbol{x}_0)}}{\sqrt{\det(-H)}}. \tag{9.2.20}$$

These combine to give the formula given by the Conjecture. □

Conjecture-Corollary 9.2.5. *Let $A, \Lambda_n, \mathcal{W}$ be as in Lemma 9.2.1 and $g, h \colon \mathcal{W} \to \mathbb{R}$ satisfies Laplace assumptions with maximizer $\boldsymbol{x}_0$. Let $B \subseteq \mathcal{W}$ be a fixed ball containing $\boldsymbol{x}_0$. Suppose $\mathscr{S}_n \colon \mathcal{W} \cap \Lambda_n \to \mathbb{R}$ has asymptotic approximation $\mathscr{S}_n(\boldsymbol{x}) \sim g(\boldsymbol{x}) e^{nh(\boldsymbol{x})}$ uniformly convergent in B, precisely:*

> *For all $\epsilon > 0$, there exists $N > 0$ such that for all $\boldsymbol{x} \in B$ and $n \geq N$, then*
>
> $$\left| \mathscr{S}_n(\boldsymbol{x}) \left(g(\boldsymbol{x}) e^{nh(\boldsymbol{x})} \right)^{-1} - 1 \right| < \epsilon. \tag{9.2.21}$$

Then as $n \to \infty$,

$$\sum_{\boldsymbol{x} \in B \cap \Lambda_n} \mathscr{S}_n(\boldsymbol{x}) \sim \frac{(2\pi n)^{d/2}}{|\det(A)|} \frac{g(\boldsymbol{x}_0)}{\sqrt{\det(-\mathcal{H}\{h\}(\boldsymbol{x}_0))}}. \tag{9.2.22}$$

Proof. Uniform convergence (Equation (9.2.21)) implies for all $\epsilon > 0$, then $(1 - \epsilon) g e^{nh} \leq \mathscr{S}_n \leq (1+\epsilon) g e^{nh}$ for all $\boldsymbol{x} \in B$, for all sufficiently large n. Hence as $n \to \infty$,

$$\sum_{\boldsymbol{x} \in B \cap \Lambda_n} \mathscr{S}_n(\boldsymbol{x}) \sim \sum_{\boldsymbol{x} \in B \cap \Lambda_n} g(\boldsymbol{x}) e^{nh(\boldsymbol{x})}. \tag{9.2.23}$$

□

9.3 Asymptotic Approximation of the big sum

Now we return to the special situation occurring in our critical threshold problem. We combine work done here with the previous work on asymptotics from Corollary 7.6.4 and Proposition 8.3.1 to obtain (in Conjecture 9.3.2) the explicit but complicated formula for $\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2}$, used as Equation (1.2.3) in the introduction. Recall from Section 8.3, the polytope $\mathcal{U}_c$ is the disjoint union

$$\mathcal{U}_c^{01} = \mathcal{U}_c^{\mathrm{Int}} \cup \mathcal{U}_c^{\partial},$$

where

$$\mathcal{U}_c^{\mathrm{Int}} := \mathrm{Int}\,\mathcal{U}_c = \mathcal{U}_c^{01} \cap \{0 < r_i < 1, 0 < \alpha_i < 1, 0 < t_i\} \tag{9.3.1}$$
$$\mathcal{U}_c^{\partial} := \mathcal{U}_c^{01} \setminus \mathcal{U}_c^{\mathrm{Int}}. \tag{9.3.2}$$

Also recall, where $\mathscr{L}_{m,n}$ is the lattice defined in Equation (7.5.2), for $c = m/n$:

$$\mathcal{U}_c^{01} := \{(\vec{r}, \vec{\alpha}) \mid \vec{r} \in \mathcal{T}, (r_i, \alpha_i) \in \mathcal{P}_c^{0,1}, i = 1, 2, 3\} \tag{9.3.3}$$
$$\mathcal{U}_{m,n}^{01} := \mathcal{U}_c^{01} \cap \mathscr{L}_{m,n} \tag{9.3.4}$$
$$\mathcal{U}_c^{\mathrm{Int}} := \mathrm{Int}\,\mathcal{U}_c = \mathcal{U}_c^{01} \cap \{0 < r_i < 1, 0 < \alpha_i < 1, 0 < t_i\} \tag{9.3.5}$$
$$\mathcal{U}_{m,n}^{\mathrm{Int}} := \mathcal{U}_c^{\mathrm{Int}} \cap \mathscr{L}_{m,n} \tag{9.3.6}$$
$$\mathcal{U}_{m,n}^{\partial} := \mathcal{U}_{m,n}^{01} \setminus \mathcal{U}_{m,n}^{\mathrm{Int}} \tag{9.3.7}$$
$$\mathcal{U}_c^{1/12} := \{(\vec{r}, \vec{\alpha}) \mid \vec{r} \in \mathcal{T}^{1/12}, (r_i, \alpha_i) \in \mathcal{P}_c^{1/12},\ i = 1, 2, 3\} \subseteq \mathcal{U}_c^{\mathrm{Int}}. \tag{9.3.8}$$

As motivation, recall from Corollary 7.6.4 that the big sum we care about is

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} = \sum_{(\vec{r},\vec{\alpha}) \in \mathcal{U}_{m,n}^{01}} \breve{\mathscr{S}}_{m,n}(\vec{r}, \vec{\alpha}).$$

Note Proposition 8.3.1 approximated $\breve{\mathscr{S}}_{m,n}(\vec{r}, \vec{\alpha})$ well on $\mathcal{U}_{m,n}^{\mathrm{Int}}$, so $\mathcal{U}_{m,n}^{\partial}$ provides the terms of the sum where the approximation does not hold.

Conjecture 9.3.1. *Fix c. Along $m = cn$,*

$$\sum_{\boldsymbol{x} \in \mathcal{U}_{m,n}^{\partial}} \breve{\mathscr{S}}_{m,n} \to 0, \quad \text{as } n \to \infty. \tag{9.3.9}$$

This is suggested by numerical plots for small n and is a topic for future work.
Finally, we state the main formula Equation (1.2.3) which underlies this thesis.

Conjecture 9.3.2. *Fix c. Along $m = cn$, as $n \to \infty$,*

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} \sim \frac{c^3}{2} (2\pi)^3 \frac{\overline{g}_c(\boldsymbol{x}_0)}{\sqrt{\det(-\mathcal{H}\{h\}(\boldsymbol{x}_0))}} \tag{9.3.10}$$

where $\boldsymbol{x}_0 = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$, and $\overline{g}_c, h_c$ are defined in Section 3.3.

Proof. (Using other conjectures). Fix c. From Corollary 7.6.4, the big sum is written as

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} = \sum_{\boldsymbol{x} \in \mathcal{U}_{m,n}^{01}} \breve{\mathscr{S}}_{m,n}(\boldsymbol{x}).$$

Conjecture 9.3.1 allows subtracting the terms in $\mathcal{U}_{m,n}^{\partial}$, leaving only the terms in $\mathcal{U}_{m,n}^{\mathrm{Int}} = \mathcal{U}_{m,n}^{01} \setminus \mathcal{U}_{m,n}^{\partial}$:

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} \sim \sum_{\boldsymbol{x} \in \mathcal{U}_{m,n}^{\mathrm{Int}}} \breve{\mathscr{S}}_{m,n}(\boldsymbol{x}).$$

Consider the asymptotic approximation

$$n^3 \breve{\mathscr{S}}_{m,n}(\vec{r}, \vec{\alpha}) \sim \overline{g}_c(\vec{r}, \vec{\alpha}) e^{n h_c(\vec{r}, \vec{\alpha})}. \tag{9.3.11}$$

The calculations in Section 4 and Section 5 imply, $\overline{g}_c, h_c$ satisfies Laplace assumptions with maximizer $\boldsymbol{x}_0 = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$.

Let $B \subseteq \mathcal{U}_c^{1/12}$ be a ball centered at $\boldsymbol{x}_0$. By Proposition 8.3.1, Equation (9.3.11) has uniformly bounded error in $\mathcal{U}_c^{\text{Int}}$, hence uniformly bounded error in $\mathcal{U}_c^{\text{Int}} \setminus B$, so Lemma 9.2.2 applies:

$$\sum_{\boldsymbol{x} \in (\mathcal{U}_c^{\text{Int}} \setminus B) \cap \mathscr{L}_{m,n}} n^3 \breve{\mathscr{S}}_{m,n}(\boldsymbol{x}) \to 0. \tag{9.3.12}$$

By Proposition 8.3.1, Equation (9.3.11) is uniformly convergent in $\mathcal{U}_c^{1/12}$, hence uniformly convergent in B, so Conjecture-Corollary 9.2.5 applies:

$$\sum_{\boldsymbol{x} \in B \cap \mathscr{L}_{m,n}} n^3 \breve{\mathscr{S}}_{m,n}(\boldsymbol{x}) \sim \frac{(2\pi n)^{d/2}}{|\det(A_c)|} \frac{\overline{g}_c(\boldsymbol{x}_0)}{\sqrt{\det(-\mathcal{H}\{h_c\}(\boldsymbol{x}_0))}}. \tag{9.3.13}$$

Simplification using $d = 6$ and $\det(A_c) = 2/c^3$ yields the result. □

10 Conclusion

In this honors thesis we gave evidence supporting Conjecture 1.2.1, and coupled with work in progress we have gone a long way toward proving the following weaker conjecture.

Conjecture 10.0.1. *For $2.5 < c$ and $m = cn$, as $n \to \infty$, random (uniformly distributed) 3-XOR-game two-core problems:*

1. *have at least one solution in $\mathbb{Z}_2$ w.h.p. provided $c < 3$.*
2. *have no solution in $\mathbb{Z}_2$ w.h.p. provided $c > 3$.*

Proof. Conjecture 9.3.2 combined with Proposition 4.3.3 tells us

$$\frac{\mathbb{E}(N^2)}{\mathbb{E}(N)^2} \sim 1. \tag{10.0.1}$$

The second moment inequality then implies $\Pr(N \geq 1) \geq 1$, so the random problems have at least one solution in $\mathbb{Z}_2$ with high probability as $n \to \infty$. □

The biggest gap in proving this is Conjecture 9.3.1, which we have not had time to consider seriously. This is work we are planning for the future.

The major difference between Conjecture 10.0.1 and Conjecture 1.2.1 is that the latter has the weaker hypothesis $m = n(c + o(1))$ instead of $m = cn$. There are ideas for approaching this, but they are relatively unexplored.

Worth pointing out is that the gaps discussed in Section 9.2.1 also apply to the classic 3-SAT proof in [DM02b], and we fill some of these gaps.

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