Properties of an Aloha-like stability region

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Abstract

A well-known inner bound on the stability region of the finite-user slotted Aloha protocol is the set of all arrival rates for which there exists some choice of the contention probabilities such that the associated worst-case service rate for each user exceeds the user’s arrival rate, denoted \( \Lambda \). Although testing membership in \( \Lambda \) of a given arrival rate can be posed as a convex program, it is nonetheless of interest to understand the geometric properties of this set. In this paper we develop new results of this nature, including i) several equivalent descriptions of \( \Lambda \), ii) a method to construct a vector of contention probabilities to stabilize any stabilizable arrival rate, iii) the volume of \( \Lambda \), iv) explicit polyhedral, spherical, and ellipsoid inner and outer bounds on \( \Lambda \), and v) characterization of the generalized convexity properties of a natural “excess rate” function associated with \( \Lambda \), including the convexity of the set of contention probabilities that stabilize a given arrival rate vector.

Index Terms

Aloha, multiple access, random access, stability region, inner bounds, outer bounds.

I. INTRODUCTION

A. Motivation and problem statement

This paper addresses membership testing and structural properties of a natural inner bound on the stability region of the finite-user slotted-time Aloha medium access control (MAC) protocol under the collision channel model, hereafter the Aloha protocol [2]. The Aloha protocol is specified by a tuple \((n, x, p)\) where \(n \in \mathbb{N}\) is the number of users wishing to communicate with a common base station, \(x \in \mathbb{R}_+^n\) denotes the arrival rate of new packets at each user’s queue (one queue per user, each queue assumed capable to hold an unlimited number of packets awaiting transmission), and \(p \in [0, 1]^n\) denotes each user’s chosen contention probability, i.e., the probability with which any user with a non-empty queue will contend for the channel. User contention decisions are synchronized at the beginning of each time slot, and, conditioned on the queue lengths, the user contention decisions are independent across users and across time slots. Each packet transmission requires exactly one time slot. Under the assumed...
collision channel model, an attempted transmission succeeds in a given time slot if and only if it is the only attempt in that time slot. Ternary channel feedback (success, collision, idle) from the base station to each user at the end of each time slot is assumed to be both instantaneous and error-free.

The stability region (of a MAC protocol) is defined as the set of arrival rate vectors (with elements corresponding to exogenous arrival rates at each user’s queue) such that by some appropriate choice of the parameter(s) no user will, as time tends to infinity, accumulate an infinite backlog of packets waiting to be transmitted. The stability region asks for necessary and sufficient conditions in order for every user’s queue to remain bounded. Let \( q_i(t) \) denote user \( i \)’s queue length at time \( t \); queue \( i \) is stable if \( \lim_{L \to \infty} \lim_{t \to \infty} \mathbb{P}(q_i(t) < L) = 1 \), and the system is considered stable if every queue is stable. Since all the states of the underlying discrete time Markov chain (DTMC) of queue length vectors (defined on \( \mathbb{Z}_n^+ \)) communicate, the stability of the system, or equivalently, the positive recurrence of the DTMC amounts to the property that each queue has a non-zero probability of being empty, i.e., \( \lim_{t \to \infty} \mathbb{P}(q_i(t) = 0) > 0 \) for all \( i \in \{1, \ldots, n\} \).

There is a significant body of work that derives bounds on the stability region of the Aloha protocol (denoted \( \Lambda_A \)) from a queueing-theoretic perspective, including [3], [4], [5]. In contrast to this approach, in this work we develop bounds and properties for an important and natural inner bound on the Aloha stability region, namely, the set of arrival rates for which there exists a vector of contention probabilities with associated worst-case service rates component-wise exceeding each arrival rate, denoted below by \( \Lambda \). Our motivation to study this inner bound \( \Lambda \) is that testing membership of a candidate arrival rate vector \( x \) in \( \Lambda \) is easier than (but nonetheless has certain challenges similar to those encountered in) testing membership in the Aloha stability region. In either case one must, either implicitly or explicitly, identify \( p \), a vector of stabilizing contention probabilities, for which \( x \) can be shown to be in \( \Lambda \) or \( \Lambda_A \). The difficulty is that the set of potential controls \( p \) is uncountably infinite, (\( p \in [0,1]^n \)), and as such, given \( x \), it is not obvious whether or not such a \( p \) exists, i.e., whether or not \( x \) is stabilizable.

Our results address this challenge in several ways. First, we give a novel characterization of membership in \( \Lambda \) in terms of whether or not a certain order-\( n \) polynomial has a positive root. Second, we give several equivalent formulations for \( \Lambda \), each with its own advantages. Third, we give a means of constructing a suitable control \( p \) for any stabilizable rate vector \( x \). Fourth, we give polyhedral, spherical, and ellipsoid inner and outer non-parametric (explicit) bounds on \( \Lambda \), which constitute, variously, necessary or sufficient conditions on membership in \( \Lambda \). These explicit inner and outer bounds partially illuminate the shape and structure of \( \Lambda \) as a function of \( n \). Finally, we present certain structural properties of certain functions and sets naturally associated with \( \Lambda \), including the excess rate function and (an inner bound of) the set of contention probabilities that stabilize a given arrival rate vector.
The inner bound \( \Lambda \subseteq \Lambda_A \subseteq \mathbb{R}^n_+ \) studied in this paper is:

\[
\Lambda = \left\{ \mathbf{x} \in \mathbb{R}^n_+ : \exists \mathbf{p} \in [0, 1]^n : x_i \leq p_i \prod_{j \neq i} (1 - p_j), \ \forall i \in \{1, \ldots, n\} \right\}. \tag{1}
\]

The expression \( p_i \prod_{j \neq i} (1 - p_j) \) is the worst-case service rate for user \( i \)’s queue, namely the service rate assuming all users have non-empty queues and thus all users are eligible for channel contention. In particular, user \( i \)’s transmission is successful in such a time slot if user \( i \) elects to contend (with probability \( p_i \)) and each other user \( j \neq i \) does not contend (each with independent probability \( 1 - p_j \) for a non-empty queue). Clearly \( \Lambda \subseteq \Lambda_A \), since an arrival rate that is stabilizable under the worst-case service rate is certainly stabilizable under a better service rate. Our aim in this paper is to establish properties of and non-parametric bounds on \( \Lambda \). We emphasize that we call sets such as \( \Lambda \) “parametric” due to the observation that asserting membership in them requires explicitly or implicitly identifying another parameter which may be viewed as auxiliary from the perspective of membership testing.

In this paper all the vectors are column vectors and inequalities between two vectors are understood to hold component-wise. A list of general notation is given in Table I.

| Symbol | Meaning |
|--------|---------|
| \( n \) | number of users, also the default length of a vector |
| \([n] = \{1, \ldots, n\}\) | set of positive integers up to \( n \) |
| \( \mathbf{x} = (x_1, \ldots, x_n) \) | vector of user’s arrival rates |
| \( \mathbf{p} = (p_1, \ldots, p_n) \) | vector of user’s chosen probabilities for channel contention |
| \( \mathbf{1} \) | a vector with 1 in all its positions |
| \( \mathbf{e}_i \) | unit vector with 1 in position \( i \in [n] \) |
| \( \mathbf{m} = m \mathbf{1}, m = \frac{1}{n} (1 - \frac{1}{n})^{n-1} \) | “all-rates-equal” point \( \mathbf{m} \) and its component value \( m \) |
| \( \pi(\mathbf{p}) = \prod_{i} (1 - p_i) \) | product of \( (1 - p_i) \)'s |
| \( \mathbf{x}(\mathbf{p}) \text{ for } x_i(\mathbf{p}) = p_i \prod_{j \neq i} (1 - p_j) \) | \( n \)-vector \( \mathbf{x}(\mathbf{p}) \) with components \( x_i(\mathbf{p}) \) determined by \( \mathbf{p} \) |
| \( \mathbf{p}(\delta, \mathbf{x}) \text{ for } p_i(\delta, \mathbf{x}) = \frac{\mathbf{1} - \delta \mathbf{x}}{1 - \delta} \) | \( n \)-vector \( \mathbf{p}(\delta, \mathbf{x}) \) with components \( p_i(\delta, \mathbf{x}) \) determined by \( \mathbf{x} \) and parameterized by \( \delta > 0 \) |
| \( \mathbb{bd} \) | topological boundary of a set |
| \( \text{int} \) | interior of a set |
| \( \text{conv} \) | convex hull of a set |
| \( A^c \) | complement of set \( A \) |
| \( \| \cdot \| \) | \( l_2 \) norm |
| \( d(x, y) = \|x - y\| \) | Euclidean distance between (geometric objects) \( x, y \) |
| \( I_3 \) | indicator function for boolean expression \( \mathcal{S} \) |
| \( \mathbb{S} = \{ \mathbf{z} \geq 0 : \sum_{i} z_i \leq 1 \} \) | closed standard unit simplex |
| \( \partial \mathbb{S} = \{ \mathbf{z} \geq 0 : \sum_{i} z_i = 1 \} \) | the facet of closed standard unit simplex in \( \mathbb{R}^n_+ \), namely the set of probability vectors |
| \( \mathcal{H}(\mathbf{n}, d) = \{ \mathbf{x} : \mathbf{n}^T \mathbf{x} = d \} \) | hyperplane with normal vector \( \mathbf{n} \) and displacement \( d \) |
| \( B(\mathbf{c}, r) = \{ \mathbf{x} : d(\mathbf{c}, \mathbf{x}) < r \} \) | open ball centered at \( \mathbf{c} \) with radius \( r \) |
| \( \mathcal{E} = \{ \mathbf{x} : (\mathbf{x} - \mathbf{c})^T \mathbf{R}^{-1} (\mathbf{x} - \mathbf{c}) < 1 \} \) | open ellipsoid centered at \( \mathbf{c} \), expressed in quadratic form |
| \( \mathcal{E}(\mathbf{c}, a_1, a_2) \) | open ellipsoid centered at \( \mathbf{c} \) with semi-axis lengths \( a_1, a_2, \ldots, a_n \) |
| \( \mathbf{Q} \) | the rotation matrix used in Prop. 12, may also encode the direction of ellipsoid axes (see §VI) |
B. Related work

The throughput analysis of the Aloha packet system with and without slots can be found in Roberts [6] and Abramson [7]. The Aloha stability region problem was posed in 1979 by Tsybakov and Mikhailov [8] who also solved the \( n = 2 \) and the homogeneous \( n \)-user case, for both of which they showed \( \Lambda = \Lambda_A \). Szpankowski [9] studied this problem when \( n > 2 \), with result expressed in terms of the joint statistics of the queue lengths. The use of the so-called “dominant system” in Rao and Ephremides [3], as well as Luo and Ephremides [4], established some important bounds on the stability region. Anantharam [10] showed \( \Lambda = \Lambda_A \) for a certain correlated arrival process by applying the Harris correlation inequality. Using mean field analysis, assuming each queue’s evolution is independent, Bordenave et al. [11] were able to show \( \Lambda = \Lambda_A \) holds asymptotically in \( n \). More recently Kompalli and Mazumdar [5] obtained bounds that are linear with respect to the users’ arrival rates, based on a Foster-Lyapunov approach. To date, characterization of \( \Lambda_A \) remains open for the general \( n \)-user case with general arrival processes, although it’s been conjectured ([3] §V, [12] §V Thm. 2) that \( \Lambda \) coincides with the Aloha stability region \( \Lambda_A \). More recently, Subramanian and Leith [13] showed structural properties such as boundary and convexity properties of the rate region of CSMA/CA wireless local-area networks which includes Aloha and IEEE 802.11 as special cases.

Besides its intimate connection with the Aloha stability region \( \Lambda_A \), the set \( \Lambda \) has also been featured in an information theoretic context. Namely, in 1985 Massey and Mathys [14] proved \( \Lambda \) is the capacity region of the collision channel without feedback. In the same issue, Post [15] established the convexity of the complement of \( \Lambda \) in the non-negative orthant \( \mathbb{R}_n^+ \).

C. Summary of bounds on \( \Lambda \)

In this paper we present a variety of inner and outer bounds on \( \Lambda \), including the “square-root-sum” inner bound \( \Lambda_{\text{srs}} \) (§III, Prop. 5), polyhedral inner \( \Lambda_{\text{pi}} \) and outer \( \Lambda_{\text{po}} \) bounds (§IV, Props. 7 and 8), spherical inner \( \Lambda_{\text{si}} \) and outer \( \Lambda_{\text{so}} \) bounds (§V, Props. 9 and 10), and ellipsoid inner \( \Lambda_{\text{ei}} \) and outer \( \Lambda_{\text{eo}} \) bounds (§VI, Props. 18 and 17). The volumes of the aforementioned bounds as a function of the number of users, \( n \), are collected in Fig. 1 and Tables II and III, where \( i \) (o) refers to inner (outer) bound respectively, and \( p, s, e \) refers to polyhedral, spherical, ellipsoid, respectively. We give both the volumes themselves, as well as the volumes normalized by the volume of the (trivial) simplex outer bound of \( 1/n! \). The volumes of \( \Lambda_{\text{srs}}, \Lambda_{\text{pi}}, \Lambda \) are computed exactly from closed-form expressions we derive in the paper. All other volumes are estimated using standard Monte-Carlo simulation. \( \Lambda_{\text{pi}}^* \) is the optimal polyhedral inner bound among its family. For the spherical bounds \( \Lambda_{\text{si}}, \Lambda_{\text{so}} \) the center of spheres are chosen such that the induced bounds are optimal within their families (hence the notation \( \Lambda_{\text{si}}^* \) and \( \Lambda_{\text{so}}^* \)). For the
ellipsoid bounds $\Lambda_{ei}$, $\Lambda_{eo}$ the center of ellipsoids are chosen by setting $c = 2$. $\Lambda_{podso}$ is constructed by using $\Lambda_{po}$ and $\Lambda_{so}^*$ in conjunction namely $\Lambda_{podso} \equiv \Lambda_{po} \cap \Lambda_{so}^*$. It is clear from Fig. 1 that the three inner bounds (polyhedral, spherical, ellipsoid) are tighter than are the four outer bounds.

For the Monte-Carlo volume estimates we generate independent points over $[0,1]^n$ uniformly at random, and use the fraction of points that fall into the region defined by the bound as our volume estimate. As the volume of the unit box $[0,1]^n$ is 1, the volume of any subset of the unit box can be viewed as the probability that a point uniformly distributed over the unit box falls into this subset, which equals the mean of a Bernoulli random variable, say $Z \sim \text{Ber}(v)$, for $v$ the volume of the subset. This justifies the use of the sample mean, $\hat{v}_k = (Z_1 + \cdots + Z_k)/k$, as our volume estimate. We also include confidence interval estimates in both tables, indicating the relative half-width, denoted $\delta$, in order for the probability that the true mean $v$ deviates from the sample mean $\hat{v}_k$ by a fraction of no more than $\delta$ is at least $1 - \alpha$. More precisely, let $n$ and the bound (with unknown volume $v$) be given, and let $k$ be the total number of trials for generating instances of i.i.d. random variables $Z \sim \text{Ber}(v)$. We want to find $\delta$ such that $\mathbb{P}(\hat{v}_k (1 - \delta) \leq v \leq \hat{v}_k (1 + \delta)) \geq 1 - \alpha$. Under a normal approximation we can derive $\delta \approx \sqrt{1 - \hat{v}_k (k - 1) \hat{v}_k} \Phi^{-1}(1 - \alpha/2)$, applying results from [16] (§9.1). In our simulations we use $k = 10^8$ and $\alpha = 5\%$. For those volumes estimated using Monte-Carlo, the corresponding entries in Table II are $\hat{v}_k$ (top) and $\delta$ (bottom), and in Table III are $n!\hat{v}_k$ (top) and $\delta$ (bottom).

As will be shown (Remarks 1, 3 and 5), the inner bounds are ordered by volume for all $n \geq 3^1$, i.e.,

$$\text{vol}(\Lambda_{srs}) \leq \text{vol}(\Lambda_{pi}^*) \leq \text{vol}(\Lambda_{si}^*) \leq \text{vol}(\Lambda_{ei}) \leq \text{vol}(\Lambda), \ n \geq 3. \quad (2)$$

Among the outer bounds ($\Lambda_{eo}$, $\Lambda_{podso}$, $\Lambda_{po}$ and $\Lambda_{so}^*$) there is no such complete ordering valid for all $n$, although $\Lambda_{podso}$ outperforms both $\Lambda_{po}$ and $\Lambda_{so}^*$ by construction, and the ellipsoid outer bound $\Lambda_{eo}$ outperforms the optimal spherical outer bound $\Lambda_{so}^*$ provided the outer bounding ellipsoid is such that its center $c = c1$ with $c \geq 1$.

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1Provided the inner bounding ellipsoid is such that its center $c = c1$ with $c \geq (1 - nm^2)/(2(1 - nm))$ where $m = m(n) \equiv \frac{1}{n} \left(1 - \frac{1}{n}\right)^{n-1}$. August 18, 2014 DRAFT
Fig. 1. The volumes (computed, or estimated from Monte-Carlo simulation) of the various inner and outer bounds $\Lambda_{\text{srs}}$, $\Lambda_{\text{pi}}^*$, $\Lambda_{\text{si}}$, $\Lambda_{\text{eo}}$, $\Lambda_{\text{po}}$, $\Lambda_{\text{so}}$, on the Aloha stability region inner bound $\Lambda$ versus the number of users, $n$. The top figure shows the volumes and the bottom figure shows the volumes normalized by the volume of the (trivial) simplex outer bound ($1/n!$). Each of the two ovals on each plot groups four curves, with the top oval indicating the four left labels and the bottom oval indicating the four right labels. The left and right label orderings reflect the ordering of the curves within the top and bottom ovals, respectively. Ellipsoids have parameter $c = 2$. DRAFT August 18, 2014
D. Organization and contributions

We now describe the major sections of the paper, highlighting our main results in each section. In §II we present a polynomial root condition for testing membership in $\Lambda$, and use this result to establish some equivalent forms of $\Lambda$. Furthermore, the root testing can be augmented so that it allows us to exclusively find the critical stabilizing control(s). In §III we compute the volume of $\Lambda$ in closed-form, meaning it is expressed as a finite (albeit
complicated) sum. We then give a simple inner bound on $\Lambda$, exact for $n = 2$, but provably quite weak for $n > 2$.

The next three sections give explicit (non-parametric) inner and outer bounds on $\Lambda$. Specifically, §IV gives the optimal polyhedral inner bound induced by a single hyperplane as well as a polyhedral outer bound in $\mathbb{R}^n_+$ induced by $n + 1$ hyperplanes, §V presents the optimal spherical inner and outer bounds each induced by a single sphere, and §VI establishes ellipsoid inner and outer bounds each induced by an ellipsoid. We include two different proofs for our ellipsoid outer bound. Our last technical section, §VII, shifts the focus to the generalized convexity properties of an “excess rate function” associated with $\Lambda$, and establishes the convexity of the set of stabilizing controls for a given rate vector assuming worst-case service rate. A brief conclusion is given in §VIII, and several of the proofs are placed in an appendix following the references.

II. POLYNOMIAL MEMBERSHIP TESTING, FORMS OF $\Lambda$, AND STABILIZING CONTROLS

This section introduces three rather distinct results which are presented together on account of the fact that their proofs rely upon closely related concepts. First, Prop. 1 demonstrates that testing membership of a rate vector $x$ in $\Lambda$ is equivalent to a certain polynomial having at least one positive root. Second, Prop. 2 establishes two set definitions similar to $\Lambda$ are in fact equivalent to $\Lambda$. Finally, Prop. 3 identifies a “critical stabilizing control” $p(x)$ (see Def. 3) for each $x \in \Lambda$. Def. 1 gives three sets, related to $\Lambda$, that will be important for what follows.

Definition 1:

$$\Lambda_{eq} \equiv \left\{ x \in \mathbb{R}^n_+ : \exists p \in [0, 1]^n : \forall i \in \{1, \ldots, n\} \right\}$$  \hspace{1cm} (3)

$$\Lambda_{\partial S} \equiv \left\{ x \in \mathbb{R}^n_+ : \exists p \in [0, 1]^n, \sum_i p_i = 1 : \forall i \in \{1, \ldots, n\} \right\}$$  \hspace{1cm} (4)

$$\partial \Lambda \equiv \left\{ x \in \mathbb{R}^n_+ : \exists p \in [0, 1]^n, \sum_i p_i = 1 : x_i = p_i \prod_{j \neq i} (1 - p_j), \forall i \in \{1, \ldots, n\} \right\}$$  \hspace{1cm} (5)

Comparison with $\Lambda$ in (1) makes clear that $\Lambda_{eq}$ replaces all the inequalities in $\Lambda$ with equalities, $\Lambda_{\partial S}$ adds to $\Lambda$ a restriction that the contention probabilities sum to one, and $\partial \Lambda$ adds both of these to $\Lambda$. We denote the set of all sub-stochastic vectors as $S \equiv \{ x \geq 0 : \sum_i x_i \leq 1 \}$, and its facet in $\mathbb{R}^n_+$, the set of all stochastic vectors (also called probability vectors) as $\partial S \equiv \{ x \geq 0 : \sum_i x_i = 1 \}$; this notation explains the label $\Lambda_{\partial S}$. The next definition introduces several quantities to be used. Let $\{ e_i \}_{i=1}^n$ denote the $n$ standard unit vectors in $\mathbb{R}^n_+$.

Definition 2: The order-$n$ polynomial in $\delta \in \mathbb{R}$ with coefficients determined by $x \in [0, 1]^n \setminus \{ e_i \}_{i=1}^n$:

$$f(\delta, x) \equiv \prod_{i=1}^n (1 + x_i \delta) - \delta.$$  \hspace{1cm} (6)
The n-vector \( \mathbf{p}(\delta, \mathbf{x}) \in [0,1]^n \) with components \( p_i(\delta, \mathbf{x}) \) determined by \( \mathbf{x} \in \mathbb{R}_+^n \) and parameterized by \( \delta \):

\[
p_i(\delta, \mathbf{x}) \equiv \frac{\delta x_i}{1 + \delta x_i}, \quad i \in [n].
\] (7)

The product of the complements of a given vector of contention probabilities \( \mathbf{p} \in [0,1]^n \):

\[
\pi(\mathbf{p}) \equiv \prod_j (1 - p_j).
\] (8)

The n-vector \( \mathbf{x}(\mathbf{p}) \in [0,1]^n \) with components \( x_i(\mathbf{p}) \) determined by \( \mathbf{p} \in [0,1]^n \):

\[
x_i(\mathbf{p}) \equiv p_i \prod_{j \neq i} (1 - p_j) = \frac{p_i}{1 - p_i} \pi(\mathbf{p}), \quad i \in [n].
\] (9)

Note the equalities in \( \Lambda_{eq} \) in (3) are \( \mathbf{x} = \mathbf{x}(\mathbf{p}) \) in (9). Our notation distinguishes between a generic vector of contention probabilities \( \mathbf{p} \in [0,1]^n \) and a specific vector \( \mathbf{p}(\delta, \mathbf{x}) \) determined by \( \delta \) and \( \mathbf{x} \), and likewise between a generic rate vector \( \mathbf{x} \in \Lambda \) and a specific vector \( \mathbf{x}(\mathbf{p}) \) determined by \( \mathbf{p} \).

**Definition 3 (stabilizability in the sense of \( \Lambda \) or its equivalent forms):** A stabilizing control for \( \mathbf{x} \in \Lambda \) is a vector of contention probabilities \( \mathbf{p} \in [0,1]^n \) that is “compatible” with \( \mathbf{x} \), meaning the pair \( (\mathbf{x}, \mathbf{p}) \) satisfies the definition of \( \Lambda \). A critical stabilizing control is a stabilizing control \( \mathbf{p} \) such that \( (\mathbf{x}, \mathbf{p}) \) satisfies the definition of \( \Lambda_{eq} \) (or \( \partial \Lambda \)).

A corollary of Prop. 1 below is that, given \( \mathbf{x} \in [0,1]^n \), there exists a stabilizing control iff there exists a critical stabilizing control.

Since \( \Lambda \subseteq \Lambda_{eq} \), the non-existence of a stabilizing control for a given \( \mathbf{x} \) in the sense of \( \Lambda \) does not necessarily mean the non-existence of one for \( \mathbf{x} \) in the sense of \( \Lambda_{eq} \) (i.e., it does not necessarily mean \( \mathbf{x} \) is not stabilizable under the Aloha protocol). Throughout this paper though, our usage of “stabilizability” and “stability controls” is tied to \( \Lambda \) or its equivalent forms.

The following proposition gives an alternative test for membership of a rate vector \( \mathbf{x} \) in \( \Lambda \) in terms of the existence of a positive root of the polynomial \( f(\delta, \mathbf{x}) \) in (6), and furthermore establishes that in fact \( \Lambda = \Lambda_{eq} \). The converse proof is constructive, meaning given a positive root \( \delta \), one can construct a \( \mathbf{p}(\delta, \mathbf{x}) \) compatible with \( \mathbf{x} \). In the forward direction, given \( \mathbf{x} \in \Lambda \) and an associated compatible \( \mathbf{p} \), we do not give an explicit expression for a positive root \( \delta \) of \( f(\delta, \mathbf{x}) \), although we can lower bound the interval containing \( \delta \). In the forward direction for \( \mathbf{x} \in \Lambda_{eq} \), however, given a compatible \( \mathbf{p} \) such that \( \mathbf{x} = \mathbf{x}(\mathbf{p}) \) as in (9), we have that one of the positive roots of \( f(\delta, \mathbf{x}) \) for \( \mathbf{x} \in \Lambda_{eq} \) will always equal \( \delta = 1/\pi(\mathbf{p}) \).

**Proposition 1 (root testing):** Membership in \( \Lambda \) (except \( \{ \mathbf{e}_i \}_i \)) is equivalent to the existence of a positive root of the polynomial equation \( f(\delta, \mathbf{x}) = 0 \).

\[
\mathbf{x} \in \Lambda \setminus \{ \mathbf{e}_i \}_i \iff \exists \delta > 0 : f(\delta, \mathbf{x}) = 0.
\] (10)
The same equivalence holds for membership in $\Lambda_{eq}$. In particular, $\Lambda = \Lambda_{eq}$.

**Proof:** We first address membership testing for $\Lambda$.

“$\Leftarrow$”: Fix $x \not\in \{e_i\}_{i=1}^n$ and suppose $\delta > 0$ satisfies $f(\delta, x) = 0$. Construct $p(\delta, x)$ as in (7), and observe the worst-case service rate for user $i$ is

$$p_i(\delta, x) \prod_{j \neq i} (1 - p_j(\delta, x)) = \frac{\delta x_i}{\prod_j (1 + \delta x_j)},$$

(11)

and for this choice of $p$ the requirement $x_i \leq p_i \prod_{j \neq i} (1 - p_j)$ simplifies to $\prod_j (1 + \delta x_j) \leq \delta$, which is true with equality by assumption that $f(\delta, x) = 0$. As this is true for each $i \in [n]$ it follows that $x \in \Lambda$.

“$\Rightarrow$”: First observe that if $p_i = 1$ for some $i \in [n]$ then the only way for $x \in \Lambda$ is to fix $x = e_i$. Similarly, if $x_i = 0$ for some $i \in [n]$, then we can work with a reduced-dimensional $x$ (i.e., the original $x$ with zero component(s) removed). Consequently, we now assume $p_i < 1$ and $x_i > 0$ for each $i \in [n]$. Suppose $x \in \Lambda \setminus \{e_i\}_{i=1}^n$ and let $p$ be compatible with $x$. Define the “inverse stability rank” vector $\Delta$ (Luo and Ephremides [4] Thm. 2) with elements

$$\Delta_i = \frac{p_i}{x_i(1 - p_i)}, \ i \in [n].$$

(12)

Then $x \in \Lambda$ may be equivalently expressed in terms of $\Delta$ via:

$$x \in \Lambda \iff \exists p : x_i \leq p_i \prod_{j \neq i} (1 - p_j), \ i \in [n]$$

$$\iff \exists p : \frac{p_i}{x_i(1 - p_i)} \geq \prod_{j \in [n]} \frac{1}{1 - p_j} = \prod_{j \in [n]} \left(1 + x_j \frac{p_j}{x_j(1 - p_j)}\right), \ i \in [n]$$

$$\iff \exists \Delta : \Delta_i \geq \prod_j (1 + x_j \Delta_j), \ i \in [n] \quad (\ast)$$

(13)

Define $\hat{\Delta} = \min_j \Delta_j$, and let $\Delta = \hat{\Delta} \mathbf{1}$ be the $n$-vector with all components equal to $\hat{\Delta}$. If $\Delta$ obeys $(\ast)$ in (13) then $\Delta$ also obeys $(\ast)$, because

$$\Delta = \Delta_i = \min_j \Delta_j \geq \prod_k (1 + x_k \Delta_k) \geq \prod_k (1 + x_k \hat{\Delta}_k) = \prod_k (1 + x_k \hat{\Delta}), \ i \in [n].$$

It follows that $f(\hat{\Delta}, x) \leq 0$. If $f(\hat{\Delta}, x) = 0$ then $\hat{\Delta}$ is the required positive root in (10). Otherwise, notice $\lim_{\Delta \to \infty} f(\hat{\Delta}, x) = \infty$, so by the intermediate value theorem there must exist some $\delta \in (\hat{\Delta}, \infty)$ so that $f(\delta, x) = 0$. This concludes the proof of the equivalence for membership testing for $\Lambda$.

We now address membership testing for $\Lambda_{eq}$.

“$\Leftarrow$”: The same proof used for membership testing for $\Lambda$ holds here.

“$\Rightarrow$”: We must show that if $x \in \Lambda_{eq} \setminus \{e_i\}_{i=1}^n$ then there exists $\delta > 0$ such that $f(\delta, x) = 0$. But the above proof for membership testing for $\Lambda$ showed such a $\delta$ always exists for each $x \in \Lambda$, and as $\Lambda_{eq} \subseteq \Lambda$, a $\delta$ must likewise
exist for each \( x \in \Lambda_{eq} \). The fact that \( f(1/\pi(p), x) = 0 \) for \( p \) compatible with \( x \in \Lambda_{eq} \) follows by substitution. This concludes the proof of the equivalence for membership testing for \( \Lambda_{eq} \).

The assertion \( \Lambda = \Lambda_{eq} \) is immediate from the two equivalences just established.

The following proposition extends the equivalence of \( \Lambda \) and \( \Lambda_{eq} \) to include \( \Lambda_{\partial S} \).

**Proposition 2:** \( \Lambda_{eq} = \Lambda = \Lambda_{\partial S} \).

**Proof:** Prop. 1 established \( \Lambda_{eq} = \Lambda \); it remains to show \( \Lambda = \Lambda_{\partial S} \). As \( \Lambda_{\partial S} \subseteq \Lambda \), we only need to show \( \Lambda \subseteq \Lambda_{\partial S} \). By Lem. 1 of [14], given \( x \in \Lambda \) (with compatible \( p \in [0, 1]^n \)), there must exist a unique \( \hat{x} \in \delta \Lambda \) (with a unique compatible \( \hat{p} \in \partial S \)) which “dominates” \( x \) in the sense that \( x \leq \hat{x} \). If in fact \( x = \hat{x} \) then \( \hat{p} = p \) as well [14]. Since \( \hat{x} \in \partial \Lambda \) and \( x \leq \hat{x} \), it follows that \( x \in \Lambda_{\partial S} \), and thus \( \Lambda \subseteq \Lambda_{\partial S} \).

We next present an augmented version of the root testing Prop. 1, which makes clear how the roots of polynomial equation \( f(\delta, x) = 0 \) map between compatible \( p \) and \( x \in \Lambda = \Lambda_{eq} \). The proofs of the (critical) stabilizing controls \( p(x) \) for a given \( x \) are constructive.

**Proposition 3 (augmented root testing):** Fix \( n \geq 2 \) and let a rate vector \( x \in [0, 1]^n \setminus \{e_i\}_{i=1}^n \) be given.

1) \( x \in \partial \Lambda \) iff there is a unique positive root \( \delta \) of \( f(\delta, x) = 0 \), denoted \( \delta_u \). Furthermore given \( x \in \partial \Lambda \), then \( p_u = p(\delta_u, x) \) given by (7) stabilizes \( x \). Finally, \( p_u \in \partial S \) and is the only (critical) stabilizing control for \( x \) among all \( p \in [0, 1]^n \).

2) Let \( x \in \Lambda \setminus \partial \Lambda \) be given. Solving \( f(\delta, x) = 0 \) on \( (0, \infty) \) for \( \delta \) yields exactly two positive roots denoted \( \delta_s \), \( \delta_l \). Each root can be used to construct a vector of contention probabilities, \( p_s = p(\delta_s, x) \), \( p_l = p(\delta_l, x) \), according to (7), that stabilizes \( x \). Furthermore, \( p_s \) is such that \( \sum_{i=1}^n p_{s,i} < 1 \) (i.e., \( p_s \in S \setminus \partial S \)) and \( p_l \) is such that \( \sum_{i=1}^n p_{l,i} > 1 \) (i.e., \( p_l \in [0, 1]^n \setminus S \)). Finally, \( p_s \), \( p_l \) are also the only two critical stabilizing controls for \( x \) among all \( p \in [0, 1]^n \).

**Proof:** See §X-A in the Appendix.

**Corollary 1:** There exist the following bijections: i) \( \partial S \leftrightarrow \partial \Lambda \), ii) \( S \setminus \partial S \leftrightarrow \Lambda \setminus \partial \Lambda \), iii) \( [0, 1]^n \setminus S \leftrightarrow \Lambda \setminus \partial \Lambda \), iv) \( S \setminus \partial S \leftrightarrow [0, 1]^n \setminus S \), v) \( S \leftrightarrow \Lambda \).

**Proof:** Massey and Mathys [14] showed i). We now show ii). From (the proof of) Prop. 3 there exists a function that maps from \( \Lambda \setminus \partial \Lambda \) to \( S \setminus \partial S \). We need to show this function mapping is one-to-one and onto. First, given two distinct points \( x, y \in \Lambda \setminus \partial \Lambda \), the function maps to \( p_{s,x}, p_{s,y} \) respectively, both in \( S \setminus \partial S \). If \( p_{s,x} = p_{s,y} \), since they are both critical stabilizing controls (according to Prop. 3) meaning they determine the corresponding rate vectors \( x = x(p_{s,x}), y = y(p_{s,y}) \) according to (9), this gives \( x = y \), which contradicts the assumption \( x \neq y \) and hence this function is one-to-one. Second, for any point \( p_s \in S \setminus \partial S \) it defines a rate vector \( x(p_s) \) according
to (9), which by definition is in $\Lambda_{eq} = \Lambda$ and in fact is in $\Lambda \setminus \partial \Lambda$ (because of the bijection $i$) [14]). Recall $p_s$ is automatically a critical stabilizing control for $x(p_s)$. That this function has to map $x(p_s)$ back to $p_s$ is due to the fact that a rate vector from $\Lambda \setminus \partial \Lambda$ has exactly two critical stabilizing controls (one in $S \setminus \partial S$, the other in $[0, 1]^n \setminus S$), as shown at the end of the proof of Prop. 3. Therefore this function is onto. Thus we have shown the bijection $ii)$. The proof of $iii)$ is similar to that of $ii)$ and is omitted. The proof of $iv)$ follows from $ii)$ and $iii)$ due to transitivity. Finally $i)$ and $ii)$ together give $v)$.

Fig. 2 illustrates the three membership possibilities ($x \in \Lambda \setminus \partial \Lambda$, $x \in \partial \Lambda$, $x \notin \Lambda$) and the corresponding polynomials $f(\delta, x)$ for the case $n = 2$. The case $n = 2$ is the only (known) value of $n$ for which $\Lambda$ can be expressed explicitly ([8], [3], [14]), i.e., $\Lambda = \Lambda_A = \{x \in \mathbb{R}^2_+: \sqrt{x_1} + \sqrt{x_2} \leq 1\}$.

III. VOLUME OF $\Lambda$ AND AN INNER BOUND ON $\Lambda$

We first give a closed-form expression for the volume of $\Lambda$. Unfortunately its computation is a formidable task.

**Proposition 4:** The set $\Lambda$ defined in (1) has volume

$$\text{vol}(\Lambda) = \sum_{k \in K_{2^n, n-2}} \binom{n-2}{k}(-1)^{\sum_{i=1}^{n} \alpha(k)_{i}} \frac{\prod_{i=1}^{n} \alpha(k)_{i}!}{(n+1+\sum_{i=1}^{n} \alpha(k)_{i})!},$$

(14)

Fig. 2. Polynomial root membership testing when $n = 2$. The green curve corresponds to the interior point $x = (1/4, 1/5) \in \Lambda \setminus \partial \Lambda$, and has two positive roots: $(11 - \sqrt{41})/2, (11 + \sqrt{41})/2 \approx (2.2984, 8.7016)$; the blue curve corresponds to the boundary point $x = (1/16, 9/16) \in \partial \Lambda$ and has a unique positive root $16/3 \approx 5.3333$; the red curve corresponds to a point $x = (1/4, 1/3) \notin \Lambda$ and hence does not have any positive root.
where \((n-2)^{k}\) is a multinomial coefficient and \(K_{r,s} \equiv \{ k = (k_1, \ldots, k_r) \in \mathbb{Z}_+^r : \sum_{i=1}^r k_i = s \}.\) Furthermore, \(\alpha(k) = \sum_{i=1}^{2^n} V_{i,k} \) for \(V\) the \(n \times 2^n\) matrix whose columns are the \(2^n\) possible length-\(n\) binary vectors.

In coding theory, the matrix \(V\) is called a binary Hamming matrix.

**Proof:** Recall there is a bijection from \(S\) to \(\Lambda\) (Cor. 1). Let \(\tilde{J}(p) \equiv J(p)/\pi(p)\), where \(J(p)\) is the Jacobian of this mapping, namely the mapping \(p \mapsto x\) given by (9) in Def. 2:

\[
x_i(p) = p_i \prod_{j \neq i} (1 - p_j), \quad \text{for all } i \in [n], \quad p \in S.
\]  

(15)

The fact that \(\det(\alpha A) = \alpha^n \det A\) for any scalar \(\alpha\) and any \(n \times n\) matrix \(A\) yields \(\det J(p) = \pi(p)^n \det \tilde{J}(p)\).

Abramson [7] showed that \(\pi(p)^2 \det \tilde{J}(p) = 1 - p^T \mathbf{1}\), which gives \(\det J(p) = \pi(p)^{n-2} (1 - p^T \mathbf{1})\). Substituting this into the general expression for volume yields

\[
\text{vol}(\Lambda) = \int_S \det J(p) \, dp = \int_S \prod_{i=1}^n (1 - p_i)^{n-2} \left(1 - \sum_{j=1}^n p_j \right) \, dp.
\]  

(16)

In order to get a better closed-form expression, we leverage results in Grundmann and Möller [17], in particular (2.3) on integration of certain functions over the standard solid unit simplex \(S\):

\[
\int_S \mathbf{p}^\alpha \left(1 - \sum_i p_i \right) \, dp = \frac{\prod_{i=0}^{n} \alpha_i!}{(n + \sum_i \alpha_i)!},
\]  

(17)

where \(\mathbf{p} = (p_1, \ldots, p_n), \ \alpha = (\alpha_1, \ldots, \alpha_n),\) and \(\mathbf{p}^\alpha = \prod_{i=1}^{n} p_i^{\alpha_i}\). To apply this general expression to our case (16), we want to put \(\prod_{i=1}^{n} (1 - p_i)^{n-2}\) into a weighted sum of terms of the form \(\mathbf{p}^\alpha\). The multi-binomial theorem states, for arbitrary \(n\)-vectors \(\mathbf{a}, \mathbf{b},\) and positive \(n\)-vector \(\mathbf{c}\):

\[
\prod_{i=1}^{n} (a_i + y_i)^{c_i} = \sum_{k_1=0}^{c_1} \cdots \sum_{k_n=0}^{c_n} \left(\begin{array}{c} c_1 \\ k_1 \end{array} \right) a_1^{c_1-k_1} y_1^{k_1} \cdots \left(\begin{array}{c} c_n \\ k_n \end{array} \right) a_n^{c_n-k_n} y_n^{k_n}.
\]  

(18)

Specializing the above expression to the case \(\mathbf{a} = \mathbf{1}\) and \(\mathbf{c} = \mathbf{1}\) and arbitrary \(n\)-vector \(\mathbf{y}\) yields:

\[
\prod_{i=1}^{n} (1 + y_i)^{1} = \sum_{k_1=0}^{1} \cdots \sum_{k_n=0}^{1} \left(\begin{array}{c} 1 \\ k_1 \end{array} \right) 1^{1-k_1} y_1^{k_1} \cdots \left(\begin{array}{c} 1 \\ k_n \end{array} \right) 1^{1-k_n} y_n^{k_n} = \sum_{\mathbf{v} \in \{0,1\}^n} \left(\begin{array}{c} 1 \\ \mathbf{v} \end{array} \right) 1^{1-\mathbf{y}^{\mathbf{v}}},
\]  

(19)

where we employ the multi-index notation \(\left(\begin{array}{c} \mathbf{a} \\ \mathbf{b} \end{array} \right) = \prod_{i=1}^{n} \left(\begin{array}{c} a_i \\ b_i \end{array} \right)\) and \(\mathbf{a}^{\mathbf{b}} = \prod_{i=1}^{n} a_i^{b_i}\), for two \(n\)-vectors \(\mathbf{a}, \mathbf{b}\). Consequently, for \(\mathbf{y} = -\mathbf{p}\),

\[
\prod_{i=1}^{n} (1 - p_i)^{n-2} = \left(\sum_{\mathbf{v} \in \{0,1\}^n} (-\mathbf{p}^{\mathbf{v}}) \right)^{n-2} = \left(\sum_{i=1}^{2^n} (-\mathbf{p}_i^{\mathbf{v}_i}) \right)^{n-2} = \left(\sum_{i=1}^{2^n} (-p_i)^{\mathbf{v}_{i,t}} \right)^{n-2},
\]  

(20)

where \(\mathbf{v}_t\) is the \(t\)th column of \(\mathbf{V}\). The multinomial theorem states, for arbitrary \(r\)-vector \(\mathbf{y}\) and positive integer \(s\),

\[
(y_1 + \cdots + y_r)^s = \sum_{\mathbf{k} \in K_{r,s}} \binom{s}{\mathbf{k}} y^{\mathbf{k}},
\]  

(21)
for $\mathcal{K}_{r,s}$ defined in the proposition. We apply the multinomial theorem to the RHS of (20) and get

$$\prod_i (1 - p_i)^{n-2} = \sum_{k \in \mathcal{K}_{2^n,n-2}} \left( \prod_{i=1}^{n-2} \left( \begin{array}{c} n-2 \\ k_{1_i}, \ldots, k_{2^n} \end{array} \right) \prod_{t=1}^{k_t} (-p_t)^{y_{t,i}} \right)^{k_t} = \sum_{k \in \mathcal{K}} \left( \prod_{i=1}^{n-2} \left( \begin{array}{c} n-2 \\ k_{1_i}, \ldots, k_{2^n} \end{array} \right) (-1)^{\sum_{i=1}^{n-2} k_i} \prod_{i=1}^{n} p_i^{\alpha_i} \right)^{k_t}, \tag{22}$$

for $\alpha_i$ defined in the proposition. Finally substitution of this expression of $\prod_i (1 - p_i)^{n-2}$ into (16) and application of (17) with $\alpha_0 = 1$ yields the desired volume expression in (14).

The number of summands in (14) is the number of multinomial coefficients. Equivalently, it is the number of ways to write $n - 2$ as an ordered sum of $2^n$ non-negative integers, and is given by $(n - 2 + 2^n - 1)$ (see e.g., Wilf [18] Ex. 3 in Chapter 2). Applying an easy lower bound on the binomial coefficient $\binom{n}{k} \geq \left( \frac{n}{k} \right)^k$, we have $(n - 2 + 2^n - 1) \geq \left( 1 + \frac{2^n - 1}{n - 2} \right)^{n-2}$, meaning it grows super-exponentially in $n$, and hence calculation of $\text{vol}(\Lambda)$ using Prop. 4 requires substantial computation for even moderate $n$.

We now initiate our pursuit of non-parametric bounds on $\Lambda$, which is the focus of the next three sections. Recall it is already known that when $n = 2$, $\Lambda$ equals a non-parametric set $\{ x \in \mathbb{R}^2_+ : \sqrt{x_1} + \sqrt{x_2} \leq 1 \}$ [8], [3], [14] for which membership testing is simple. Naturally one might wonder how the natural extension of this sum relates to $\Lambda$ for higher values of $n$. This motivates the following definition of the “square root sum” set. The proposition below shows in general this set is only an inner bound on $\Lambda$. In the subsequent proof and elsewhere throughout the paper, we use the fact that $\Lambda$ is coordinate convex, meaning if $x \in \Lambda$ then $x' \in \Lambda$ for all $0 \leq x' \leq x$.

**Definition 4:**

$$\Lambda_{\text{srs}} \equiv \left\{ x \in \mathbb{R}^+_n : \sum_{i=1}^n \sqrt{x_i} \leq 1 \right\}. \tag{23}$$

**Proposition 5 (“square root sum” inner bound):** The set $\Lambda_{\text{srs}}$ is an inner bound on $\Lambda$ for $n \geq 2$.

**Proof:** Fix a point $x' \in \Lambda_{\text{srs}}$. Due to the coordinate convexity of $\Lambda$ and $\Lambda_{\text{srs}}$, it suffices to produce a point $x \in \Lambda$ so that $x \geq x'$. Set $p_i = \sqrt{x_i'}$ for each $i$ and set $x = x(p)$ according to (9) in Def. 2. Clearly $x \in \Lambda$. It remains to show $x_i \geq x_i'$ for each $i \in [n]$. Note $x' \in \Lambda_{\text{srs}}$ ensures $\sum_{i=1}^n p_i \leq 1$. Define independent events $A_1, \ldots, A_n$ with $\mathbb{P}(A_i) = 1 - p_i$ for each $i \in [n]$. Denote the complement of event $A_i$ by $A_i^c$. It follows that

$$1 - \mathbb{P} \left( \bigcup_{j \neq i} A_j^c \right) = \mathbb{P} \left( \bigcap_{j \neq i} A_j \right) = \prod_{j \neq i} \mathbb{P}(A_j) = \prod_{j \neq i} (1 - p_j). \tag{24}$$

Then for any $i$, reversely applying (24) to $x_i$ followed by the union bound and then the fact $\sum_{i=1}^n p_i \leq 1$, we have

$$x_i = p_i \left( 1 - \mathbb{P} \left( \bigcup_{j \neq i} A_j^c \right) \right) \geq p_i \left( 1 - \sum_{j \neq i} \mathbb{P}(A_j^c) \right) = p_i \left( 1 - \sum_{j \neq i} p_j \right) \geq p_i^2 = x_i'. \tag{25}$$

\[\blacksquare\]
Proposition 6: The volume of the inner bound \( \Lambda_{\text{srs}} \) is

\[
\text{vol}(\Lambda_{\text{srs}}) = \frac{2^n}{(2n)!}. \tag{26}
\]

Proof: Use the change of variable \( y_i = \sqrt{x_i}, \forall i \in [n] \) so that the volume integration becomes

\[
\text{vol}(\Lambda_{\text{srs}}) = \int_{[0,1]^n} \prod_{i=1}^n \sqrt{x_i} \, dx_1 \cdots dx_n = 2^n \int_{[0,1]^n} \prod_{i=1}^n y_i \, dy_1 \cdots dy_n
\]

\[
= 2^n \int_0^1 y_n \int_0^{1-y_n} \cdots \int_0^{1-y_n-\cdots-y_3} y_2 \int_0^{1-y_n-\cdots-y_2} y_1 \, dy_1 dy_2 \cdots dy_{n-1} dy_n. \tag{27}
\]

It will be useful to first compute an integral denoted \( I(d,k) = \int_0^d y(d-y)^k \, dy \) for \( d \geq 0, \ k \in \mathbb{Z}_+ \): instead of expanding the integrand using binomial theorem and then handling some alternating sum, we proceed as follows:

\[
-I(d,k) + \int_0^d d(d-y)^k \, dy = \int_0^d (d-y)^{k+1} \, dy = \frac{1}{k+2} d^{k+2}
\]

\[
\Rightarrow \quad I(d,k) = \int_0^d (d-y)^k \, dy - \frac{1}{k+2} d^{k+2} = d \frac{1}{k+1} d^{k+1} - \frac{1}{k+2} d^{k+2} = \frac{1}{(k+1)(k+2)} d^{k+2}. \tag{28}
\]

For \( j \in [n] \) define \( k_j = 2(j-1) \) and for \( j \in [n-1] \) define \( d_j = 1 - y_n - \cdots - y_{j+1} \), and \( d_n = 1 \). Observe the recurrences \( k_j + 2 = k_{j+1}, \ d_j = d_{j+1} - y_{j+1} \). Specializing (28) with parameters \( d_j, k_j \) and dummy integrating variable \( y_j \), we have

\[
I(d_j, k_j) = \int_0^{d_j} y_j(d_j - y_j)^{k_j} \, dy_j = \frac{1}{(k_j + 1)(k_j + 2)} d_j^{k_j+2}, \ \forall j \in [n]. \tag{29}
\]

Now we are ready to resume the computation of \( \text{vol}(\Lambda_{\text{srs}}) \) in (27). Using our new notation, we have:

\[
\text{vol}(\Lambda_{\text{srs}}) = 2^n \int_0^1 y_n \int_0^{d_n-1} y_{n-1} \cdots \int_0^{d_2} y_2 \int_0^{d_1} y_1 (d_1 - y_1)^{k_1} \, dy_1 dy_2 \cdots dy_{n-1} dy_n. \tag{30}
\]

We can then repeatedly apply (29) with \( j \in [n] \). To see this, observe after the \( j^{\text{th}} \) innermost integration, the new innermost integration is

\[
\int_0^{d_{j+1}} \prod_{s=1}^j \frac{1}{(k_s + 1)(k_s + 2)} y_j+1 d_{j+1}^{k_{j+2}} dy_{j+1} = \prod_{s=1}^j \frac{1}{(k_s + 1)(k_s + 2)} \int_0^{d_{j+1}} \ y_{j+1} (d_{j+1} - y_{j+1})^{k_{j+1}} \, dy_{j+1}, \tag{31}
\]

which is \( \prod_{s=1}^j \frac{1}{(k_s + 1)(k_s + 2)} I(d_{j+1}, k_{j+1}) \).

Therefore, after the \( j = (n-1)^{\text{st}} \) innermost integration, we have

\[
\text{vol}(\Lambda_{\text{srs}}) = 2^n \int_0^1 \frac{1}{(k_s + 1)(k_s + 2)} \int_0^{d_n} y_n d_n^{k_n+2} \, dy_n = 2^n \int_0^1 \frac{1}{(k_s + 1)(k_s + 2)} \int_0^{d_n} y_n (d_n - y_n)^{k_n} \, dy_n
\]

\[
= 2^n \prod_{s=1}^{n-1} \frac{1}{(k_s + 1)(k_s + 2)} I(d_n, k_n) = 2^n \prod_{s=1}^n \frac{1}{(k_s + 1)(k_s + 2)} d_n^{k_n+2} = 2^n \prod_{s=1}^n \frac{1}{(2s-1)(2s)}
\]

\[
= \frac{2^n}{(2n)!} \tag{32}
\]
Although simple, as has been seen in Fig. 1 (in §I), $\Lambda_{srs}$ is a poor inner bound. In the following three sections we present various inner and outer bounds on $\Lambda$ based on polyhedra (§IV), spheres (§V), and ellipsoids (§VI).

IV. POLYHEDRAL INNER AND OUTER BOUNDS ON $\Lambda$

In this section we form inner and outer bounds on $\Lambda$ using polyhedra. The inner bound is formed using a single hyperplane, i.e., a generalized simplex, while the outer bound is formed using the intersection of a collection of $n + 1$ hyperplanes in $\mathbb{R}_+^n$.

**Definition 5:**

$$\Lambda_{pi}(p) \equiv \left\{ x \in \mathbb{R}_+^n : (1-p)^T x \leq \prod_{i}(1-p_i) \right\}, \text{ where } p \in \partial S. \quad (33)$$

Geometrically, the set $\Lambda_{pi}(p)$ is a generalized simplex bounded by the $n$ coordinate hyperplanes and the hyperplane with normal vector $1 - p$. All such hyperplanes are tangent to $\partial \Lambda$ with a tangency point at $x(p)$ in (9) in Def. 2. The following proposition asserts for each given $p$ this set is an inner bound on $\Lambda$, indicates the $p^*$ that achieves the largest volume bound over this family of inner bounds, and also computes the corresponding volume.

**Proposition 7 (polyhedral inner bound):** For each $p \in \partial S$, the set $\Lambda_{pi}(p)$ is an inner bound on $\Lambda$ for $n \geq 2$.

Among these, the tightest is given when $p = p^* = \frac{1}{n} 1$, namely,

$$\Lambda_{pi}^* = \Lambda_{pi}(p^*) = \left\{ x \in \mathbb{R}_+^n : \sum_{i=1}^{n} x_i \leq \left(1 - \frac{1}{n}\right)^{n-1} \right\}. \quad (34)$$

and the corresponding volume of this set is $\text{vol}(\Lambda_{pi}^*) = \frac{1}{n!} \left(1 - \frac{1}{n}\right)^{n(n-1)}$.

**Proof:** Recall Post [15] established that the complement of $\Lambda$ in $\mathbb{R}_+^n$ is convex, and gave the tangent hyperplane at a point $x(p)$ on $\partial \Lambda$: $\{ x : (1-p)^T x = \prod_{i}(1-p_i) \}$, where $p \in \partial S$ is the unique vector associated with a point $x \in \partial \Lambda$. Since this hyperplane is a supporting hyperplane, this open convex set $\Lambda^c \cap \mathbb{R}_+^n$ lies entirely on one “side”, i.e., the open halfspace $\{ x : (1-p)^T x > \prod_{i}(1-p_i) \}$, of the hyperplane. This means points on the other side of this hyperplane are not in $\Lambda^c \cap \mathbb{R}_+^n$, and hence are in $\Lambda$, i.e., $\Lambda_{pi}(p) \subseteq \Lambda$.

Now notice $L_{pi}(p)$ is a generalized simplex, and its volume is given by ([19]):

$$\text{vol}(\Lambda_{pi}(p)) = \frac{1}{n!} \prod_{i=1}^{n} \prod_{j \neq i}^{n} (1 - p_j) = \frac{1}{n!} \left( \prod_{i=1}^{n} (1 - p_i) \right)^{n-1}. \quad (35)$$

It is easily shown that the function $\prod_{i=1}^{n} (1 - p_i)$ is maximized over $p \in \partial S$ at $p = \frac{1}{n} 1$, and hence the best $\Lambda_{pi}$ (in terms of achieving the largest volume) is given by (34).
Remark 1: Using upper and lower bounds on the factorial [20], one can show \( \text{vol}(\Lambda^*_p) \leq \text{vol}(\Lambda_{\text{rs}}) \) for all \( n \geq 3 \).

Next we construct a polyhedral outer bound. If we restrict ourselves to only using a single halfspace, the best choice is the standard simplex, \( S \), which is a very loose outer bound. Consequently, we consider a specific construction using \( 2n + 1 \) hyperplanes. The convex polytope given below is a subset of \( S \) (and in fact a subset of \( S \setminus \Lambda \)), has \( \partial S \) as a facet, and an additional \( n \) facets each defined by a hyperplane, \((H^+_1, \ldots, H^+_n)\), where \( H^+_i \) is the hyperplane passing through \( e_i, m \), and \( \alpha e_j \) for all \( j \neq i \), for \( \alpha \) given below.

Definition 6: The halfspace representation of the convex polytope \( P \) in \( \mathbb{R}^n \) consists of the following halfspaces:

\[
H^+_i = \left\{ \mathbf{x} \in \mathbb{R}^n : x_i + \frac{1}{\alpha(n)} \sum_{j \neq i} x_j \geq 1 \right\}, \quad i \in [n],
\]

\[
H^0 \equiv \mathbf{x} \in \mathbb{R}^n : x_i \geq 0, \quad i \in [n],
\]

\[
H^{\partial S} = \left\{ \mathbf{x} \in \mathbb{R}^n : \sum_{i=1}^n x_i \leq 1 \right\},
\]

where

\[
\alpha(n) = \frac{n-1}{1 - \frac{1}{n}} - \frac{n-1}{m(n) - 1} = \frac{n - 1}{(1 - \frac{1}{n})^{n-1} - 1},
\]

and the superscript \( + \) indicates an “upward” halfspace and \( - \) indicates a “downward” halfspace. More compactly,

\[
P = \left\{ \mathbf{x} \in \mathbb{R}^n : \mathbf{x} \in \bigcap_{i \in [n]} H^+_i \bigcap_{i \in [n]} H^+ \setminus H^{\partial S} \right\}.
\]

Furthermore, the corresponding hyperplane is denoted by dropping these superscripts, meaning the inequality in the definition holds with equality. For example, \( H^+_i \) denotes the coordinate hyperplane \( \{ \mathbf{x} \in \mathbb{R}^n : x_i = 0 \} \).

Proposition 8 (polyhedral outer bound): The convex polytope \( P \) defined above induces an outer bound on \( \Lambda \). More precisely, \( \Lambda \subseteq \Lambda_{\text{po}} = S \setminus P \).

To prove the correctness of this bound it will be essential to establish the monotonicity of \( \alpha(n) \) (37).

Lemma 1: The function \( \alpha(n) \) (37) is monotone increasing for \( n \geq 2 \). In particular, \( \alpha(2) = 1/3, \alpha(3) = 8/23, \alpha(\infty) = 1/e \).

Proof: The derivative of \( \alpha(n) \) (37) is

\[
\frac{d\alpha(n)}{dn} = \frac{(n-1)^2}{n} \left( 1 - \frac{1}{n} \right)^{n-1} \left( 1 - \frac{1}{n} \right)^{n-1} + (n-1) \log \left( 1 - \frac{1}{n} \right),
\]

for which the sign is determined by the sign of \( g(n) = 1 - \frac{1}{n} \left( 1 - \frac{1}{n} \right)^{n-1} + (n-1) \log \left( 1 - \frac{1}{n} \right) \). To show the positivity of \( g(n) \) for all \( n \geq 2 \), first observe \( \lim_{n \to \infty} g(n) = 0 \). It therefore suffices to show \( g(n) \) is itself monotone...
decreasing in $n$, which is shown below:

$$
\frac{n \log(n)}{dn} = 1 + n \left( 1 - \frac{1}{n} \right) \left( 1 - \frac{1}{n} \right)^{n-1} \log \left( 1 - \frac{1}{n} \right)
\leq (a) 1 + n \left( 1 - \frac{1}{n} \right) \left( 1 - \frac{1}{n} \right)^{n-1} \left( - \frac{1}{n} - \frac{1}{2n^2} - \frac{1}{3n^3} \right)
\leq (b) 1 + n \left( 1 - \frac{1}{2n} \right) \left( - \frac{1}{n} - \frac{1}{2n^2} - \frac{1}{3n^3} \right) = - \frac{n - 2}{12n^3} \leq 0,
$$

where we use in $(a)$ the inequality $\log(1+x) \leq x - \frac{x^2}{2} + \frac{x^3}{3}$ for all $x \in (-1, 0)$ and $(b)$ the property that $(1 - \frac{1}{n})^{n-1}$ is monotone decreasing in $n$ from $1/2$ (when $n = 2$) to $1/e$ (when $n = \infty$).

**Proof:** (of Prop. 8) Our approach is to show all the vertices of the convex polytope $P$ are in $X^c$, it then follows from the convexity of $X^c \cap \mathbb{R}^n_+$ that $P \subseteq X^c \cap \mathbb{R}^n_+$ which implies $\Lambda_{po} \equiv S \setminus P \supseteq \Lambda$.

To find a vertex, we first choose $n$ out of the $2n + 1$ hyperplanes defining $P$. If there is a solution to this linear system which is a single point that also obeys the remaining $n + 1$ halfspace constraints, then this solution is a valid vertex (indicated below as underlined cases). Furthermore, since our primary goal is to show all the vertices are in $X^c$, rather than to list all the vertices, for simplicity we only consider the scenario where those $n$ selected hyperplanes do not include $H^{\partial S}$. This is justified since the intersection of $H^{\partial S}$ and $n$ halfspaces $H_i^{c+}$, namely $\partial S$, lies completely in $X^c$, so if there exists a valid vertex on $H^{\partial S}$ it is guaranteed to be in $X^c$.

Consequently, we choose a set of hyperplanes from $\{ H_i^{c+} \}_{i=1}^n$ (denoted $S$) and a set of hyperplanes from $\{ H_i^{c+} \}_{i=1}^n$ (denoted $T$) so that their cardinalities $|S|$ and $|T|$ sum to $n$. We also assume we choose the first $|S|$-indexed hyperplanes from $\{ H_i^{c+} \}_{i=1}^n$; this holds no loss of generality as we may always permute the indices of the hyperplanes, and the polytope $P$ is symmetric with respect to such permutations. For notational convenience define $I_S$ and $I_T$ as the set of indices appearing as subscripts of the elements in the set $S$ and $T$ respectively. For example, if $S = \{ H_1^{c+}, H_2^{c+} \}$, then $I_S = \{ 1, 2 \}$; if $T = \{ H_1^{c+} \}$, then $I_T = \{ 1 \}$. Recall, $m(k) = \frac{1}{k} (1 - \frac{1}{k})^{k-1}$ for $k \in [n]$ stands for the coordinate of the all-rates-equal point on $\partial \Lambda$ in a $k$-dimensional space.

We discuss cases based on the pair $(|I_S \cap I_T|, |S|)$

- **case 1:** $|I_S \cap I_T| = 0, |S| = n$. Namely we choose all $n$ $H_i^{c+}$’s, to which the only solution is all-rates-equal point $m = m_1$, which is in $X^c$.

- **case 2:** $|I_S \cap I_T| = 0, |S| = k$ for $1 \leq k < n$. Namely $S = \{ H_1^{c+}, \ldots, H_k^{c+} \}$, $T = \{ H_{k+1}^{c+}, \ldots, H_n^{c+} \}$. The only solution can be shown to be $x = \left( 1 + \frac{k-1}{n} \right)^{-1} \sum_{j=1}^k e_j$. To verify this point $x$ is in $P$, we first verify it satisfies the halfspace constraint $H_i^{c+}$, i.e., $x_{k+1} + \frac{1}{n} \sum_{j \neq k+1} x_j \geq 1$, which applied to this point becomes $\alpha(n) \leq 1$. Similarly $x$ also satisfies the halfspace constraints associated with $H_{k+2}^{c+}, \ldots, H_n^{c+}$. Next, for $x$
to satisfy the halfspace constraint $\mathcal{H}^{\partial S}$, we again only need $\alpha(n) \leq 1$. Finally the nonnegativity constraint for each coordinate axis $\mathcal{H}_i^{e+}$ is satisfied, so this solution is a valid vertex. We now need to show $x \in \overline{\mathcal{X}}$. Observe this vertex’s effective length is $k$ so we need to check $\overline{\mathcal{X}}$ in the corresponding $k$-dimensional space; furthermore, all the non-zero components of $x$ are identical meaning $x$ lies along the all-rates-equal ray in this $k$-dimensional space so we only need to show $x$ extends beyond the corresponding all-rates-equal point $m = m(k)1$ for a $k$-vector of all 1’s. Applying Lem. 1, we have $(1 + \frac{k-1}{\alpha(n)})^{-1} \geq (1 + \frac{k-1}{\alpha(k)})^{-1} = m(k)$.

Thus we’ve shown this case does produce a valid vertex in $\overline{\mathcal{X}}$.

- case 3: $|\mathcal{I}_S \cap \mathcal{I}_T| = 0$, $|S| = 0$. Namely we choose all $n$ coordinate hyperplane $\mathcal{H}_i^{e+}$’s. The only solution is the origin $0$, which is not in $P$, hence this is an invalid vertex.

- case 4: $|\mathcal{I}_S \cap \mathcal{I}_T| = 1$, $|S| = k$ for $1 \leq k < n$. In this case, in order to further satisfy $|S| + |T| = n$, there must exist some index $k' \geq k + 1$ such that $\mathcal{H}_{k'}^{e} \notin T$. In fact if we assume $\mathcal{H}_i^{0} \in T$, this determines $T = \{\mathcal{H}_1^{c}, \mathcal{H}_{k+1}^{c}, \ldots, \mathcal{H}_{n}^{c}\} \setminus \{\mathcal{H}_{k'}^{c}\}$. The solution can be shown to be $x = \alpha e_{k'}$, which is not in $P$, and hence is not a valid vertex. Note this conclusion does not depend on our choice of $\mathcal{H}_i^{0}$ to be included in $T$.

- case 5: $|\mathcal{I}_S \cap \mathcal{I}_T| > 1$, $|S| = k$ for $1 < k < n-1$. In this case, in order to further satisfy $|S| + |T| = n$, there must exist $l = |\mathcal{I}_S \cap \mathcal{I}_T|$ indices such that the corresponding coordinate hyperplanes are not in $T$. Attempt to solve this system shows this is an underdetermined system because the solution is given by a hyperplane instead of a point.

Furthermore, if we want to ensure the solution is in $P$, we find there is no consistent solution. As $S = \{\mathcal{H}_1^{e}, \ldots, \mathcal{H}_k^{e}\}$, suppose $T$ does not include, say, $\mathcal{H}_{k+1}^{e}, \ldots, \mathcal{H}_{k+l}^{e}$ (as well as $\mathcal{H}_{l+1}^{e}, \ldots, \mathcal{H}_{n}^{e}$), so $T = \{\mathcal{H}_1^{e}, \ldots, \mathcal{H}_k^{e}, \mathcal{H}_{k+l+1}^{e}, \ldots, \mathcal{H}_{n}^{e}\}$. Solving these $n$ equations gives an $l$-dimensional hyperplane: $\{x : x_{k+1} + \cdots + x_{k+l} = \alpha\}$.

Satisfying the halfspace constraint $\mathcal{H}_{k+1}^{e+}$ as well as each nonnegativity component constraints $\mathcal{H}_i^{e+}$ requires $x_{k+1} = 0$. Similarly, due to each other halfspace constraint $\mathcal{H}_{k+2}^{e+}, \ldots, \mathcal{H}_{k+l}^{e+}$, each other component $x_{k+2}, \ldots, x_{k+l}$ would also need to be set to zero, which altogether leads to no valid (vertex) solution.

To summarize, each valid vertex solution we have found is such that: i) its non-zero components are all equal, and ii) this non-zero component value is no smaller than the coordinate of all-rates-equal point in the corresponding possibly reduced-dimensional space, which means all those vertices are in $\overline{\mathcal{X}}$. More precisely, each vertex extends beyond (or coincides with) the corresponding all-rates-equal point (which lies on the boundary of $\Lambda$), and can be written as (up to permutation of the indices) $x = \left(1 + \frac{k-1}{\alpha(n)}\right)^{-1} \sum_{j=1}^{k} e_j$ for $k \in [n]$. In particular, when $k = 1$, $x = e_1$; when $k = n$, $x = m$.

Remark 2: One can perform a similar analysis considering the scenario where $\mathcal{H}^{\partial S}$ is selected. The only valid vertex solutions consist of just $e_i$’s for all $i \in [n]$. 

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We give the vertex representation of the convex polytope $P$ when $n = 2$ and $n = 3$ in the following example. The bounds $\Lambda_{\text{pi}}$ and $\Lambda_{\text{po}}$ together with $\partial \Lambda$ are illustrated in Fig. 3.

**Example 1:** When $n = 2$, since $\alpha(2) = 1/3$, the vertices of $P$ are $\{e_1, e_2, m\}$, here $m = m(2)1$ for $m(2) = 1/4$.

When $n = 3$, since $\alpha(3) = 8/23$, the vertices of $P$ are $\{e_1, e_2, e_3, (8/31)(e_1 + e_2), (8/31)(e_1 + e_3), (8/31)(e_2 + e_3), m\}$, here $m = m(3)1$ for $m(3) = 4/27$. Those vertices are also shown in Fig. 3. Note $8/31 > 1/4$ thus each of the three green points in the right subfigure extends beyond the all-rates-equal point on the corresponding 2-dimensional plane namely the orange point in the left subfigure.

![Fig. 3. Polyhedral bounds for $n = 2$ (left) and 3 (right).](image)

In this section we consider bounds induced by spheres. More specifically we want $S \setminus B(c, r)$ to be included in (for inner bounding) or to include (for outer bounding) $\Lambda$, where $B(c, r)$ denotes the open ball in $\mathbb{R}^n$ with center $c$ and radius $r$, and $\partial B(c, r)$ is its boundary. By symmetry, we restrict our attention to balls with centers on the all-rates-equal ray, i.e., $c = e1$ for some $c > 0$. In the following, Prop. 9 establishes a family of inner bounds...
induced by balls centered at $c = c1$ with radius $r(c) = d(c, m)$ (i.e., $m \in \partial B(c, r)$), and among them the best one (in the sense of giving the best approximation of the volume of $\Lambda$) is obtained by $c = (1 - nm^2)/(2(1 - nm))$, which is indeed the minimum $c$ for $\Lambda$.

Prop. 10, establishes a family of outer bounds induced by balls centered at $c = c1$ with radius defined as $r(c) = d(c, e_i)$ (i.e., $e_i \in \partial B(c, r)$ for $i \in [n]$), and among them the best one is given when $c = 1$, which is also the minimum $c$ in order to produce a valid spherical outer bound in this family.

**Definition 7:** $\Lambda_{si}(c) \equiv S \setminus B(c, r_{in}(c))$, where the center of the ball is $c = c1$ for all $c \geq c^*_{in} \equiv (1 - nm^2)/(2(1 - nm))$, and its radius $r_{in}(c) \equiv d(c, m) = \sqrt{n}(c - m)$.

**Proposition 9 (spherical inner bound):** For each $c \geq c^*_{in}$, the set $\Lambda_{si}(c)$ is an inner bound on $\Lambda$ for $n \geq 2$.

Among these, the tightest is given when $c = c^*_{in}$:

$$\Lambda^*_i = \Lambda_{si}(c^*_{in}) = \{x \in S : \|x - c^*_{in}1\| \geq \sqrt{n}(c^*_{in} - m)\}. \tag{41}$$

**Proof:** Here is an overview of the proof. First, we observe the correctness of the spherical inner bound with some $c$ implies the correctness of an inferior bound with a larger $c$ (Lem. 2), so we only need to show the correctness of the bound with the minimum $c$ namely $c^*_{in}$. Second, by inspecting the Karush-Kuhn-Tucker (KKT) conditions, we argue a potential local extremizer can have at most two distinct non-zero component values, and also obtain a condition the components of this extremizer must satisfy ((54)). Third, we address the case when a potential extremizer does not have zero component and has exactly two distinct non-zero component values, and we show such a point can be safely ruled out for the optimization problem set up in Step 2. Fourth, we consider the case when a potential extremizer has zero component(s), and show this point can be removed too (unless it reduces to $e_i$). Finally, it is clear we only need to evaluate the objective function at $m$ and $e_i$.

**Step 1:** correctness of the bound with small $c$ implies correctness and inferiority of the bound with larger $c$. Lem. 2 below establishes that $c_2 \geq c_1 \geq m$ implies $B(c_2, d(c_2, m)) \supseteq B(c_1, d(c_1, m))$, i.e., the balls in this family are nested in $c$. Since $\Lambda_{si}(c) = S \setminus B(c, r_{in}(c))$, it follows that $c_2 \geq c_1 \geq m$ implies $\Lambda_{si}(c_1) \supseteq \Lambda_{si}(c_2)$, i.e., the induced bounds are likewise nested, and thus the optimal (largest) bound in this family is obtained by the smallest $c$ in the family. Because of this, we need only establish that $\Lambda_{si}(c) \subseteq \Lambda$ for this smallest $c$ in the family. To establish $c^*_{in}$ is the minimum $c$, it suffices to verify the following:

$$d(c, m) <, =, > d(c, e_i) \text{ if and only if } c <, =, > c^*_{in} \text{ respectively.} \tag{42}$$

This is straightforward to establish, and the proof is omitted. Assuming (42) to be true, it follows that if $c < c^*_{in}$ then each $e_i$ will not be included in the closed ball $\overline{B}(c, r_{in})$, implying the induced bound $S \setminus B(c, r_{in})$ is invalid.
(since each $e_i \in \Lambda$).

**Lemma 2:** $B(c_2, d(c_2, m)) \supseteq B(c_1, d(c_1, m))$ for $c_2 \geq c_1 \geq m$.

**Proof of Lem. 2:** For simplicity we shift the origin of coordinate system along the all-rates-equal ray $1$ so that it overlaps with $m$ in the original system. In the new system we have $c'_2 = c_2 - m$, $c'_1 = c_1 - m$, and $m' = 0$, and we need to show $B(c'_2, d(c'_2, o')) \supseteq B(c'_1, d(c'_1, o'))$ for $c'_2 \geq c'_1 \geq 0$, where $o'$ denotes the origin of the new system. Observe $d(c'_j, o') = \sqrt{n}c'_j$ for $j = 1, 2$. So we need to verify for all $x$ satisfying $\sum_i (x_i - c'_1)^2 \leq nc'_1^2$, it holds that $\sum_i (x_i - c'_2)^2 \leq nc'_2^2$. Towards this, we write

$$\sum_i (x_i - c'_2)^2 = \sum_i (x_i - c'_1)^2 + n(c'_2 - c'_1)^2 - 2(c'_2 - c'_1) \sum_i (x_i - c'_1) \leq nc'_2^2 + n(c'_2 - c'_1)^2 - 2(c'_2 - c'_1) \sum_i (x_i - c'_1).$$

(43)

So it suffices to show the RHS is no larger than $nc'_2^2$, which is equivalent to showing $\sum_i x_i \geq 0$. We claim this is true, because the hyperplane $\{x \in \mathbb{R}^n : \sum_i x_i = 0\}$ is tangent with $B(c'_1, d(c'_1, o'))$ at $o'$, and in fact it is a supporting hyperplane of the convex body $B(c'_1, d(c'_1, o'))$. □

Steps 2, 3, and 4 are actually valid for $\Lambda_{si}(c)$ for all $c$, not just $c = c^*_m$, and so we consider an arbitrary $\Lambda_{si}(c)$ in what follows.

**Step 2:** properties of a potential extremizer for $\Lambda_{si}$. By Prop. 15 in §VI-A, it suffices to establish $\partial \Lambda \subseteq \overline{B}(c, r_m)$, i.e., given any point $x \in \partial \Lambda$, its distance to the center of the sphere is no larger than the sphere’s radius:

$$\max_{x \in \partial \Lambda} d(c, x)^2 \leq r_m^2. \tag{44}$$

Recall from Cor. 1 (§II) the bijection between $\partial \Lambda$ and $\partial S$, and write $x(p)$ to denote the unique $x \in \partial \Lambda$ associated with each $p \in \partial S$. Under this bijection, the LHS of (44) becomes

$$\max_{p \in \partial S} f(p) \equiv d(c, x(p))^2 = \sum_{i=1}^n \left( c - \frac{1}{n-1} \prod_{j \neq i}^n (1-p_j) \right)^2. \tag{45}$$

Introducing Lagrange multipliers $\mu$, $(\lambda_i, i \in [n])$ for the equality constraint and $n$ inequality constraints in $\partial S$, respectively, the Lagrangian of this maximization problem becomes:

$$\mathcal{L}(p, \mu, \lambda) = f(p) + \mu \left( \sum_{i=1}^n p_i - 1 \right) + \sum_{i=1}^n \lambda_i (-p_i). \tag{46}$$
The first-order Karush-Kuhn-Tucker (KKT) necessary conditions for a local maximizer are:

stationarity \[ \frac{dL}{dp_i} = 0, \quad i \in [n] \quad (47) \]

primal feasibility \[ \sum_{i=1}^{n} p_i - 1 = 0, \quad -p_i \leq 0, \quad i \in [n] \quad (48) \]

dual feasibility \[ \lambda_i \leq 0, \quad i \in [n] \quad (49) \]

complementary slackness \[ \lambda_i (-p_i) = 0, \quad i \in [n]. \quad (50) \]

Note the regularity condition LICQ (linear independence constraint qualification) is satisfied.

Observe \( \frac{dL}{dp_i} = \frac{df}{dp_i} + \mu - \lambda_i \). Therefore, if a potential local maximizer \( \mathbf{p} \) has two distinct non-zero components \( 0 < p_k < p_l \) then, by complementary slackness, stationarity of the Lagrangian reduces to the equality of derivatives of the objective function w.r.t. \( p_k \) and \( p_l \):

\[ \frac{dL}{dp_k} = \frac{dL}{dp_l} = 0 \Leftrightarrow \frac{df}{dp_k} = \frac{df}{dp_l} = -\mu. \quad (51) \]

The derivative of \( f \) w.r.t. \( p_k \) is

\[ \frac{1}{2} \frac{df}{dp_k} = -\frac{\pi_k}{1 - p_k} (c - p_k \pi_k) + \frac{1}{1 - p_k} \sum_{i=1}^{n} p_i (c - p_i \pi_i) \pi_i, \quad (52) \]

where \( \pi_i = \pi_i(\mathbf{p}) \equiv \pi(\mathbf{p})/(1 - p_i) \). Similarly we can write out the derivative w.r.t. \( p_l \). Equating the two by further multiplying both sides by \( (1 - p_k)(1 - p_l) \) gives

\[ (1 - p_l) (\eta_c - (c - p_k \pi_k) \pi_k) = (1 - p_k) (\eta_c - (c - p_l \pi_l) \pi_l), \quad (53) \]

where \( \eta_c \equiv \sum_{i=1}^{n} p_i (c - p_i \pi_i) \pi_i \) and hence \( \eta_c \) can be viewed as the expectation of a discrete random variable \( Z \) with support \( \{(c - p_i \pi_i) \pi_i, \; i \in [n]\} \) and associated PMF \( \mathbb{P}(Z = (c - p_i \pi_i) \pi_i) = p_i \) for each \( i \in [n] \). So the only way to satisfy the above equality (for all \( k, l \) such that \( 0 < p_k < p_l \)) is by requiring \( (c - p_i \pi_i) \pi_i \) to be all equal for \( i \)'s such that \( p_i \neq 0 \) (because otherwise we can always choose \( k', l' \) so that \( \eta_c \) lies between \( (c - p_{k'} \pi_{k'}) \pi_{k'} \) and \( (c - p_{l'} \pi_{l'}) \pi_{l'} \)). In particular, \( (c - p_i \pi_i) \pi_i = (c - p_k \pi_k) \pi_k \), which simplifies, after some algebra, to:

\[ c = \frac{\pi(\mathbf{p})}{(1 - p_k)(1 - p_l)} (1 - p_k p_l). \quad (54) \]

Because of the constraint enforced by (54), we claim there are at most two distinct values among all the non-zero components of a potential local extremizer. To see this, we prove by contradiction. Assume there exist \( p_j, p_k, p_l \) such that \( 0 < p_j < p_k < p_l < 1 \). Then (54) must hold with indices \( \{j, k\} \) replacing indices \( \{k, l\} \). Equating the two resulting expressions for \( c \) gives \( p_j = p_l \), a contradiction.
With the above claim, we only need to consider points that have at most two distinct non-zero component values. Define \( \mathcal{V}(p) = \{a \in (0, 1) : \exists i \in [n] : p_i = a\} \) as the set of non-zero values taken by a \( p \in \partial \mathcal{S} \), and \( \mathcal{Z}(p) = \{i \in [n] : p_i = 0\} \) as the set of indices where \( p \) has a zero value. The set of probability vectors taking at most two distinct non-zero component values is then denoted \( \mathcal{P}^{(2)} = \{p \in \partial \mathcal{S} : |\mathcal{V}(p)| \in \{1, 2\}\} \). We partition this set into two subsets, \( \mathcal{P}^{(2)} = \mathcal{P}^{(2)}_a \cup \mathcal{P}^{(2)}_b \), which are in turn each partitioned into two subsets, \( \mathcal{P}^{(2)}_a = \mathcal{P}^{(2)}_{a,1} \cup \mathcal{P}^{(2)}_{a,2} \) and \( \mathcal{P}^{(2)}_b = \mathcal{P}^{(2)}_{b,1} \cup \mathcal{P}^{(2)}_{b,2} \), where

\[
\begin{align*}
\mathcal{P}^{(2)}_a &= \{p \in \mathcal{P}^{(2)} : \mathcal{Z}(p) = \emptyset\} & \mathcal{P}^{(2)}_b &= \{p \in \mathcal{P}^{(2)} : \mathcal{Z}(p) \neq \emptyset\} \\
\mathcal{P}^{(2)}_{a,1} &= \{p \in \mathcal{P}^{(2)} : |\mathcal{V}(p)| = 1\} & \mathcal{P}^{(2)}_{a,2} &= \{p \in \mathcal{P}^{(2)} : |\mathcal{V}(p)| = 2\} \\
\mathcal{P}^{(2)}_{b,1} &= \{p \in \mathcal{P}^{(2)} : |\mathcal{Z}(p)| = n - 1\} & \mathcal{P}^{(2)}_{b,2} &= \{p \in \mathcal{P}^{(2)} : |\mathcal{Z}(p)| \in \{1, \ldots, n - 2\}\}.
\end{align*}
\]

In words, \( \mathcal{P}^{(2)}_a \) holds \( p \in \partial \mathcal{S} \) with no component equal to zero and at most two distinct (non-zero) values, while \( \mathcal{P}^{(2)}_b \) holds those with at least one component equal to zero and at most two distinct non-zero values. Likewise, \( \mathcal{P}^{(2)}_{a,1} \) holds \( p \) with no zero components and only one (non-zero) value, meaning \( \mathcal{P}^{(2)}_{a,1} = \{1/2\} \), and \( \mathcal{P}^{(2)}_{a,2} \) holds \( p \) with all components taking one of two non-zero values, and both values held by some component. Finally, \( \mathcal{P}^{(2)}_{b,1} \) holds \( p \) with all but one of the \( n \) entries holding value zero, meaning \( \mathcal{P}^{(2)}_{b,1} = \{e_1, \ldots, e_n\} \), and \( \mathcal{P}^{(2)}_{b,2} \) holds \( p \) with between one and \( n - 2 \) components taking value zero, and all non-zero components taking at most two distinct (non-zero) values. The next step (Step 3) in the proof focuses on \( \mathcal{P}^{(2)}_{a,2} \), while Step 4 focuses on \( \mathcal{P}^{(2)}_{b,2} \); the simpler cases \( \mathcal{P}^{(2)}_{a,1} \) and \( \mathcal{P}^{(2)}_{b,1} \) will be left until the end.

**Step 3:** Any \( p \in \mathcal{P}^{(2)}_{a,2} \) cannot be a global maximizer. We define the subset \( \mathcal{P}^{(2),*}_{a,2} \subseteq \mathcal{P}^{(2)}_{a,2} \) as the collection of points from \( \mathcal{P}^{(2)}_{a,2} \) that also satisfies (54), which is a necessary condition for any such \( p \) to be a potential extremizer. In order to rule out the possibility that a point from \( \mathcal{P}^{(2)}_{a,2} \) can be a global maximizer, based on the KKT condition analysis, we only need to show the original objective function \( f \) maximized over \( p \in \mathcal{P}^{(2),*}_{a,2} \) is no larger than say \( f(e_i) = d(c, e_i)^2 \), equivalently we show another function \( \tilde{f} \) maximized over \( p \in \mathcal{P}^{(2),*}_{a,2} \) is no larger than \( f(e_i) \) where \( \tilde{f} = f \) for all \( p \in \mathcal{P}^{(2),*}_{a,2} \). It suffices to work with an enlarged feasible set, meaning we shall show \( \tilde{f} \) maximized over \( p \in \mathcal{P}^{(2)}_{a,2} \) is still smaller than \( f(e_i) \).

As \( p \in \mathcal{P}^{(2)}_{a,2} \) by assumption, there is no loss in generality in denoting the two non-zero values it takes by \( \mathcal{V}(p) = \{p_s, p_l\} \) for \( 0 < p_s < p_l < 1 \), where \( s \) stands for small and \( l \) for large (and do not denote indices). Assume there are \( k \) (\( 1 \leq k \leq n - 1 \)) components that equal \( p_s \) and hence \( (n - k) \) components equal \( p_l \). Then \( kp_s + (n - k)p_l = 1 \), and it follows from these assumptions that \( 0 < p_s < \frac{1}{n} < p_l < 1 \), where we emphasize the
satisfy (56). We now express the original objective function obtained by further optimizing \( u \), August 18, 2014 DRAFT

Therefore showing it is straightforward to establish that it follows that, for fixed \( p \), only points from the subset \( P^{(2)\ast}_a \) also satisfy (56). We now express the original objective function \( f \) from (45) as another function, \( \tilde{f}(p_s,k) \), where \( f(p) = \tilde{f}(p_s,k) \) for all \( p \in P^{(2)\ast}_a \), i.e., for all \( p \) for which both \( kp_s + (n-k)p_l = 1 \) and (56) hold:

\[
\tilde{f}(p_s,k) = k \left( c - p_s(1-p_s)^{k-1}(1-p_l)^{n-k} \right)^2 + (n-k) \left( c - p_l(1-p_s)^{k-1}(1-p_l)^{n-k} \right)^2 \\
= k \left( (1-p_s)^{k-1}(1-p_l)^{n-k-1}(1-p_sp_l) - p_s(1-p_s)^{k-1}(1-p_l)^{n-k-1} \right)^2 + \\
(n-k) \left( (1-p_s)^{k-1}(1-p_l)^{n-k-1}(1-p_sp_l) - p_l(1-p_s)^{k-1}(1-p_l)^{n-k-1} \right)^2 \\
= ((1-p_s)^{k-1}(1-p_l)^{n-k-1})^2 (k(1-p_s)^2 + (n-k)(1-p_l)^2) \\
= \left( c / (1-p_sp_l) \right)^2 \cdot \frac{(n+kp_s^2 + (n-k)p_l^2 - 2(kp_s + (n-k)p_l))}{(n-k-p_s+kp_s^2)}.
\]

Fixing \( p_s \in (0, \frac{1}{n}) \) temporarily, we now show \( \tilde{f} \) is monotone increasing in \( k \) for \( k \in \{1, \ldots, n-1\} \). Denote \( u = u(p_s,k) = (n-k)(n-2) + 1 - 2kp_s + knp_s^2 \) and \( v = v(p_s,k) = n-k - p_s + kp_s^2 \) so that

\[
\tilde{f}(p_s,k) = c^2(n-k) \frac{u(p_s,k)}{v(p_s,k)^2}.
\]

It is straightforward to establish that \( u \geq 0, v \geq 0 \) under the given assumptions. Taking the derivative of \( \tilde{f} \) w.r.t. \( k \):

\[
\frac{d}{dk} \tilde{f}(p_s,k) = \left( c^2 / (n-p_s-k(1-p_s^2)) \right) \left( -uv + (n-k)v(np_s^2 - 2p_s - (n-2)) - 2(n-k)u(p_s^2 - 1) \right) \\
= \left( c^2 / (n-p_s-k(1-p_s^2)) \right) h(p_s,k)
\]

Therefore showing \( \frac{d}{dk} > 0 \) is equivalent to showing \( h(p_s,k) > 0 \). Towards this, observe the third summand in \( h(p_s,k) \) can be split evenly to be combined with the first and second summands, thus

\[
h(p_s,k) = (1-np_s) \frac{up_s + (n-k)(1-p_s^2)}{2} > 0.
\]

It follows that, for fixed \( p_s \in (0, \frac{1}{n}) \), \( \tilde{f}(p_s,k) \) is maximized at \( k = n-1 \). The global maximum of \( \tilde{f}(p_s,k) \) is obtained by further optimizing \( \tilde{f}(p_s,n-1) \) over \( p_s \in (0, \frac{1}{n}) \). Setting \( k = n-1 \) in (57) gives

\[
\tilde{f}(p_s,n-1) = c^2(n-1) \frac{np_s^2 - 2p_s + 1}{((n-1)p_s^2 - p_s + 1)^2}.
\]
for which
\[
\left. \frac{\partial \tilde{f}(p_s, k)}{\partial p_s} \right|_{k=n-1} = -2c^2(n-1)^2 \frac{p_s (np_s^2 - 3p_s + 1)}{n} < 0.
\]

The inequality holds since the quadratic \( np_s^2 - 3p_s + 1 \) can be verified to be positive for \( n \geq 2 \) and \( p_s \in (0, \frac{1}{n}) \).

Therefore, the maximum (indeed supremum) of \( \tilde{f}(p_s, n-1) \) is obtained when \( p_s \to 0 \) (meaning in the limit \( e_i \) is the maximizer although \( e_i \) itself does not satisfy (54)), which according to (61) is \( (n-1)c^2 \). These monotonicities are illustrated in Fig. 4.

Observe when we maximize \( \tilde{f}(p_s, k) \) we effectively enlarge the feasible set from \( \mathcal{P}_{a,2}^{(2),*} \) to be \( \mathcal{P}_{a,2}^{(2)} \) because we do not check whether (54) is satisfied. Recall \( f \) is identically equal to \( \tilde{f} \) only for \( p \in \mathcal{P}_{a,2}^{(2),*} \) because \( \tilde{f} \) is derived from \( f \) by applying (54). Therefore we have
\[
f(p') = \tilde{f}(p') \leq \max_{p \in \mathcal{P}_{a,2}^{(2),*}} \tilde{f}(p) \leq \max_{p \in \mathcal{P}_{a,2}^{(2)}} \tilde{f}(p) = (n-1)c^2, \quad \forall p' \in \mathcal{P}_{a,2}^{(2),*}.
\]

Summarizing, so far we have shown, suppose there exists a potential extremizer \( p \) whose components are all non-zero but not all identical, then in order to satisfy the first-order KKT necessary conditions, the original objective function \( f \) evaluated at such a point is upper bounded by \( \tilde{f}(0, n-1) = (n-1)c^2 \). Now since \( f(e_i) = d(c, e_i)^2 = (n-1)c^2 + (c-1)^2 \), this means no \( p \in \mathcal{P}_{a,2}^{(2)} \) can achieve a higher objective value than \( e_i \) (i.e., case \( \mathcal{P}_{b,1}^{(2)} \) in
terms of globally maximizing the original objective function. In fact, this property does not depend on choosing the thresholding $c^*_m = (1 - nm^2)/(2(1 - nm))$. This property is useful in Step 4 below.

**Step 4:** Any $p \in \mathcal{P}_{b,2}^{(2)}$ cannot be a global maximizer. Fix $p \in \mathcal{P}_{b,2}^{(2)}$ and let $s = n - |Z(p)| \in \{2, \ldots, n-1\}$ be the number of non-zero components. Evaluating the original objective function, (45), for such a point yields

$$f(p) = (n - s)(c - 0)^2 + \sum_{i=1}^{s} (c - p_i \prod_{j \neq i} (1 - p_j))^2. \quad (63)$$

For each given $s$, $f(p)$ is maximized iff the second summand above is maximized. Maximizing the above second summand can be thought of as performing the same optimization problem in an $s$-dimensional space where the $s$-vector $p$ duplicates all the $s$ non-zero components from the original $n$-vector $p$. Then, one may view this $s$-vector with no zero components as a member of $\mathcal{P}_a^{(2)}$, but with the dimension reduced from $n$ to $s$. There are two possibilities: this point is either in $\mathcal{P}_{a,2}^{(2)}$ or in $\mathcal{P}_{a,1}^{(2)}$.

Consider the first possibility, i.e., $\mathcal{P}_{a,2}^{(2)}$. Based on the analysis of this case in Step 3 (with the dimension reduced from $n$ to $s$), and the upper bound (62) in particular, it follows that

$$\sum_{i=1}^{s} \left( c - p_i \prod_{j \neq i} (1 - p_j) \right)^2 \leq (s - 1)c^2,$$

and hence $f(p) \leq (n - s)(c - 0)^2 + (s - 1)c^2 = (n - 1)c^2$, which is the same upper bound for candidates in case $\mathcal{P}_{a,2}^{(2)}$ in the original $n$-dimensional space. It follows that, in this reduced dimensional space, points in $\mathcal{P}_{a,2}^{(2)}$ cannot achieve a higher objective value than that achieved by the points $e_i$ in the original space.

Consider the second possibility, i.e., $\mathcal{P}_{a,1}^{(2)}$, namely the all-rates-equal point in this $s$-dimensional space. There are two subcases: $i)$ $c \leq c^*_m(s) = (1 - sm(s)^2)/(2(1 - sm(s)))$, and $ii)$ $c > c^*_m(s)$. Note we write $c^*_m(s)$ to highlight it is a function of $s$, the corresponding dimension. Case $i)$ can be skipped, due to (42) and the observation that the $e_i$ in this $s$-dimension is also the $e_i$ in the original $n$-dimensional space. Recall, $e_i$ (in the set $\mathcal{P}_{b,1}^{(2)}$) will be addressed in the final step. For case $ii)$ we now directly show the all-rates-equal point in this $s$-dimensional space cannot achieve a higher objective value than that in the original space. First, it is straightforward to establish the inequality

$$n \left( c - \frac{1}{n} \left( 1 - \frac{1}{n} \right)^{n-1} \right)^2 = f(m(n)) \geq f(m(s)) = (n - s)c^2 + s \left( c - \frac{1}{s} \left( 1 - \frac{1}{s} \right)^{s-1} \right)^2 \quad (64)$$

holds iff

$$2c(sm(s) - nm(n)) \geq sm^2(s) - nm^2(n). \quad (65)$$
Since $c > c_m^*(s)$, (65) is equivalent to
\[
sm(s)(1 - m(s)) - nm(n)(1 - m(n)) + sm(s)m(n)(m(s) - m(n)) \geq 0.
\] (66)

Since $sm(s)m(n)(m(s) - m(n)) \geq 0$, to show (66) it suffices to show the function $g(n) \equiv nm(n)(1 - m(n))$ is monotone decreasing in $n$ for $n \geq 3$ (recall $2 \leq s \leq n - 1$). Towards this we find the derivative of $g(n)$ as
\[
\frac{dg(n)}{dn} = \frac{1}{2n^2} \left(1 - \frac{1}{n}\right)^{n-1} \left[-2 \left(1 - \frac{1}{n}\right)^{n-1} + 2n + 2n^2 \left(1 - \frac{2}{n} \left(1 - \frac{1}{n}\right)^{n-1}\right) \log \left(1 - \frac{1}{n}\right)\right]
\]
\[
= \frac{1}{2n^2} \left(1 - \frac{1}{n}\right)^{n-1} \tilde{g}(n).
\] (67)

It now suffices to show $\tilde{g}(n) < 0$. For $n = 3, 4$ this can be verified; for $n \geq 5$ we apply the inequality $\log(1 + x) \leq x - \frac{x^2}{2}$ for all $x \in (-1, 0]$ and get
\[
\tilde{g}(n) \leq 2 \left(1 - \frac{1}{n}\right)^{n-1} \left(1 + \frac{1}{n}\right) - 1 \leq 0,
\] (68)
where the inequality follows from the monotonicity in $n$ of the upper bound on $\tilde{g}(n)$. Therefore we have shown the desired inequality (66). This means that, even if a point is from $P_{a,1}$, it cannot be an extremizer as it cannot achieve a higher objective value than $e_i$ (case $i$)) and/or $m$ (case $ii$) in the original $n$-dimensional space. This concludes Step 4.

Finally, we are left with only cases $P_{a,1}^{(2)}$ and $P_{b,1}^{(2)}$. We can verify by checking the KKT conditions that $m$ is always eligible to be a local extremizer, while $e_i$ is eligible to be a local maximizer iff $c \leq 1$. Therefore, we conclude the global maximum of the original optimization problem can be obtained by evaluating and comparing $f$ at two points $m$, $e_i$. Furthermore, recall the objective function is defined as $d(c, x)^2$ for $x \in \partial \Lambda$. Then as a consequence of (42), we can actually conclude in a more general manner: the global maximum occurs at $i$ any $e_i$ when $c < c_{in}$, $ii$) any $e_i$ and $m$ when $c = c_{in}$, and $iii$) $m$ when $c > c_{in}$. See Fig. 5 for an illustration. For $\Lambda_m^*$, the global maximizers are both $e_i$ and $m$ giving the maximum of $f$ as $(n - 1) c_{in}^2 + (c_{in}^* - 1)^2 = n(c_{in}^* - m)^2$, as desired in (41).

Remark 3: Since the hyperplane inducing the optimal polyhedral inner bound $\Lambda_{pi}^*$ is a supporting hyperplane of the convex body $B(c, r_{in}(c))$, due to the constructions of $\Lambda_{pi}^*$ and $\Lambda_{si}$ it follows that $\Lambda_{si}$ always outperforms $\Lambda_{pi}^*$ in terms of volume approximation to $\Lambda$.

We now proceed to the spherical outer bound. There are many similarities between the definitions, propositions and proof techniques for the spherical inner and outer bound. In both cases there exists a set inclusion relationship which implies the optimal bound arises when $c$ is chosen to be the minimum possible.
Fig. 5. Original objective function $f(p)$ for $\Lambda_{si}$ when $n = 3$ for various $c$. Horizontal axes are $p_2$, $p_3$. **Left:** $c = 0.99c_{in}^*$ with global maximizers: $e_i$. **Middle:** $c = c_{in}^*$, with global maximizers: $e_i$ & $m$. **Right:** $c = 1.02c_{in}^*$, with global maximizer: $m$.

**Definition 8:** $\Lambda_{so}(c) \equiv S \setminus B(c, r_{out}(c))$, where the center of the ball $c = c_1$ for all $c \geq 1$, and its radius $r_{out}(c) \equiv d(c, e_i) = \sqrt{(c-1)^2 + (n-1)c^2}$.

**Proposition 10 (spherical outer bound):** For each $c \geq 1$, the set $\Lambda_{so}(c)$ is an outer bound on $\Lambda$ for $n \geq 2$. Among these, the tightest is given when $c = c_{out}^*$:

$$\Lambda_{so}^* = \Lambda_{so}(c_{out}^*) = \{x \in S : \|x - 1\| \geq \sqrt{n-1}\}.$$ (69)

**Proof:** By Def. 8, in order to induce an outer bound we must have $c > m$. Moreover, $d(c, m) > d(c, e_i) = r_{out}$, which is equivalent to $c > (1 - nm^2)/(2(1 - nm))$. This means there remain two possible intervals for $c$: (i) $(1 - nm^2)/(2(1 - nm)) < c < 1$ and (ii) $c \geq 1$. For each one we investigate whether a ball with parameter $c$ in that interval induces a valid outer bound for $\Lambda$.

For case (i), we can compute that $e_1, x_0 \in \partial B(c, r_{out})$ for $x_0 \equiv (2c-1)e_1$, i.e., the boundary of the ball intersects the first coordinate axis at these two points. As $c > (1 - nm^2)/(2(1 - nm)) > 1/2$, the line segment $x_0 e_1 \subseteq \Lambda$ due to $\Lambda$’s coordinate convexity. Furthermore, since the open line segment $x_0 e_1 \subseteq B(c, r_{out})$, we find $\Lambda \not\subseteq S \setminus B(c, r_{out})$ namely $B(c, r_{out})$ does not induce a valid outer bound.

It remains to investigate case (ii). In the rest of this proof we first show every $c$ in this category gives a valid outer bound and, furthermore, $c = c_{out}^* = 1$ yields the tightest bound. We first show $c = c_{out}^* = 1$ yields the tightest bound, i.e., we show $\Lambda_{so}^* \subseteq \Lambda_{so}(c)$ for each $c \geq 1$. Note the equivalence

$$\Lambda_{so}^* \subseteq \Lambda_{so}(c) \iff S \setminus (B(1, \sqrt{n-1}) \cap S) \subseteq S \setminus (B(c, r_{out}(c)) \cap S)$$

$$\iff B(c, r_{out}(c)) \cap S \subseteq B(1, \sqrt{n-1}) \cap S.$$ (70)
Therefore we seek to prove: \( \forall x \in S, \text{ if } d(c, x)^2 < r_{out}(c)^2 \) (i.e., \( x \in B(c, r_{out}(c)) \cap S \)), then \( d(1, x)^2 < (\sqrt{n} - 1)^2 \) (i.e., \( x \in B(1, \sqrt{n} - 1) \cap S \)). Suppose \( x \in S \) is such that \( d(c, x)^2 < r_{out}(c)^2 \). Then, we compute:

\[
d(1, x)^2 = \sum_{i=1}^{n} (1 - x_i)^2 = \sum_{i=1}^{n} ((c - x_i) - (c - 1))^2 = \sum_{i=1}^{n} (c - x_i)^2 + n(c - 1)^2 - 2(c - 1) \left( nc - \sum_{i=1}^{n} x_i \right) < (c - 1)^2 + (n - 1)c^2 + n(c - 1)^2 - 2(c - 1)(nc - 1) = n - 1, \tag{71}
\]

where the inequality follows from \( d(c, x)^2 < r_{out}(c)^2 \) and \( \sum_{i=1}^{n} x_i \leq 1 \). This shows the desired set inclusion, meaning \( \Lambda^{*}_{so} \) is the smallest set among \( \{ \Lambda_{so}(c), c \geq 1 \} \).

It remains to show that \( \Lambda^{*}_{so} \) is a valid outer bound on \( \Lambda \). For any \( x \in \Lambda = \Lambda_{eq} \) we must show \( x \in \Lambda^{*}_{so} \), namely \( x \) is outside the open ball \( B(c, 1) \), or equivalently \( \min_{x \in \Lambda} \|1 - x\|^2 \geq n - 1 \). This latter expression may be cast as an optimization problem w.r.t. \( p \):

\[
\min_{p \in [0, 1]^n} f(x(p)) = \frac{1}{2} \sum_{i=1}^{n} \left( 1 - p_i \prod_{j \neq i} (1 - p_j) \right)^2 \geq n - 1, \tag{72}
\]

Observe if any component of \( p \) equals 1 or if \( p = 0 \) then \( f \geq n - 1 \) immediately holds. So below we assume \( p < 1 \) and \( p \) has non-zero component(s). Recall we defined \( \mathcal{V}(p) = \{ a \in (0, 1] : \exists i \in [n] : p_i = a \} \) in the proof of Prop. 9 as the set of non-zero values taken by a vector \( p \). We categorize based on how many distinct non-zero values the components of \( p \) assume: a) \( |\mathcal{V}(p)| > 1 \) or b) \( |\mathcal{V}(p)| = 1 \).

Consider first case a) (\( |\mathcal{V}(p)| > 1 \)), i.e., \( p \) has two or more distinct non-zero component values, say \( 0 < p_k < p_l < 1 \). We will show that all such \( p \)'s cannot be local extremizers due to the violation of Karush-Kuhn-Tucker (KKT) conditions required for optimality (note regularity is guaranteed in this case). An equivalent form of the KKT stationarity condition is that

\[
\frac{1}{2} \left( \frac{\partial f}{\partial p_k} - \frac{\partial f}{\partial p_l} \right) (1 - p_k)(1 - p_l) = 0, \quad 0 < p_k < p_l < 1, \tag{73}
\]

which, after some algebra, may be shown to be equivalent to:

\[
(1 - p_l)(\eta - \pi_k(1 - p_k \pi_k)) = (1 - p_k)(\eta - \pi_l(1 - p_l \pi_l)), \tag{74}
\]

where \( \eta \equiv \sum_i \pi_i(1 - p_i \pi_i)p_i, \pi_i = \pi_i(p) \equiv \pi(p)/(1 - p_i) \). Note \( \eta \) can be interpreted as the expectation of a discrete random variable \( Z \) with support \( \{ \pi_i(1 - p_i \pi_i), i \in [n] \} \) and associated PMF \( \mathbb{P}(Z = \pi_i(1 - p_i \pi_i)) = p_i \) for each \( i \in [n] \). Therefore, stationarity will not be satisfied as long as we can choose indices \( k', l' \) such that \( 0 < p_{k'} < p_{l'} < 1 \), and \( \eta \) lies strictly between \( \pi_{k'}(1 - p_{k'} \pi_{k'}) \) and \( \pi_{l'}(1 - p_{l'} \pi_{l'}) \). But, we can always find such indices since, following Lem. 3 (which can be easily verified), we can show the ordering: \( \pi_{k'}(1 - p_{k'} \pi_{k'}) < \pi_{l'}(1 - p_{l'} \pi_{l'}) \). This rules out the possibility that an extremizer can come from case a).
Consider next case $b$) ($|\mathcal{V}(p)| = 1$), i.e., $p$ has only one distinct non-zero component value (we call such $p$ “quasi-uniform”). Lem. 4 below states that for any such $p$, the objective $f(p)$ equals $n - 1$, the lower bound in (72). Observe $\{e_i\}_{i=1}^n$ satisfy $|\mathcal{V}(e_i)| = 1$ and so $f(e) = n - 1$.

These two cases establish the validity of the inequality (72), and thereby establish the fact that $\Lambda_{x_0}^*$ is a valid outer bound for $\Lambda$.

The following two lemmas are used in the preceding proof of Prop. 10.

**Lemma 3:** If two non-zero components of $p$ satisfy $p_i > p_k$, then

$$x_l > x_k, \quad \pi_l > \pi_k, \quad \frac{x_l}{x_k} > \frac{p_l}{p_k}, \quad x_l - x_k < p_l - p_k. \tag{75}$$

**Proof:** Omitted.

**Lemma 4:** Fix $t \in (0, 1]$ and $k \in [n]$. Suppose $p < 1$ ($p \neq 0$) takes only one non-zero value (i.e., $|\mathcal{V}(p)| = 1$), and $p_i \in \{0, t\}$ for $i \in [n]$, and this value is taken by $k$ components of $p$. Then $f(p) \geq n - 1$ (for $f$ in (72)), with equality iff $k = t = 1$, i.e., $f(p) = n - 1$ iff $p \in \{e_i\}_{i=1}^n$.

**Proof:** Wlog let $p = t \cdot \sum_{i=1}^k e_i$ for $k \in [n], t \in (0, 1]$. Substitution of such a $p$ into (72) yields the following inequality

$$t(1 - t)^{k-1} \leq 1 - \sqrt{1 - 1/k}, \tag{76}$$

meaning the lemma will be established if we can show (76) holds for all valid $(t, k)$, and holds with equality iff $k = t = 1$. The inequality (76) is easily verified to hold strictly for a) $k = 1 \neq t$ and b) $t = 1 \neq k$. If $k = t = 1$ (namely $p = e_1$) the original objective function in (72) evaluates to $n - 1$, the desired minimum. It remains to study the case $k \in \{2, \ldots, n\}$ and $0 < t < 1$. Define $g(t) \equiv t(1 - t)^{k-1}$. The only stationary point of $g$ on $t \in [0, 1)$ is $t^* = 1/k$, at which the second derivative can be verified to be strictly negative, meaning $t^*$ is the unique maximizer. And hence we need to show (76) when $t = 1/k$, namely $(1 - 1/k)^{k-1} \leq k \left(1 - \sqrt{1 - 1/k}\right)$. The derivative of its LHS can be shown to be negative using the inequality $\log(1 + x) \leq x$ for $x > -1$. Thus the sequence $\{(1 - 1/k)^{k-1}\}$ is upper bounded by $\left(1 - 1/2\right)^{2-1} = 1/2$. On the other hand, using AM-GM inequality $\sqrt{1 - 1/k} < (1 - 1/k + 1)/2$, one can see the RHS is strictly lower bounded by $1/2$. This shows the desired inequality (76), thus proving this lemma.

**Remark 4:** The Cauchy-Schwarz inequality gets close to proving the desired inequality (72), but is insufficient by itself (note $\sum_i x_i \leq 1$ as $\Lambda \subseteq S$):

$$\sum_{i=1}^n (1 - x_i)^2 \geq \frac{(\sum_{i=1}^n 1 \cdot (1 - x_i))^2}{\sum_{i=1}^n 1^2} = \frac{(n - \sum_{i=1}^n x_i)^2}{n} \geq \frac{(n - 1)^2}{n}, \tag{77}$$

which is slightly weaker than the bound of $n - 1$ required to show (72).
The optimal spherical inner and outer bounds $\Lambda_{\text{in}}^*$, $\Lambda_{\text{out}}^*$, together with $\partial \Lambda$ are shown in Fig. 6 for $n = 2$ and 3.

It seems hard to obtain the volume of these spherical bounds in closed-form for arbitrary $n$. Essentially, the problem is one of integrating over the intersection of a (solid) hypersphere within $[0,1]^n$. It is natural to attempt to bound the volume. Below, we illustrate such an attempt using $\Lambda_{\text{out}}^*$ as an example.

We take a probabilistic approach. As the volume of the unit box $[0,1]^n$ always equals 1, and as $\Lambda_{\text{out}}^* \subseteq [0,1]^n$, it follows that its volume can be interpreted as the probability that a point uniformly distributed over $[0,1]^n$ falls into the set $\Lambda_{\text{out}}^*$. More precisely, for i.i.d. $\text{Unif}[0,1]$ random variables (RV) $y_1, \ldots, y_n$,

$$\text{vol}(\Lambda_{\text{out}}^*) = \mathbb{P}(y \in \mathcal{S}, \ y \notin B(1, \sqrt{n-1})) \overset{(a)}{=} \mathbb{P}(y \notin B(1, \sqrt{n-1})) = \mathbb{P}\left(\sum_{i}(1-y_i)^2 \geq n-1\right) \overset{(b)}{=} \mathbb{P}\left(\sum_{i}y_i^2 \geq n-1\right),$$

where (a) follows from Lem. 5 given below and (b) is due to the observation that $1-y_i$ are i.i.d. $\text{Unif}[0,1]$ RV's too. We note the uniform sum distribution (also known as Irwin-Hall distribution), $\sum_i y_i$, has a known closed-form density function, yet this does not seem to be the case for $\sum_i y_i^2$. Then one natural thing to do is to bound this tail probability. A typical form of the Chernoff bound states that for a random variable $Z$ (usually expressed as a sum of independent RVs), an upper bound on the (upper) tail probability is $\mathbb{P}(Z \geq t) \leq \inf_{s \geq 0} e^{-st}\mathbb{E}[e^{sZ}]$.

Substituting $\sum_i y_i^2$ for $Z$ yields:

$$\text{vol}(\Lambda_{\text{out}}^*) \leq \inf_{s \geq 0} e^{-s(n-1)}\mathbb{E}\left[e^{s\sum_i y_i^2}\right] = \inf_{s \geq 0} e^{-s(n-1)}\prod_i \mathbb{E}\left[e^{sy_i^2}\right] = \inf_{s \geq 0} e^{-s(n-1)}\left(\int_0^1 e^{sy^2}dy\right)^n.$$  \hspace{1cm} (79)

The minimizer $s^*$ is hard to be obtained in closed-form. Worse still, the numerically optimized upper bound is not close to the actual tail probability (i.e., the volume of $\Lambda_{\text{out}}^*$).

**Lemma 5:** $[0,1]^n \setminus \mathcal{S} \subseteq B(1, \sqrt{n-1})$. In words this says the unit box with the unit simplex subtracted lies completely inside the ball $B(1, \sqrt{n-1})$.

**Proof:** Given $x \in [0,1]^n$, $\sum_i x_i > 1$, we need to show $\sum_i (1-x_i)^2 < n-1$, which is easily verifiable since

$$\sum_{i}(1-x_i)^2 = n - 2 \sum_{i} x_i + \sum_{i} x_i^2 \leq n - 2\sum_{i} x_i + \sum_{i} x_i = n - \sum_{i} x_i < n-1.$$ \hspace{1cm} (80)

Note this lemma can be equivalently stated as $[0,1]^n \setminus B(1, \sqrt{n-1}) \subseteq \mathcal{S}$ which implies if a point is from $[0,1]^n$ but not in $B(1, \sqrt{n-1})$ then it’s guaranteed to be in $\mathcal{S}$. This observation is used step (a) in (78).

VI. Ellipsoid inner and outer bounds on $\Lambda$

We now turn to the third, and final, class of bounds on $\Lambda$. In this section we establish inner and outer bounds, each induced by a parameterized family of ellipsoids. This section is organized into three subsections. First, in §VI-A we
prove three results: \( i \) that the set of ellipsoids that inherit all the permutation symmetries of \( \Lambda \) are characterized by three scalars \((c, a_1, a_2)\) (Prop. 11), \( ii \) the sufficiency of working only with \( \partial \Lambda \) for the purpose of proving the correctness of the induced bound (Props. 14 and 15), and \( iii \) a property of a local extremizer from \( \partial \Lambda \) (Prop. 16).

Next, in §VI-B we present the parameterized families of ellipsoid inner (Prop. 18) and outer (Prop. 17) bounds. The derivation is based on the Karush-Kuhn-Tucker (KKT) optimality conditions. Finally, in §VI-C, we provide an alternate proof of the ellipsoid outer bound by working in a transformed space and leveraging Schur-convexity.

A. Simplification of parameter space

The contributions of this section were outlined above. We consider open ellipsoids \( \mathcal{E} \) of the form ([21]):

\[
\mathcal{E} = \{ x : (x - c)^T R^{-1} (x - c) < 1 \}.
\] (81)

Here \( c \) is the center of the ellipsoid and the \( n \times n \) symmetric and positive definite matrix \( R \) has the spectral decomposition \( R = Q D Q^T \) where \( Q = [q_1 \cdots q_n] \) is orthonormal and holds the eigenvectors of \( R \) (which are the directions of the \( n \) axes of the ellipsoid), and \( D = \text{diag}(\lambda_1, \ldots, \lambda_n) \) holds the eigenvalues of \( R \). Each \( a_i = \sqrt{\lambda_i} \) is the semi-axis length in the direction \( q_i \). Denote the boundary of \( \mathcal{E} \) by \( \partial \mathcal{E} = \{ x : (x - c)^T R^{-1} (x - c) = 1 \} \).
Our approach is to approximate the surface $\partial \Lambda$ with part of the surface of an ellipsoid, and then form inner and outer bounds on $\Lambda$ by subtracting these ellipsoids from the unit simplex $\mathcal{S}$. This is the same approach that was used in constructing the spherical bounds (§V). More concretely, we want to find inner and outer bounding ellipsoids $E_{in}, E_{out}$ such that $\Lambda_{ei} \subseteq \Lambda \subseteq \Lambda_{eo}$, where $\Lambda_{ei} = \mathcal{S} \setminus E_{in}$, $\Lambda_{eo} = \mathcal{S} \setminus E_{out}$.

Although we are not able to characterize them further, we define the optimal inner and outer bounding ellipsoids:

$$E_{in}^* = \arg \min_{E_{in}} \operatorname{vol}(E_{in} \cap \mathcal{S}) = \arg \min_{E_{in}} \operatorname{vol}(E_{in} \cap \mathcal{S})$$

$$E_{out}^* = \arg \min_{E_{out}} \operatorname{vol}(E_{out} \setminus \Lambda) = \arg \max_{E_{out}} \operatorname{vol}(E_{out} \cap \mathcal{S})$$

where the second equality in (82) follows from Lem. 11.

A result in convex geometry states that for any convex body there exists a unique maximum (resp. minimum) volume inscribed (resp. circumscribing) ellipsoid, called the \textit{Löwner-John ellipsoid}. Although we have a convex body $\Lambda^c \cap \mathcal{S}$, our objective is not to identify an inscribed/circumscribed ellipsoid with extremized volume for this set. Rather, our figure of merit (in (82) and (83)) is to extremize the volume of the intersection between the ellipsoid and the simplex. For example, our $E_{out}$ need not lie entirely within the convex body.

In general, analytical characterization of the Löwner-John ellipsoid is hard (see e.g., [22] [21]). One constructive result, though, is that the Löwner-John ellipsoid is an \textit{invariant ellipsoid}, meaning it inherits all the symmetries of the convex body [22]. The intuition is that if there were some symmetry that the volume optimal ellipsoid is not endowed with, then using that particular symmetry one can construct another distinct volume optimal ellipsoid, hence contradicting the uniqueness of the Löwner-John ellipsoid.

In the spirit of the above result, we restrict our attention to ellipsoids that inherit all the symmetries of the convex body $\Lambda^c \cap \mathcal{S}$. Note $\Lambda^c \cap \mathcal{S}$, $\Lambda$ and $\mathcal{S}$ all have full permutation symmetry. Prop. 11 below states some consequences of inheriting this permutation symmetry. Its proof uses the following three lemmas. The proof of Lem. 6 is given in §X-B and the proof of Lem. 8 is omitted as it is easy to verify.

\textbf{Lemma 6:} Fix an ellipsoid $E = \{x : (x - c)^T R^{-1} (x - c) < 1\}$ in $\mathbb{R}^n$ with center $c$. A hyperplane passing through $c$ with its normal vector being one of the axis/eigenvectors of $R$ is a reflecting hyperplane for $E$, i.e., $E$ is symmetric w.r.t. this hyperplane. Conversely, the normal vector of any reflecting hyperplane of $E$ can be considered as an axis/eigenvector of $R$.

Note that in the context of a full-dimensional ellipsoid, the axis (direction), eigenvector, and reflecting hyperplane’s normal vector are all essentially the same thing.
Lemma 7: For a symmetric matrix $R$, if the two eigenvalues associated with two of the eigenvectors of $R$ are distinct, then these two eigenvectors must necessarily be orthogonal (not just linearly independent).

Proof: Suppose eigenvectors $v, w$ have associated distinct eigenvalues $\lambda_v, \lambda_w$, meaning $Rw = \lambda_w w, \, Rv = \lambda_v v$. First we write $w^T R v = \lambda_v w^T v$. Next since $R$ is symmetric, we can also write $w^T R v = (Rw)^T v = \lambda_w w^T v$. These two give $(\lambda_w - \lambda_v) w^T v = 0$. As $\lambda_w \neq \lambda_v$, it has to holds that $w^T v = 0$.

Lemma 8: The linear combination of some eigenvectors associated with the same eigenvalue is also an eigenvector (with the same eigenvalue). In fact, all such eigenvectors are in the same eigen-subspace.

Proposition 11: The class of ellipsoids invariant under permutations of the coordinate axes is the set of ellipsoids parameterized by $(c, a_1, a_2) \in \mathbb{R}^3$ with the properties that

1) the center is at $c = c1$
2) one axis is along the all-rates-equal ray with direction $1$ and has semi-axis length $a_1$
3) the $n-1$ remaining axes are arbitrary (provided they, along with the axis aligned with $1$, form an orthonormal set) and have common semi-axis lengths $a_2$.

Proof: A set $S \subseteq \mathbb{R}^n$ is invariant under permutations if for any permutation $\sigma$ of $[n]$ we have $x = (x_1, \ldots, x_n) \in S$ iff $\sigma(x) = (x_{\sigma(1)}, \ldots, x_{\sigma(n)}) \in S$. It is straightforward to see that any ellipsoid parameterized by $(c, a_1, a_2)$ obeying the properties in the proposition is in fact permutation invariant. It remains to show each invariant ellipsoid has to possess the properties stated in the proposition.

Proof of Property 1. Any permutation $\sigma$ is a composition of transpositions, where a transposition is a permutation that only exchanges the positions of two elements. Let $\mathcal{H}(n, d) = \{x : n^T x = d\}$ be a hyperplane with normal vector $n$ and displacement $d$. For an ellipsoid centered at the origin, a transposition $\tau_{i,j}$ that exchanges axes $i,j$ geometrically corresponds to a reflection w.r.t. the hyperplane $\mathcal{H}(e_i - e_j, 0) = \{x : x_i = x_j\}$. Any reflection w.r.t. a hyperplane is an affine transformation $T$. The center $c$ of an invariant ellipsoid $\mathcal{E}$ must be fixed for any affine transformation $T$ in its automorphism group $\text{Aut}(\mathcal{E})$ [22], i.e., $T(c) = c$ for all $T \in \text{Aut}(\mathcal{E})$. In particular, $T_{\tau_{i,j}}(c) = c$ for each $T_{\tau_{i,j}}$ corresponding to reflection w.r.t. $\mathcal{H}(e_i - e_j, 0)$, i.e., for each transposition $\tau_{i,j}$. Equivalently, $c$ is unchanged by reflection w.r.t. $\mathcal{H}(e_i - e_j, 0)$. Therefore $c \in \mathcal{H}(e_i - e_j, 0)$, and thus $c_i = c_j$. As this is true for all $i,j$ it follows that $c_1 = \cdots = c_n = c$, i.e., $c = c1$.

Proof of Property 2. We need to use the following facts and/or claims:

- A matrix $R$ is diagonalizable (which is the case here since $\mathcal{E}$ is full-dimensional) if and only if all its eigenvectors span $\mathbb{R}^n$.
- The $\binom{n}{2}$ by $n$ matrix with each row being the normal vector of a reflecting hyperplane $\mathcal{H}(e_i - e_j, 0)$ ($\forall i,j \in \mathbb{N}$).
\[ n, i \neq j \] for \( E \) (or \( \Lambda \)) has rank \( n - 1 \). More concretely, these \( n - 1 \) linearly independent row vectors can be: \( (e_i - e_{i+1})^T, i \in [n - 1] \). It is then easy to see how the rest rows of the matrix can be constructed from linear combination (just summation suffices) of these \( n - 1 \) rows.

- Lemma 6 says that these normal vectors \( (e_i - e_{i+1}), i \in [n - 1] \) can be treated as eigenvectors of \( R \).
- Since these eigenvectors can span a subspace (or many subspaces) whose dimension (sum) is at most \( n - 1 \), there must exist another eigenvector which is orthogonal to all these eigenvectors. Because 1 is the unique (up to normalization) vector orthogonal to all of them, 1 has to be one eigenvector of \( R \), meaning one axis of the ellipsoid is along the “ray” with direction 1 and associated semi-axis length \( a_1 \).

**Proof of Property 3.** Denote \( \lambda_{i+1} \) to be the eigenvalue associated with eigenvector \( (e_i - e_{i+1}) \) for \( i \in [n - 1] \). Because \( (e_i - e_{i+1}) \not\perp (e_{i+1} - e_{i+2}) \), it follows from Lem. 7 that \( \lambda_{i+1} = \lambda_{i+2} \forall i \in [n - 2] \). This means there actually exists a single eigen-subspace of dimension \( n - 1 \), hence regardless of how the \( n - 1 \) eigenvectors in this subspace are chosen, the ellipsoid’s semi-axis lengths along these \( n - 1 \) directions are all equal: \( a_2 = \cdots = a_n \). ■

Lem. 9 below gives an explicit construction for \( R^{-1} \), and its Cor. 2 allows us to characterize the ellipsoid that passes through \( \{e_i\}_{i=1}^n \). Finally, Lem. 10 gives an expression that must be satisfied in order for \( \partial E \) and \( \partial \Lambda \) to share a common tangent point.

**Lemma 9:** For any ellipsoid in the form of (81), if \( q_1 = \frac{1}{\sqrt{n}}1 \) and \( D = \text{diag}(a_1^2, a_2^2, \ldots, a_n^2) \), then \( R^{-1} = \zeta 1_{n \times n} + a_x^2 I_{n \times n} \), where \( \zeta \equiv \frac{1}{n} (a_1^{-2} - a_x^{-2}) \). \( 1_{n \times n} \) is an \( n \times n \) matrix with each element being 1 and \( I_{n \times n} \) is the \( n \times n \) identity matrix.

The proof of Lem. 9 is straightforward and omitted.

**Corollary 2:** For any \( c > 1/n \) and \( a_1 > \sqrt{n(c - 1/n)} \), setting \( a_2^2 \) as below ensures \( e_i \in \partial E \) for \( i \in [n] \)

\[
 a_2^2 = \frac{(n - 1)a_1^2}{na_1^2 - (nc - 1)^2} \tag{84}
\]

**Lemma 10:** Define \( \bar{p}_t \equiv 1 - p_t \). Then \( \partial E \) and \( \partial \Lambda \) share a point of tangency at \( x_t = x(p_t) \) if for each \( i \in [n - 1] \):

\[
 \left( \frac{a_2}{a_1} \right)^2 = \frac{(\bar{p}_t,i - \bar{p}_t,n)\Sigma_{j=1}^n x_{t,j} + n(\bar{p}_t,n x_{t,i} - \bar{p}_t,i x_{t,n})}{(\bar{p}_t,i - \bar{p}_t,n)(\Sigma_{j=1}^n x_{t,j} - nc)} \tag{85}
\]

**Proof:** Recall the bijection between \( p_t \in \partial \mathcal{S} \) and \( x_t \in \partial \Lambda \) (Cor. 1) established in [14]. Post [15] established that the tangent hyperplane to \( \Lambda \) at a point \( x_t \in \partial \Lambda \) with \( x_t \mapsto p_t \) is \( \{x : (1 - p_t)^T x = \prod_{i}(1 - p_{t,i})\} \). Next, using the implicit function theorem it is straightforward to establish that the tangent hyperplane to an arbitrary ellipsoid \( E \) (81) at a point \( x_t \in \partial E \) is given by \( \{x : w_t^T x = b\} \), where

\[
 w_t = \frac{R^{-1}(x_t - c_0)}{R_n^{-1}(x_t - c_0)}, \quad b = w_t^T x_t. \tag{86}
\]
Here $R_n^{-1}$ is the $n$th row of $R^{-1}$. Finally equating (after appropriate normalization) these two tangent hyperplane equations yields the lemma.

Because of the symmetries present in $E(c, a_1, a_2)$, if we use a hyperplane with normal vector 1 to "slice" $E(c, a_1, a_2)$ we get an $(n - 1)$-dimensional ball. This is particularly intuitive in light of the following Prop. 12 for which we need to introduce the concept of rigid rotation of coordinate system.

**Definition 9 (rigid rotation of coordinate system):** Denote the original coordinate system as $X$. A rigid rotation of the coordinate system about the origin is specified by two vectors $v_s$ and $v_t$ such that after the rotation $v_s$ overlaps with $v_t$ while during the rotation the relative position of $v_s$ w.r.t. the coordinate axes remains unchanged. Denote this rotated coordinate system as $U$, in which $v_s$ was denoted (before rotation) as $v_t$ in the original system $X$. Alternatively, a rigid rotation is specified by a rotation matrix $M_{\text{rot}}$ (that can be determined by the starting and terminating vectors $v_s, v_t$ [23]) satisfying $v_t = M_{\text{rot}}v_s$. All rotation matrices are orthonormal.

According to this definition, we perform a rigid rotation of the original coordinate system $X$ such that $e_1$ overlaps with $1/\sqrt{n}$ (i.e., $v_s = e_1$, $v_t = 1/\sqrt{n}$), we then shift the origin to $c = c1$. Denote this rotated and translated system as $U$, then the two systems are related by $X = QU + c$ where $Q$ is the associated rotation matrix.

**Proposition 12:** In the above rotated and translated coordinate system $U$, $A$ has permutation symmetry among coordinates $\{2, \ldots, n\}$. If we let $T_u(\cdot)$ denote this transformation from $X$ to $U$, namely $u = T_u(x) = Q^{-1}(x - c)$, then:

$u = (u_1, u_2, \ldots, u_n)^T \iff \sigma(u) = (u_1, u_{\sigma(2)}, \ldots, u_{\sigma(n)})^T \in T_u(\Lambda), \forall \sigma \in S_{[n]\{1\}}$, \hspace{1cm} (87)

where $S_{[n]\{1\}}$ is the permutation group whose members permute coordinate indices from $\{2, \ldots, n\}$ arbitrarily.

**Proof:** Denote by $S_A$ the permutation group of set $A$. Each member of this group can be viewed as a bijection. We overload the notation $\sigma(\cdot)$. First, if the input parameter is an $n$-vector it outputs the vector after permuting its coordinate components according to $\sigma$. Second, if the parameter is a natural number $k \in \{2, \ldots, n\}$ it only indicates how the $k$th component is permuted, i.e., it gives the index of the coordinate taking the $k$th position after permutation (assuming the original indexing is in natural order: $2, 3, \cdots$). According to this notation, for any vector $v = (v_1, v_2, \ldots, v_n)^T$, we write $\sigma(v) = (v_1, v_{\sigma(2)}, \ldots, v_{\sigma(n)})^T$. Our goal is to show (87) namely $T_u(x) \in T_u(\Lambda) \iff \sigma(T_u(x)) \in T_u(\Lambda), \forall \sigma \in S_{[n]\{1\}}$.

What we know can be seen from the following

$T_u(x) \in T_u(\Lambda) \iff (b) \ x \in \Lambda \iff (a) \ \sigma(x) \in \Lambda \iff (b) \ T_u(\sigma(x)) \in T_u(\Lambda)$, \hspace{1cm} (88)

where $(a)$ holds because of the natural inclusion for the symmetric group $S_n \supseteq S_{[n]\{1\}}$, and $(b)$ holds because
affine transformation preserves set membership. It therefore suffices to show
\[ T_u(\sigma(x)) = \sigma(T_u(x)). \] (89)

Recall \( T_u(x) = u(x) = (u_1(x), u_2(x), \ldots, u_n(x))^T \) where we now highlight each component of \( u \) is a function of the entire vector \( x \). We have
\[
\begin{align*}
T_u(\sigma(x)) &= (u_1(\sigma(x)), u_2(\sigma(x)), \ldots, u_n(\sigma(x)))^T \\
\sigma(T_u(x)) &= \sigma(u_1(x), u_2(x), \ldots, u_n(x))^T = (u_1(x), u_{\sigma(2)}(x), \ldots, u_{\sigma(n)}(x))^T.
\end{align*}
\] (90) (91)

We need to show that
\[
u_1(\sigma(x)) = u_1(x), \quad \text{and} \quad u_j(\sigma(x)) = u_{\sigma(j)}(x), \quad \forall j \in [n] \setminus \{1\}
\] (92)

for all \( \sigma \in S_{[n]\setminus\{1\}} \). Observe that obeying the symmetry condition (92) depends on the rotation and shift transformation \( T_u \). Define a matrix \( Q \) to be:
\[
Q_{ij} = \begin{cases} 
\frac{1}{\sqrt{n}}, & i = 1, \ldots, n, \ j = 1 \\
-\frac{1}{\sqrt{n}}, & i = 1, \ j = 2, \ldots, n \\
-\frac{1}{\sqrt{n}} + \frac{1}{1+\sqrt{n}}, & i \neq j, \ i = 2, \ldots, n, \ j = 2, \ldots, n \\
1 - \frac{1}{\sqrt{n}} + \frac{1}{1+\sqrt{n}}, & i = j, \ i = 2, \ldots, n.
\end{cases}
\] (93)

Namely, \( Q \) is the rotation matrix associated with the rigid rotation such that \( e_1 \) becomes \( 1/\sqrt{n} \) (Mortari [23] Eq. (10) pp. 7).

Therefore the two coordinate systems are related by \( X = QU + c \). Being a rotation matrix, \( Q^{-1} = Q^T \), so
\[
Q_{i,j}^{-1} = Q_{j,i}^T = Q_{j,i}.
\]

For any given point \( x, u = Q^T(x - c) \) and its components are:
\[
u_1(x) = \sum_{i=1}^{n} Q_{1,i}^T(x - c)_i = \sum_{i=1}^{n} Q_{i,1}(x - c)_i = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (x_i - c)
\] (94)
\[
u_j(x) = \sum_{i=1}^{n} Q_{j,i}^T(x - c)_i = Q_{j,1}^T(x - c)_1 + Q_{j,j}^T(x - c)_j + \sum_{i=2, i \neq j}^{n} Q_{i,j}^T(x - c)_i
\]
\[
= Q_{1,j}(x - c)_1 + Q_{j,j}(x - c)_j + \sum_{i=2, i \neq j}^{n} Q_{i,j}(x - c)_i
\]
\[
= -\frac{1}{\sqrt{n}}(x_1 - c) + \left(1 - \frac{1}{\sqrt{n}} + \frac{1}{1+\sqrt{n}}\right)(x_j - c) + \left(-\frac{1}{\sqrt{n}} + \frac{1}{1+\sqrt{n}}\right) \sum_{i=2, i \neq j}^{n} (x_i - c)
\]
\[
= -\frac{1}{\sqrt{n}} \sum_{i=1}^{n} (x_i - c) + \frac{1}{1+\sqrt{n}} \sum_{i=2}^{n} (x_i - c) + (x_j - c), \quad \forall j \in [n] \setminus \{1\}.
\] (95)
Condition (92) can now be verified to be true. Hence we have shown (89) and this completes the proof.

The previous proposition seems to suggest some loss of permutation symmetry. This is answered in the negative by the following.

**Proposition 13 (conservation of symmetry):** The permutation symmetry of the set $\Lambda$ is preserved under rotation of the coordinate system.

**Proof:** Let $S_{[n]}$ be the symmetric group of cardinality $n$, meaning its members permute coordinate indices from $[n]$ arbitrarily. A set $G$ has permutation symmetry for coordinate indices $A \subseteq [n]$ if $G$ has permutation symmetry for $\Pi \subseteq S_{[n]}$ where $\Pi = \{ \sigma : \sigma(k) = k, \ \forall k \notin A \}$ (namely fixing the indices in $A^c \equiv [n] \setminus A$), meaning $x \in G \iff \sigma(x) \in G$, $\forall \sigma \in \Pi$. Any permutation can be decomposed as the product of a sequence of (disjoint) transpositions, where each transposition swaps two indices and keeps the remaining indices fixed. Since $G$ is symmetric w.r.t. transposition of a pair of indices $(i, j)$, this implies $G$ has reflective symmetry w.r.t. the hyperplane $H(n_{i,j}, 0)$ for $n_{i,j} = e_i - e_j$. It follows that if $G$ has permutation symmetry for $k$ out of $n$ coordinates, then it has reflective symmetry w.r.t. each of the $\binom{n}{2}$ reflecting hyperplanes.

Now consider our particular transformation $T_u$, as defined in Prop. 12. In the transformed space $U$, $T_u(\Lambda)$ has permutation symmetry w.r.t. coordinates $[n] \setminus \{1\}$, which gives $\binom{n-1}{2}$ degrees of reflective symmetry. Furthermore, $T_u(\Lambda)$ retains reflective symmetry w.r.t. $T_u(H(n_{1,j}, 0))$ for $j \in [n] \setminus \{1\}$ and this adds another $\binom{n-1}{1}$ degrees of symmetry. The total is $\binom{n-1}{2} + \binom{n-1}{1} = \binom{n}{2}$, which agrees with the fact that $\Lambda$, in the original space $X$, has full permutation symmetry (hence $\binom{n}{2}$ reflecting hyperplanes).

The following two propositions comprise the second major contribution in this subsection. They justify why, for both $E_{\text{out}}$ (Prop. 14) and $E_{\text{in}}$ (Prop. 15), it suffices (necessity is clear) to only consider $\partial \Lambda$ in verifying an ellipsoid induces a valid inner or outer bound on $\Lambda$. This observation reduces the set of points that must be checked from $x \in \Lambda$ to $x \in \partial \Lambda$. More importantly, the characterization of $\partial \Lambda$ is amenable to analysis using majorization inequalities, which enables us to provide an alternate proof of the proposed ellipsoid outer bound in §VI-C.

**Proposition 14:** Fix $c > \frac{1}{n} \left(1 - \frac{1}{n}\right)^{n-1}$. Then $\Lambda \subseteq \Lambda_{eo} \iff \partial \Lambda \cap E_{\text{out}} = \emptyset$.

**Proof:** “$\Rightarrow$” Because $\Lambda \subseteq S$, so $\Lambda \subseteq \Lambda_{eo} = S \setminus E_{\text{out}}$ means $\Lambda \cap E_{\text{out}} = \emptyset$, hence $\partial \Lambda \cap E_{\text{out}} = \emptyset$.

“$\Leftarrow$” (We prove the contrapositive version namely $\Lambda \not\subseteq \Lambda_{eo} \Rightarrow \partial \Lambda \cap E_{\text{out}} \neq \emptyset$):

Suppose $\Lambda \not\subseteq \Lambda_{eo}$, then $\Lambda \cap E_{\text{out}} \neq \emptyset$, meaning there exists $x_0 \in \Lambda \cap E_{\text{out}}$. If $x_0 \in \partial \Lambda$, this already says $\partial \Lambda \cap E_{\text{out}} \neq \emptyset$. If $x_0 \notin \partial \Lambda$, due to the convexity of $E_{\text{out}}$, line segment $x_0c \in E_{\text{out}}$, where $c$ is the center of $E_{\text{out}}$. Since $c = c1$ where $c > \frac{1}{n} \left(1 - \frac{1}{n}\right)^{n-1}$, so $c \notin \Lambda$. But because $x_0 \in \Lambda$, the line segment $x_0c$ must necessarily cross $\partial \Lambda$.
Proposition 15: Fix \( c > \frac{1}{n} \left( 1 - \frac{1}{n} \right)^{n-1} \). Then \( \Lambda_{ei} \subseteq \Lambda \iff \partial \Lambda \subseteq \overline{E_{in}} \).

Proof: This proof (converse part) directly invokes Lem. 11 and 15 where the proof of Lem. 15 uses Lem. 11, 12, 13 and 14. All these five lemmas are shown below within the proof of this proposition. In this proof, all set complements are w.r.t. the simplex \( \mathcal{S} \). Recall \( \Lambda \subseteq \mathcal{S} \).

\[ \Rightarrow \]:

\[ \Lambda_{ei} \subseteq \Lambda \iff \Lambda^c \subseteq \Lambda_{ei}^c = (\mathcal{S} \setminus E_{in})^c = E_{in} \cap \mathcal{S} \subseteq \overline{E_{in}} \]  \hspace{1cm} (96)

\[ (a) \quad \overline{\Lambda^c} \subseteq \overline{E_{in}} \quad (b) \quad \partial \Lambda \subseteq \overline{E_{in}}, \]  \hspace{1cm} (97)

where \( (a) \) is because for all sets \( A, B \) we have \( A \subseteq B \Rightarrow \overline{A} \subseteq \overline{B} \), and \( (b) \) is due to the definition \( \text{bd}(A) = \overline{A} \cap \overline{A^c} \).

\[ \Leftarrow \]: Given \( \partial \Lambda \subseteq \overline{E_{in}} \), we need to show \( \forall x_0 \in \Lambda_{ei} \equiv \mathcal{S} \setminus E_{in} \), it holds true that \( x_0 \not\in \Lambda \). Note \( x_0 \in \mathcal{S} \) and because \( \mathcal{S} \) can be written as the disjoint union \( \Lambda \cup (\mathcal{S} \cap \Lambda^c) \), so equivalently we need to show \( x_0 \not\in \mathcal{S} \cap \Lambda^c \) is impossible. We prove by contradiction. Assuming \( x_0 \in \mathcal{S} \cap \Lambda^c \), because \( \overline{\Lambda^c} \cap \mathcal{S} = \text{conv} (\partial \Lambda) \) (Lem. 11) and the fact \( \text{bd}(\Lambda^c) = \text{bd}(\Lambda) \), we have (where the last step follows from Lem. 15)

\[ x_0 \in (\overline{\Lambda^c} \cap \mathcal{S}) \setminus \text{bd}(\Lambda^c) = \text{conv}(\partial \Lambda) \setminus \partial \Lambda \subseteq \overline{E_{in}}. \]  \hspace{1cm} (98)

But this contradicts the assumption \( x_0 \in \mathcal{S} \setminus E_{in} \).

We now present the five lemmas mentioned above.

Lemma 11: \( \overline{\Lambda^c} \cap \mathcal{S} = \text{conv}(\partial \Lambda) \).

Proof of Lem. 11: Since \( \partial \Lambda \) is also the boundary of the closed set \( \overline{\Lambda^c} \), we have: \( \partial \Lambda \subseteq \overline{\Lambda^c} \). Because \( \partial \Lambda \subseteq \mathcal{S} \subseteq \Lambda \), we have \( \partial \Lambda \subseteq \overline{\Lambda^c} \cap \mathcal{S} \), and hence \( \text{conv}(\partial \Lambda) \subseteq \overline{\Lambda^c} \cap \mathcal{S} \). The proof will be complete if we show \( \overline{\Lambda^c} \cap \mathcal{S} \subseteq \text{conv}(\partial \Lambda) \). Given \( x \in \overline{\Lambda^c} \cap \mathcal{S} \), we distinguish cases: \( i \) if \( x \in \text{bd}(\Lambda) = \partial \Lambda \), done; \( ii \) if \( x \in \partial \mathcal{S} \), since \( \partial \mathcal{S} = \text{conv}(e_1, \ldots, e_n) \subseteq \text{conv}(\partial \Lambda) \), it follows \( x \in \text{conv}(\partial \Lambda) \); \( iii \) otherwise we can draw a line along the direction \( 1 \) that passes \( x \), since (in this case) this line must necessarily intersect at distinct points on \( \partial \mathcal{S} \) and \( \partial \Lambda \), this shows \( x \in \text{conv}(\partial \Lambda) \) again.

Lemma 12: Fix two closed sets \( \overline{A}, \overline{B} \). Then \( \overline{A} \subseteq \overline{B} \Rightarrow \overline{A} \setminus \text{bd}(\overline{A}) \subseteq \overline{B} \setminus \text{bd}(\overline{B}) \).

Proof of Lem. 12: Equivalently, we show \( \overline{A} \subseteq \overline{B} \Rightarrow \text{int}(\overline{A}) \subseteq \text{int}(\overline{B}) \). Given \( x_0 \in \text{int}(\overline{A}) \) meaning there exists an open ball \( b(x_0, \epsilon) = \{ x : \|x - x_0\| < \epsilon \} \subseteq \overline{A} \subseteq \overline{B} \), this then directly says \( x_0 \in \text{int}(\overline{B}) \).

Lemma 13: Fix sets \( A, B, C \) satisfying \( C \subseteq A \). Then \( A \setminus B = (A \setminus (B \cup C)) \cup (C \setminus B) \).

Proof of Lem. 13: \( \subseteq \): Given \( x_0 \in A \setminus B \), there are two cases: \( i \) \( x_0 \notin C \), and hence \( x_0 \in A, \notin B \cup C \) namely \( x_0 \in A \setminus (B \cup C) \); \( ii \) \( x_0 \in C \), and hence \( x_0 \in A, C \notin B \) namely \( x_0 \in A \cap (C \setminus B) = C \setminus B \) because
Lemma 14: If $\partial S \subseteq \overline{E}$, then $\partial S \cap \partial E \subseteq \{e_1, \ldots, e_n\}$.

Proof of Lem. 14: Suppose $\partial S \cap \partial E \not\subseteq \{e_1, \ldots, e_n\}$, then $\exists y \in \partial S \cap \partial E$ that is not an extreme point (i.e., $e_i$’s) of $\partial S$, meaning $y$ can be represented as a convex combination of two distinct points $y_1, y_2 \in \partial S$. As $\partial S \subseteq \overline{E}$, this then implies $y$ is not an extreme point of $\overline{E}$ either. However, it is clear that all points on $\partial E$ (including $y$) are extreme points of $\overline{E}$, contradiction.

Lemma 15: If $\partial \Lambda \subseteq \overline{E}$, then $\text{conv}(\partial \Lambda) \cap \partial \Lambda \subseteq \overline{E}$.

Proof of Lem. 15: Given $\partial \Lambda \subseteq \overline{E}$, it follows $\text{conv}(\partial \Lambda) \subseteq \overline{E}$, namely (Lem. 11) $\overline{X} \cap S \subseteq \overline{E}$. As $\text{bd}(\text{conv}(\partial \Lambda)) = \partial \Lambda \cup \partial S$, Lem. 12 then gives $\text{conv}(\partial \Lambda) \setminus (\partial \Lambda \cup \partial S) \subseteq \overline{E}$. Applying Lem. 13 with $A = \text{conv}(\partial \Lambda)$, $B = \partial \Lambda$ and $C = \partial S$, we have $\text{conv}(\partial \Lambda) \cap \partial \Lambda = (\text{conv}(\partial \Lambda) \setminus (\partial \Lambda \cup \partial S)) \cup (\partial S \cap \partial \Lambda)$, so to finish the proof we need to show $\partial S \cap \partial \Lambda \subseteq \overline{E}$. Towards this, recall $\partial S \subseteq \text{conv}(\partial \Lambda) \subseteq \overline{E}$, for a point $x \in \partial S \subseteq \overline{E}$, either $x \not\in \partial E$ or $x \in \partial E$. If $x \not\in \partial E$ this means $x \in \overline{E}$. If $x \in \partial E$ then $x \in \partial S \cap \partial E$ and hence (Lem. 14) $x \in \{e_1, \ldots, e_n\}$ which means $x \in \partial \Lambda$. We have proved $\partial S \cap \partial \Lambda \subseteq \overline{E}$. This concludes the proof of Prop. 15.

The following proposition concludes this subsection; it further reduces the search space of points that must be checked to establish the correctness of a bound on $\Lambda$ induced by an ellipsoid $E(c, a_1, a_2)$. Define $V(p) = \{a \in (0, 1] : \exists i \in [n] : p_i = a\}$ as the set of non-zero values taken by a $p \in \partial S$. Further define $P^{(2)} = \{p \in \partial S : |V(p)| \in \{1, 2\}\}$ as those $p$ taking at most two distinct non-zero values, and $P^{(1)} = \{p \in \partial S : |V(p)| = 1\}$ as those $p$ taking exactly one non-zero value; we refer to $P^{(1)}$ as the set of quasi-uniform (QU) vectors. The following proposition reduces the search space from $\partial \Lambda$ to $\{x(p) : p \in P^{(2)}\}$.

Proposition 16: Fix an ellipsoid $E(c, a_1, a_2)$. A potential extremizer of the maximization or minimization problem

$$
\max_{p \in \partial S} \ (\min_{p \in \partial S}) \ f(x(p)) = (x(p) - c)^T R^{-1} (x(p) - c) \tag{99}
$$

can have at most two distinct values among all its non-zero component(s), i.e., $p \in P^{(2)}$.

Proof: For an ellipsoid in the form of (81), membership testing is by comparing the objective function $f(x(p))$ (99) with 1. Restricting the feasible set in (99) to $p \in \partial S$ follows from the results in §VI-A (Prop. 14 and 15). Note maximization and minimization is for inner and outer bounding ellipsoid, respectively. Introducing Lagrange multipliers $\mu$, ($\lambda_i, i \in [n]$) for the equality constraint and each inequality constraint respectively, the Lagrangian of...
this optimization problem is:

\[ \mathcal{L}(p, \mu, \lambda) = f + \mu \left( \sum_{i=1}^{n} p_i - 1 \right) + \sum_{i=1}^{n} \lambda_i (-p_i). \tag{100} \]

The first-order Karush-Kuhn-Tucker (KKT) necessary conditions for a local extremizer are:

- **stationarity** \( \frac{\partial \mathcal{L}}{\partial p_i} = 0, \ i \in [n] \)
- **primal feasibility** \( \sum_{i=1}^{n} p_i - 1 = 0; \ -p_i \leq 0, \ i \in [n] \)
- **dual feasibility** \( \lambda_i \leq (or \geq) 0, \ i \in [n] \)
- **complementary slackness** \( \lambda_i (-p_i) = 0, \ i \in [n]. \)

Fix \( p \in \partial S \) such that \( |\mathcal{V}(p)| \geq 2 \). As \( \frac{\partial \mathcal{L}}{\partial p_i} = \frac{\partial f}{\partial p_i} + \mu - \lambda_i \), it follows that if a potential local extremizer \( p \) has two distinct non-zero components, say \( 0 < p_k < p_l < 1 \), then, due to complementary slackness, the stationarity of the Lagrangian reduces to the equality of derivatives of the objective function w.r.t. \( p_k \) and \( p_l \):

\[ \frac{\partial \mathcal{L}}{\partial p_k} = \frac{\partial \mathcal{L}}{\partial p_l} = 0 \iff \frac{\partial f}{\partial p_k} - \frac{\partial f}{\partial p_l} \left(1 - p_k \right) \left(1 - p_l \right) = 0. \tag{101} \]

Let \( x = x(p) \). For notational convenience, we make the following definitions:

\[ \Sigma \equiv \sum_{i} x_i, \ S \equiv \sum_{i} x_i^2, \ \pi_i \equiv \prod_{j \neq i} (1 - p_j), \ \pi_{ik} \equiv \prod_{j \neq i,k} (1 - p_j), \ \forall i, k \in [n] \tag{102} \]

\[ \beta_i \equiv \frac{1}{na_1^2} (\Sigma - nc) + \frac{1}{a_2^2} \left( x_i - \frac{1}{n} \Sigma \right), \ i \in [n]; \ \alpha \equiv \frac{1}{na_1^2} (\Sigma^2 + nc \Sigma) + \frac{1}{a_2^2} \left( -S + \frac{1}{n} \Sigma^2 \right). \tag{103} \]

Applying Lem. 9, we compute

\[ f(x(p)) = (x - c)^T (\zeta I_{n \times n} + a_2^{-2} I_{n \times n}) (x - c) = \frac{1}{n} (\Sigma - nc)^2 a_1^{-2} + \left( S - \frac{1}{n} \Sigma^2 \right) a_2^{-2}. \tag{104} \]

We can also check

\[ \frac{\partial \Sigma}{\partial p_i} = -\frac{1}{1 - p_i} \Sigma + \frac{1}{p_i (1 - p_i)} x_i \tag{105} \]
\[ \frac{\partial S}{\partial p_i} = 2 \left( -\frac{1}{1 - p_i} S + \frac{1}{p_i (1 - p_i)} x_i^2 \right) \tag{106} \]
\[ \frac{\partial f}{\partial p_i} = \frac{1}{na_1^2} 2 (\Sigma - nc) \frac{\partial \Sigma}{\partial p_i} + \frac{1}{a_2^2} \left( \frac{\partial S}{\partial p_i} - \frac{1}{n} 2 \Sigma \frac{\partial \Sigma}{\partial p_i} \right) \tag{107} \]

\[ \frac{\partial f}{\partial p_i} \frac{1}{a_2} (1 - p_i) = \alpha + \pi_i \beta_i. \tag{108} \]
Using these expressions, the RHS of (101) may be written as
\[(1 - p_i)(\alpha - (-\pi k \beta_k)) = (1 - p_k)(\alpha - (-\pi l \beta_l)).\] (109)

It can be shown that \(\alpha = \sum_{i=1}^{n} p_i (-\pi_i \beta_i) = \mathbb{E}_p(-\pi_i \beta_i),\) so the only way to satisfy equality (109) is to require \((-\pi_i \beta_i)'s\) associated with every non-zero components of \(p \notin \mathcal{P}^{(1)}\) to be all equal, i.e., at this point we have established

\[p : |\mathcal{V}(p)| \geq 2 \text{ and } p \text{ satisfies } (101) \Rightarrow \pi_i(p) \beta_i(p) \text{ are equal for all } i \in [n] : p_i > 0.\] (110)

We next investigate the consequence of this property. First observe \(\pi_i \neq 0\) always holds. There are two possibilities: i) there exists some \(i \in [n]\) with \(\beta_i = 0,\) or ii) \(\beta_i \neq 0\) for all \(i \in [n].\) First consider case i). If some \(\beta_i = 0,\) then all \(\beta_i's\) must equal zero (as otherwise \(\pi_i \beta_i = \pi_j \beta_j\) won’t hold). It then follows from the definition of \(\beta_i\) that all the non-zero components of \(p\) are the same (since all the \(x_i's\) are the same), meaning \(|\mathcal{V}(p)| = 1,\) contradicting the assumption that \(|\mathcal{V}(p)| \geq 2.\)

It remains to consider case ii), i.e., \(\pi_i \neq 0\) and \(\beta_i \neq 0\) for all \(i\) such that \(p_i \neq 0.\) W.l.o.g., let \(i, j\) be indices associated with two non-zero components of \(p.\) Manipulations of the expressions for \(\pi_i\) and \(\beta_i\) yield

\[\frac{\pi_i}{\pi_j} = \frac{\beta_j}{\beta_i} \text{ and } p_i \neq p_j \Rightarrow \frac{\pi_i}{\pi_j} = \frac{\beta_j}{\beta_i} = -a_2^2.\] (111)

But the LHS of the above equation holds for the assumed indices \(i, j\) because of (110). The RHS of (111) therefore holds, and we can prove by contradiction that there are at most two distinct values among all the non-zero components of a potential local extremizer. Namely, if there are indices \(i, j, k\) with \(0 < p_i < p_j < p_k < 1,\) then applying the RHS of (111) to each of the three pairs of indices, i.e., \(\{i, j\}, \{i, k\}, \{j, k\},\) will necessarily violate the assumption \(0 < p_i < p_j < p_k < 1.\) This completes the proof that a potential extremizer \(p\) with \(|\mathcal{V}(p)| \geq 2\) must have \(|\mathcal{V}(p)| = 2,\) i.e., \(p \in \mathcal{P}^{(2)}.\)

We have now established Prop. 16; the remainder of this proof will establish some expressions that will be of use in Props. 18 and 17. A consequence of the above proof is the following. Suppose \(p\) has \(|\mathcal{V}(p)| = 2\) and let \(i, j\) be indices such that \(0 < p_i < p_j < 1.\) Then

\[\frac{nc - \sum}{a_1^2} = \frac{n(\pi_i + x_j) - \sum}{a_2^2} = \frac{n(\pi_j + x_i) - \sum}{a_2^2}.\] (112)

Substitutions of the expressions in (102) and (103) to the objective function \(f\) in (104) yields

\[f(x(p)) = -\alpha + \frac{c}{a_1^2} (nc - \Sigma).\] (113)
If an extremizer $p$ has $|V(p)| = 2$ and satisfies (112), then the objective function may be expressed as

$$f(x(p)) = \frac{1}{a_2^2} \left( -\pi_i \pi_j + cn \left( \pi_i + x_j - \frac{\Sigma}{n} \right) \right).$$  \hspace{1cm} (114)

We emphasize however that this expression for $f$ is derived under the assumptions and constraints associated with (111), and is not valid in general.

\[\Box\]

### B. Explicit ellipsoid induced bounds

The key contributions of this subsection are Props. 18 and 17, which leverage the results from the previous subsection to provide an explicit construction for ellipsoid induced inner and outer bounds on $\Lambda$. As with the proofs of the spherical inner and outer bounds, $\Lambda_{si}$ and $\Lambda_{so}$, the key proof technique we use is by exploiting the implications of Karush-Kuhn-Tucker first order necessary conditions. In the next subsection ($\S$VI-C) we establish the ellipsoid outer bound using a different proof technique.

**Proposition 17 (ellipsoid outer bound):** The ellipsoid $E_{\text{out}}(c, a_{1,\text{out}}(c), a_{2,\text{out}}(c))$ (in the class of $E(c, a_1, a_2)$ ellipsoids) with

$$a_{1,\text{out}}(c) = \sqrt{(nc - 1)c}, \quad a_{2,\text{out}}(c) = \sqrt{\frac{(n-1)}{na_{1,\text{out}}^2 - (nc-1)^2} a_{1,\text{out}}} = \sqrt{(n-1)c}$$  \hspace{1cm} (115)

induces an outer bound $\Lambda_{\text{eo}} = S \setminus E_{\text{out}}$ on $\Lambda$, for all $c > 1/n$.

**Proposition 18 (ellipsoid inner bound):** The ellipsoid $E_{\text{in}}(c, a_{1,\text{in}}(c), a_{2,\text{in}}(c))$ (in the class of $E(c, a_1, a_2)$ ellipsoids) with

$$a_{1,\text{in}}(c) = \sqrt{n(c-m)}, \quad a_{2,\text{in}}(c) = \sqrt{\frac{(n-1)}{na_{1,\text{in}}^2 - (nc-1)^2} a_{1,\text{in}}}$$  \hspace{1cm} (116)

induces an inner bound $\Lambda_{\text{si}} = S \setminus E_{\text{in}}$ on $\Lambda$, for all $c > 1/n$.

**Remark 5:** The ellipsoid inner bound $\Lambda_{\text{si}}$ recovers the optimal spherical inner bound $\Lambda_{\text{si}}^*$ by setting $c$ to be the critical $c_{\text{in}}^* = (1 - nm^2)/(2(1 - nm))$ (note $c_{\text{in}}^* > 1/n$ for all $n \geq 2$); the ellipsoid outer bound $\Lambda_{\text{eo}}$ recovers the optimal spherical outer bound $\Lambda_{\text{so}}^*$ by setting $c = c_{\text{out}}^* = 1$. Furthermore, as a consequence of the tightness monotonicity Prop. 19, any $\Lambda_{ci}$ with $c > c_{\text{in}}^*$ is better than $\Lambda_{si}^*$ and any $\Lambda_{eo}$ with $c > 1$ is better than $\Lambda_{so}^*$ in terms of volume approximation to $\Lambda$.

In words, $E_{\text{in}}$ is such that its boundary $\partial E_{\text{in}}$ passes through $e_1, \ldots, e_n$ and the all-rates-equal point $m$. It can be shown that $\partial E_{\text{in}}$ is tangent at $m$ with $\partial \Lambda$ (recall Lem. 10). $E_{\text{out}}$ is such that its boundary $\partial E_{\text{out}}$ passes through each $e_i$ and is further tangent with $\partial \Lambda$ at each $e_i$ (recall Lem. 10).
The ellipsoid bounds $\Lambda_{ei}, \Lambda_{eo}$ together with $\partial \Lambda$ are shown in Fig. 7 for $n = 2$ and 3, where the center is chosen to be $c = 2$. Improvements can be seen by comparing this figure with the optimal spherical bounds shown in Fig. 6. Furthermore, the quality of the ellipsoid bounds are improved by increasing $c$, as stated below.

**Fig. 7.** Ellipsoid bounds for $n = 2$ (left) and 3 (right) when $c = 2$: inner bound and the complement (w.r.t. $S$) of outer bound are shown in solid; in between sits $\partial \Lambda$. Also shown are the all-rates-equal point $m$ (orange) and corner points $e_i$’s (black).

**Proposition 19:** For all $c > 1/n$, the tightness of both $\Lambda_{ei}$ and $\Lambda_{eo}$ increases in $c$.

This result is illustrated in Fig. 8.

**Proof:** It will be easier to work in a rotated coordinate system, and further to consider all possible “cross-sections” of an ellipsoid $E$, obtained by intersecting $E$ with the hyperplane with normal vector 1. First, perform a rigid rotation of the original coordinate system $X$ according to Def. 9 such that $e_1$ overlaps with $1/\sqrt{n}$ (as in Prop. 12). Second, shift the origin to the point $1/n$, namely the intersection of $\partial S$ and vector 1. Relabel this coordinate system as $X$. Consequently, the original $\partial S$ completely resides in the new coordinate hyperplane $\{x : x_1 = 0\}$, and the equation for the boundary of ellipsoid $E(c, a_1, a_2)$ has a standard form

$$\frac{(x_1 - \sqrt{n}(c - \frac{1}{n}))^2}{a_1^2} + \frac{1}{a_2^2} \sum_{i=2}^{n} x_i^2 = 1.$$  \hfill (117)
By construction of the inner bound, establishing the proposition requires we show that if \( c_1 < c_2 \) then \( \Lambda_{\text{ei}}(c_1) \subseteq \Lambda_{\text{ei}}(c_2) \), namely, if \( c_1 < c_2 \) then \( E_{\text{in}}(c_1) \cap S \supseteq E_{\text{in}}(c_2) \cap S \). Likewise, by construction of the outer bound, establishing the proposition requires we show that if \( c_1 < c_2 \) then \( \Lambda_{\text{eo}}(c_1) \supseteq \Lambda_{\text{eo}}(c_2) \), namely, if \( c_1 < c_2 \) then \( E_{\text{out}}(c_1) \cap S \subseteq E_{\text{out}}(c_2) \cap S \).

Because the ellipsoid \( E(c, a_1, a_2) \) is spherical on the cross-section and for co-centered spheres the relative largeness of radius is the sole indicator of inclusion relationship, we can work with the cross-section where the displacement is negative (corresponding to sitting inside \( S \), recall we rotated the system). From the standard form equation (117) we can solve for the square of the radius of the sphere (with height \( x_1 \)) on the cross-section as

\[
r_2^2 = a_2^2 \left( 1 - \frac{(x_1 - \sqrt{n} (c - \frac{1}{n}))^2}{a_1^2} \right) = \frac{n - 1}{n} \frac{a_1^2 - (x_1 - \sqrt{n} (c - \frac{1}{n}))^2}{a_1^2 - (\sqrt{n} (c - \frac{1}{n}))^2} \tag{118}
\]

where we substitute the expressions from Props. 18 and 17.

Thus for \( \Lambda_{\text{ei}} \) we need to show for \( x \in E_{\text{in}}(c, a_1, a_2) \) with \( x_1 \leq 0 \), the above \( r_2 \) is decreasing in \( c \); for \( \Lambda_{\text{eo}} \) we need to show for \( x \in E_{\text{out}}(c, a_1, a_2) \) with \( x_1 \leq 0 \), the above \( r_2 \) is increasing in \( c \).

We first check \( \Lambda_{\text{ei}} \). To ensure \( x \in E_{\text{in}} \), we must have \( x_1 \geq -\sqrt{n}(1/n - m) \). Substituting \( a_{1,\text{in}}^2 \) from (116) in Prop. 18 into (118), we have

\[
r_{2,\text{in}}^2 = \frac{n - 1}{n} \frac{2(c - (m + y_{1,\text{in}})) (y_{1,\text{in}} - m)}{(2c - (m + \frac{1}{n})) (\frac{1}{n} - m)}, \quad \text{where } y_{1,\text{in}} = \frac{x_1}{\sqrt{n}} + \frac{1}{n} \in \left[ m, \frac{1}{n} \right]. \tag{119}
\]

We take the derivative of \( \frac{(2c - (m + y_{1,\text{in}})) (y_{1,\text{in}} - m)}{(2c - (m + \frac{1}{n})) (\frac{1}{n} - m)} \) w.r.t \( c \) and obtain \( \frac{2(y_{1,\text{in}} - \frac{1}{n})}{(2c - (m + \frac{1}{n}))^2} \leq 0 \) for all \( y_{1,\text{in}} \in \left[ m, \frac{1}{n} \right] \). This shows \( r_{2,\text{in}}^2 \) is decreasing in \( c \) for the regimes of interest.

We next check \( \Lambda_{\text{eo}} \). To ensure \( x \in E_{\text{out}} \), we must have \( x_1 \geq -\sqrt{n}(c - \frac{1}{n}) \) (this is obtained by solving for the intersecting point of \( \partial E_{\text{out}} \) with coordinate axis \( X_1 \)). Substituting \( a_{2,\text{out}}^2 \) from (115) in Prop. 17 into (118), we have

\[
r_{2,\text{out}}^2 = (n - 1) \left( c - \frac{(c - y_{1,\text{out}})^2}{c - \frac{1}{n}} \right), \quad \text{where } y_{1,\text{out}} = \frac{x_1}{\sqrt{n}} + \frac{1}{n} \in \left[ \sqrt{c} - \sqrt{c - \frac{1}{n}}, \frac{1}{n} \right]. \tag{120}
\]

We take the derivative of \( \left( c - \frac{(c - y_{1,\text{out}})^2}{c - \frac{1}{n}} \right) \) w.r.t \( c \) and obtain \( 1 - \frac{c - y_{1,\text{out}}}{(c - \frac{1}{n})^2} (2 \left( c - \frac{1}{n} \right) - (c - y_{1,\text{out}})) \) which is always non-negative since its non-negativeness is equivalent to \( (y_{1,\text{out}} - 1/n)^2 \geq 0 \). This also says we don’t need to restrict our attention to \( S \) (corresponding to \( y_{1,\text{out}} \leq 1/n \)). There is a complete enclosing relationship as \( c \) increases.

Thus \( \partial \Lambda \) is increasingly tightly “sandwiched” between part of \( \partial E_{\text{in}} \) and \( \partial E_{\text{out}} \) as \( c \to \infty \). This sandwiching is asymptotically tight at the all-rates-equal point \( m \) (and by construction always tight at each \( e_i \)). Specifically, the
ellipsoids $E_{\text{in}}, E_{\text{out}}$ viewed in the limit as $c \to \infty$ have axes ratios given by

$$
\lim_{c \to \infty} \frac{a_{1,\text{in}}(c)}{a_{1,\text{out}}(c)} = 1, \quad \lim_{c \to \infty} \frac{a_{2,\text{in}}(c)}{a_{2,\text{out}}(c)} = \left(2 \left(1 - \left(1 - \frac{1}{n} \right)^{n-1}\right)\right)^{-\frac{1}{2}}
$$

for each $n$, where the $a_2$ axes ratio is a monotone decreasing function of $n$, starting with value 1 at $n = 2$. Thus when $n = 2$, the $E_{\text{in}}, E_{\text{out}}$ are asymptotically equal as $c \to \infty$. It follows that the asymptotic in $n$ and $c$ $a_2$ axes ratio is

$$
\lim_{n \to \infty} \lim_{c \to \infty} \frac{a_{2,\text{in}}(n,c)}{a_{2,\text{out}}(n,c)} = \sqrt{\frac{e}{2(e - 1)}} \approx 0.8894.
$$

C. An alternate proof of the outer bound

This subsection supplies an alternate approach to proving the outer bound in Prop. 17. It originates from this observation: membership testing for a ball is even simpler than that for an ellipsoid in that the Euclidean distance to the center of the ball is the sole indicator of set membership. Also, recall our ellipsoid parameterized by $(c, a_1, a_2)$ is already spherical in the subspace spanned by its $2^{\text{nd}}, \ldots, n^{\text{th}}$ axes, so the required transformation converting the ellipsoid to a ball is expected to be simple, too. Of course, ultimately we care about bounding $\Lambda$ rather than membership testing for ellipsoid. The gap is filled in by the following lemma, which uses Prop. 14.
Let $T_{\text{out}}$ be an affine transformation that transforms $E_{\text{out}}$ (with center $c = c1$ and $c > \frac{1}{n}(1 - \frac{1}{n})^{n-1}$) to the unit ball at the origin, i.e., $T_{\text{out}}(E_{\text{out}}) = B(0,1)$. For any $x_t \in \partial \Lambda$ denote by $H_t = H_t(x_t)$ the hyperplane tangent to $\Lambda$ at $x_t$. In the transformed space, this hyperplane is denoted $\hat{H}_t = T_{\text{out}}(H_t)$.

**Lemma 16:** Under the above transformation,

\[ d(\hat{H}_t, o) \geq 1 \text{ holds for all } x_t \in \partial \Lambda \Rightarrow \Lambda \subseteq \Lambda_{\text{eo}}. \tag{123} \]

If $E_{\text{out}}$ is confined within $\mathbb{R}^n_+$, then we also have a converse, namely

\[ \text{If } E_{\text{out}} \subseteq \mathbb{R}^n_+, \text{ then } \Lambda \subseteq \Lambda_{\text{eo}} \Rightarrow d(\hat{H}_t, o) \geq 1 \text{ holds for all } x_t \in \partial \Lambda. \tag{124} \]

**Proof:** “forward part (i.e., (123))”: As affine transformations preserve tangency and set inclusion, it follows that

\[ d(\hat{H}_t, o) \geq 1 \iff d(H_t, \overline{E_{\text{out}}}) > 0 \text{ or } H_t \text{ is tangent with } \overline{E_{\text{out}}}. \tag{125} \]

The RHS of (125) says $H_t \cap \overline{E_{\text{out}}} \subseteq \partial E_{\text{out}}$, since $x_t \in H_t$ it follows $x_t \notin E_{\text{out}}$. So $d(\hat{H}_t, o) \geq 1$ implies $\forall x_t \in \partial \Lambda, x_t \notin E_{\text{out}}$, meaning $\partial \Lambda \subseteq \Lambda_{\text{eo}}$. Observe $\partial \Lambda \subseteq \Lambda_{\text{eo}} \iff \partial \Lambda \cap E_{\text{out}} = \emptyset$, it then follows from Prop. 14 that $\Lambda \subseteq \Lambda_{\text{eo}}$.

“converse part (i.e., (124))”: $\Lambda \subseteq \Lambda_{\text{eo}}$ means $E_{\text{out}} \subseteq \Lambda^c$, so $E_{\text{out}} \subseteq \Lambda^c \cap \mathbb{R}^n_+$, a convex set ([15]). Thus $H_t$ is a supporting hyperplane for the convex set $\Lambda^c \cap \mathbb{R}^n_+ \supseteq E_{\text{out}}$, so $d(\hat{H}_t, \overline{E_{\text{out}}}) > 0$ or $H_t$ is tangent with $\overline{E_{\text{out}}}$, then the properties of affine transformation ensures $d(\hat{H}_t, \overline{B(o,1)}) > 0$ or $\hat{H}_t$ is tangent with $\overline{B(o,1)}$, which can be summarized as $d(\hat{H}_t, o) \geq 1$.

**Remark 6:** The intuition behind Lem. 16 is that the intersection between any tangent hyperplane of $\partial \Lambda$ and $\mathbb{R}^n_+$ is included in $\Lambda$ (proof similar to part of the proof of Prop. 7), hence the intersection is disjoint from (or at most tangent with) any $\overline{E_{\text{out}}}$. If further $E_{\text{out}}$ is entirely confined within $\mathbb{R}^n_+$, then for any $x_t \in \partial \Lambda$, any part of the associated tangent hyperplane $H_t(x_t)$ beyond $\mathbb{R}^n_+$ cannot touch $E_{\text{out}}$. Consequently, the entire tangent hyperplane is disjoint from (or at most tangent with) such $\overline{E_{\text{out}}}$.

The following proposition will be used in our alternate proof of the $\Lambda_{\text{eo}}$ bound. For notational convenience, we define following functions, assuming $(c, a_1, a_2)$ is given.

**Definition 10:**

\[ g(p) \equiv \frac{(n - 1)^2}{n} a_1^2 + a_2^2 \sum_{i=2}^n \left( \frac{1}{\sqrt{n}} - p_i - \frac{1}{1 + \sqrt{n}} (1 - p_1) \right)^2, \quad f(p) \equiv \sqrt{g(p)} + \pi(p) \tag{126} \]

\[ \hat{g}(p) \equiv \frac{(n - 1)^2}{n} a_1^2 + \left( -\frac{1}{n} + \sum_{i=1}^n p_i \right) a_2^2, \quad \hat{f}(p) \equiv \sqrt{\hat{g}(p)} + \pi(p). \tag{127} \]
It can be verified that
\[ g(p) = \tilde{g}(p), \quad \text{if} \quad \sum_{i=1}^{n} p_i = 1. \quad (128) \]

**Proposition 20:** Fix an ellipsoid \( E(c, a_1, a_2) \). Define \( \Lambda_e \equiv S \setminus E \). Assume \( c > \frac{1}{n}(1 - \frac{1}{n})^{n-1} \). We have
\[ f(p) \leq c(n - 1) \quad \text{for all} \quad p \in \partial S \Rightarrow \Lambda \subseteq \Lambda_e. \quad (129) \]

Conversely,
\[ \text{If} \quad E \subseteq \mathbb{R}^n_+, \quad \text{then} \quad \Lambda \subseteq \Lambda_e \Rightarrow f(p) \leq c(n - 1) \quad \text{for all} \quad p \in \partial S. \quad (130) \]

**Proof:** Recall all rotation matrices are orthonormal, as one consequence of Prop. 11 the rotation matrix given in (93) can be used as the \( Q \) in the decomposition of \( R \) as shown in (81). An ellipsoid (in the form (81)) can be viewed as the image of a unit ball after some affine transformation:
\[ E = \{ x : x = c + Av \mid \|v\| < 1 \}, \quad (131) \]
where \( A \) is the matrix associated with this affine transformation, and \( c \) is the center of the ellipsoid. It is easy to verify the two forms of an ellipsoid are related by \( A = QD^2 \). Furthermore, the hyperplane \( \{ x : n^T x = d \} \) corresponds to \( \{ v : n_v^T v = d_v \} \) in the pre-image space \( V \) (where \( E \) becomes a unit ball centered at the origin) and they are related by:
\[ n_v^T = n^T A, \quad d_v = d - n^T c. \quad (132) \]
Recall from [15] that the tangent hyperplane at a point \( x(p) \) on \( \partial A \): \( \{ x : (1 - p)^T x = \pi(p) \} \) where \( p \in \partial S \).
Specializing \( n = 1 - p, \quad d = \pi(p) \), we can verify:
\[ (n_v)_i = \begin{cases} \frac{1}{\sqrt{n}} a_1(n - 1), & i = 1 \\ a_2 \left( \frac{1}{\sqrt{n}} - p_i - \frac{1}{1 + \sqrt{n}} (1 - p_1) \right), & i = 2, \ldots, n \end{cases} \quad (133) \]

We apply Lem. 16 with \( \hat{H}_t = \{ v : n_v^T v = d_v \} \), using a formula (see e.g., [24] §1.4) for computing the absolute distance between a point \( y \) and the hyperplane \( \hat{H}_t : |y^T n_v - d_v|/\|n_v\| \) and observing setting \( y = \mathbf{0} \) and assuming \( c > \frac{1}{n}(1 - \frac{1}{n})^{n-1} \) allows the sign to be determined. Algebra shows the following equivalent condition:
\[ d(\hat{H}_t, \mathbf{0}) \geq 1 \iff f(p) \leq c(n - 1). \quad (134) \]

The proof is now complete.

Prop. 20 asks us to check the inequality \( f(p) \leq c(n - 1) \) holds for all \( p \in \partial S \). As before, we formulate this as a constrained optimization problem. Unlike before, though, Schur-convexity now makes our job a lot easier. For this we need to state an equivalent condition for verifying Schur-convexity.
Proposition 21 ([25], Ch. 3, Thm. A.4): Let $D \subseteq \mathbb{R}$ be an open interval and let a symmetric function $f : D^n \rightarrow \mathbb{R}$ be continuously differentiable. Then $f$ is Schur-convex on $D^n$ if and only if for all distinct indices $k, l \in [n]$: 
\[ (x_k - x_l) \left( \frac{\partial f}{\partial x_k} - \frac{\partial f}{\partial x_l} \right) \geq 0, \quad \forall x \in D^n. \]  
(135)

We now apply Prop. 20, meaning we need to solve 
\[ \max_{p \in \partial S} \tilde{f}(p) = \sqrt{g(p)} + \pi(p), \]  
(136)
where $g(p)$ ($f(p)$) is replaced by $\tilde{g}(p)$ ($\tilde{f}(p)$) due to (128). Note $\tilde{f}(p)$ is symmetric.

Algebra gives:
\[ (p_k - p_l) \left( \frac{\partial \tilde{f}}{\partial p_k} - \frac{\partial \tilde{f}}{\partial p_l} \right) = (p_k - p_l)^2 \left( \frac{\alpha^2}{\sqrt{g}} - \frac{\pi(p)}{(1 - p_k)(1 - p_l)} \right). \]  
(137)

In order to show the RHS of (137) is non-negative, it suffices to show $\frac{\alpha^2}{\sqrt{g}} \geq 1$, for which we specialize with the expressions for $E_{\text{out}}$ given in (115) and get:
\[ \left( \frac{\alpha^2_{\text{out}}}{\sqrt{g}} \right)^2 = \frac{(n - 1)c}{nc - 1 - c + \sum_{i=1}^n p_i} \geq \frac{(n - 1)c}{nc - 1 - c + \sum_{i=1}^n p_i} = 1. \]  
(138)

Therefore, Prop. 21 tells $\tilde{f}$ in (136) specialized to our $E_{\text{out}}$ is Schur-convex. It then follows from the definition of Schur-convexity and the fact $e_i$ majorizes every other point in the feasible set $\partial S$ that the global maximum of $\tilde{f}$ is attained at each $e_i$. Finally, evaluating $\tilde{f}$ at $e_i$ gives $c(n - 1)$, the desired global maximum (according to Prop. 20). This then completes our alternate proof that our proposed ellipsoid outer bound is valid.

Remark 7: The Schur-convexity approach would not be directly applicable to the proposed ellipsoid inner bound in Prop. 18. Because even if we could have a parallel result to Prop. 20 for inner bounding ellipsoids, the fact that our inner bounding ellipsoid in (116) is tight at $m$ as well as at $e_i$ precludes Schur-convexity, since $m$ is strictly majorized by every other point and $e_i$ majorizes every other point.

VII. GENERALIZED CONVEXITY PROPERTIES

Given an arrival rate vector $x = (x_1, \ldots, x_n)$, define the set of stabilizing controls $P(x)$ assuming the worst-case service rate:
\[ P(x) \equiv \left\{ p \in [0, 1]^n : x_i \leq p_i \prod_{j \neq i} (1 - p_j), \quad i \in [n] \right\}. \]  
(139)

This set is related to $\Lambda$ in that $P(x) = \emptyset$ iff $x \notin \Lambda$. Whereas $\Lambda$ is an important inner bound for the Aloha stability region $\Lambda_A$, the set $P(x)$ can be viewed as the set of control options given a desired arrival rate vector $x$. To proceed,
we now view \( x \) as parameters (instead of \( p \), as was done previously) and define an “excess rate” function for each \( i \in [n] \):

\[
f_i(p) = x_i - p_i \prod_{j \neq i} (1 - p_j), \quad i \in [n].
\] (140)

The excess rate functions are closely related to the set of stabilizing controls. To see this, define the \( \alpha \)-sublevel sets of each excess rate function

\[
S_{i,\alpha} \equiv \{ p \in [0,1]^n : f_i(p) \leq \alpha \}, \quad \alpha \in \mathbb{R}.
\] (141)

Denote by \( S_\alpha = \cap_{i=1}^n S_{i,\alpha} \); then \( \mathcal{P}(x) = S_0 = \cap_{i=1}^n S_{i,0} \). In words, the set of stabilizing controls associated with \( \Lambda \) is the intersection of \( 0 \)-sublevel sets of these \( n \) excess rate functions.

For simplicity and sometimes, well-definedness, throughout this section we will work with the open convex domain \((0,1)^n\). The following propositions show these excess rate functions are not convex (Prop. 22), but are quasiconvex (Prop. 23), pseudoconvex (Prop. 24), and invex (Prop. 25).

*Proposition 22:* For any \( i \in [n] \), the excess rate function \( f_i(p) \) in (140) is not convex on \((0,1)^n\).

*Proof:* In fact we can work with an additional constraint \( \sum_{i=1}^n p_i = 1 \), i.e., with \( \partial S \) being the domain.

Wlog let us show this for \( f_1(p) = x_1 - p_1 \prod_{j \neq 1} (1 - p_j) \). Let \( \epsilon \in (0,1) \) be determined later. Denote \( p_{1,\epsilon} = (1 - \epsilon, \epsilon/(n-1), \ldots, \epsilon/(n-1)) \), \( p_2 = (1/n)1 \). Form the convex combination \( p_{\theta,\epsilon} = \theta p_{1,\epsilon} + (1 - \theta) p_2 \) for \( \theta \in (0,1) \). We shall show for all \( n \) the existence of \( \epsilon \) and \( \theta \) in order for the following inequality to hold:

\[
f_1(p_{\theta,\epsilon}) > \theta f_1(p_{1,\epsilon}) + (1 - \theta) f_1(p_2).
\] (142)

After substituting definitions and \( \theta = 1/2 \), the above inequality becomes:

\[
(1 - \epsilon + \frac{1}{n}) \left( 1 - \frac{n(\epsilon + 1) - 1}{2n(n-1)} \right)^{n-1} < (1 - \epsilon) \left( 1 - \frac{\epsilon}{n-1} \right)^{n-1} + \frac{1}{n} \left( 1 - \frac{1}{n} \right)^{n-1}.
\] (143)

Manipulation of the above equation gives the equivalent form

\[
\sqrt[n-1]{\frac{1 - \epsilon + \frac{1}{n}}{(1 - \epsilon) \left( 1 - \frac{\epsilon}{n-1} \right)^{n-1} + \frac{1}{n} \left( 1 - \frac{1}{n} \right)^{n-1}}} < \frac{1}{\sqrt[2n(n-1)]{n(\epsilon + 1) - 1}}.
\] (144)

Applying the AM-GM inequality to the LHS:

\[
\sqrt[n-1]{\frac{1 - \epsilon + \frac{1}{n}}{(1 - \epsilon) \left( 1 - \frac{\epsilon}{n-1} \right)^{n-1} + \frac{1}{n} \left( 1 - \frac{1}{n} \right)^{n-1}}} \leq \frac{1 - \epsilon + \frac{1}{n}}{(1 - \epsilon) \left( 1 - \frac{\epsilon}{n-1} \right)^{n-1} + \frac{1}{n} \left( 1 - \frac{1}{n} \right)^{n-1}} + n - 2 \leq \frac{1 - \epsilon + \frac{1}{n}}{\frac{1}{n-1}} + n - 2 \leq \frac{1 - \epsilon + \frac{1}{n}}{\frac{1}{n-1}} + n - 2 \leq > \frac{1}{n-1}.
\] (145)
It is easily verified that the sequence \((1 - \frac{1}{n})^{n-1}\) monotonically decreases to \(1/e\), and that \(\left(1 - \frac{\varepsilon}{n-1}\right)^{n-2}\) monotonically decreases to \(1/e^\varepsilon\). Because of this, it suffices to show
\[
\frac{1 - \varepsilon + \frac{1}{n}}{(1 - \varepsilon) \left(1 - \frac{\varepsilon}{n-1}\right)^{n-2} + \frac{1}{n}} + n - 2 < \frac{1}{1 - n^{(n+1)-1}},
\]
which after rearrangement becomes
\[
\frac{1 - \varepsilon + \frac{1}{n}}{(1 - \varepsilon) \left(1 - \frac{\varepsilon}{n-1}\right)^{1/e^\varepsilon} + \frac{1}{n}} - 3n - 2 < 0.
\]
Denote \(h_1(n, \varepsilon) = \frac{1 - \varepsilon + \frac{1}{n}}{(1 - \varepsilon) \left(1 - \frac{\varepsilon}{n-1}\right)^{1/e^\varepsilon} + \frac{1}{n}}\) and \(h_2(n) = \frac{3n-2}{2n-1}\). One can verify that, given \(\varepsilon \in (0, 1)\), \(h_1(n, \varepsilon)\) and \(h_2(n)\) are monotonically decreasing and increasing in \(n\) \((n \geq 2)\), respectively. Thus it suffices to show (147) holds when \(n = 2\). Observe given \(n\), the LHS of (147) i.e., \(h_1(n, \varepsilon) - h_2(n)\) is a continuous function of \(\varepsilon\) for \(\varepsilon \in (0, 1)\), since \(h_1(2, 0) - h_2(2) < 0\), \(h_1(2, 1) - h_2(2) > 0\), there exist various choices of \(\varepsilon\) so that (147) holds for \(n = 2\), and hence for all \(n \geq 2\) (with the same choice of \(\varepsilon\)).

Recall a function is called quasiconvex (or unimodal) if its domain and all its sublevel sets are convex [21].

**Proposition 23:** The excess rate function is quasiconvex on \((0, 1^n)\) for all \(i \in [n]\).

**Proof:** Our approach is to show the convexity of the sublevel sets \(S_{i,\alpha}\) for which we discuss two cases: \(i)\) \(\alpha \geq x_i\), and \(ii)\) \(\alpha < x_i\). Consider case \(i)\). If \(\alpha \geq x_i\) then \(f_i(p) \leq \alpha\) always holds, and therefore \(S_{i,\alpha} = \text{dom } f = (0, 1)^n\), which is convex. It remains to consider case \(ii)\), with \(\alpha < x_i\). Construct \(g_i(p_{\setminus i}) = \prod_{j \neq i} (1 - p_j)\), where \(p_{\setminus i}\) is formed from the vector \(p\) by dropping component \(i\). Observe
\[
S_{i,\alpha} = \{p \in (0, 1)^n : f_i(p) \leq \alpha\} = \{(p_{\setminus i}, p_i) \in (0, 1)^n : g_i(p_{\setminus i}) \leq p_i\}.
\]
Thus \(S_{i,\alpha}\) can be interpreted as the epigraph of the function \(g_i(p_{\setminus i})\). Since a function is convex iff its epigraph is a convex set, we then need to show this function \(g_i(p_{\setminus i})\) is convex. Towards this, we take the logarithm and write:
\[
\log g_i(p_{\setminus i}) = \log(x_i - \alpha) - \sum_{j \neq i} \log(1 - p_j) = \log(x_i - \alpha) + \sum_{j \neq i} -\log \left(1 - (e_j)_{\setminus i}^T p_{\setminus i}\right),
\]
where \((e_j)_{\setminus i}\) is the \((n-1)\)-vector by peeling off the \(i^{th}\) component of \(e_j\). This shows the RHS of the above equation is convex by recognizing the convexity of \(-\log(\cdot)\) and certain function compositions that preserve convexity. Finally since the function \(g_i(p_{\setminus i})\) is log-convex, this means \(g_i(p_{\setminus i})\) is itself convex, which means its epigraph, or equivalently the sublevel set \(S_{i,\alpha}\), is convex.

**Corollary 3:** Recall \(\mathcal{P}(x) = S_0 = \cap_{i=1}^n S_{i,0}\). It follows that the set of stabilizing controls \(\mathcal{P}(x)\) associated with \(x \in \Lambda\) is convex, as convexity is preserved under set intersection.

**Proposition 24:** The excess rate function is pseudoconvex on \((0, 1^n)\) for all \(i \in [n]\).
Proof: We apply Cor. 10.1 of Diewert et al. [26] (note it is stated for pseudoconcavity), or Cambini and Marten [27] (Thm. 3.4.6 and 3.4.7). Essentially, we shall show that given \( i \in [n] \) and \( \mathbf{p} \in \text{dom} f = (0, 1)^n \), then for all \( \mathbf{q} \) such that \( \|\mathbf{q}\| = 1 \), \( \mathbf{q}^T \nabla f_i(\mathbf{p}) = 0 \) implies \( \mathbf{q}^T \nabla^2 f_i(\mathbf{p}) \mathbf{q} > 0 \).

The gradient of \( f_i(\mathbf{p}) \) is:

\[
\frac{\partial}{\partial p_k} f_i(p) = \begin{cases} 
\frac{f_i(p) - x_i}{p_i}, & k = i \\
\frac{f_i(p) - x_j}{1 - p_k}, & k \neq i
\end{cases}
\]

(150)

The Hessian of \( f_i(\mathbf{p}) \) is:

\[
\frac{\partial^2}{\partial p_k \partial p_l} f_i(p) = \begin{cases} 
0, & k = l, (i, k, l) \text{ distinct} \\
-\frac{p_i \prod_{j \neq i, k, l} (1 - p_j)}{p_k (1 - p_k)}, & k = i \neq l \\
-\frac{p_i \prod_{j \neq i, k, l} (1 - p_j)}{p_k (1 - p_k)}, & l = i \neq k
\end{cases}
\]

(151)

Given \( \mathbf{q} \), \( \mathbf{q}^T \nabla f_i(\mathbf{p}) = 0 \) means

\[
q_i \frac{f_i(p) - x_i}{p_i} + \sum_{k \neq i} q_k \left( -\frac{f_i(p) - x_j}{1 - p_k} \right) = 0,
\]

(152)

or equivalently:

\[
q_i \left( -\prod_{j \neq i} (1 - p_j) \right) + \sum_{k 
eq i} q_k \left( p_i \prod_{j \neq k, i} (1 - p_j) \right) = 0,
\]

(153)

which gives (since \( \mathbf{p} \in (0, 1)^n \)):

\[
\sum_{k \neq i} \frac{q_k}{1 - p_k} = \frac{q_i}{p_i}.
\]

(154)

To verify \( \mathbf{q}^T \nabla^2 f_i(\mathbf{p}) \mathbf{q} > 0 \), i.e., \( \sum_{k,l} q_k q_l \frac{\partial^2}{\partial p_k \partial p_l} f_i(\mathbf{p}) > 0 \), we break this sum into four parts. For any \( i \in [n] \), the set \( \mathcal{I} = \{(k, l) : k, l \in [n]\} \) may be partitioned into four parts:

\[
\mathcal{I}_{i,1} = \{(k, k) : k \in [n]\}, \quad \mathcal{I}_{i,2} = \{(k, l) : k, l, i \text{ distinct}\}, \quad \mathcal{I}_{i,3} = \{(i, l) : l \in [n]\setminus\{i\}\}, \quad \mathcal{I}_{i,4} = \{(k, i) : k \in [n]\setminus\{i\}\}.
\]

(155)

Then

\[
\sum_{k,l} q_k q_l \frac{\partial^2}{\partial p_k \partial p_l} f_i(\mathbf{p}) = \sum_{(k, l) \in \mathcal{I}_{i,1}} \frac{\partial^2}{\partial p_k \partial p_l} f_i(\mathbf{p}) + \sum_{(k, l) \in \mathcal{I}_{i,2}} \frac{\partial^2}{\partial p_k \partial p_l} f_i(\mathbf{p}) + \sum_{(k, l) \in \mathcal{I}_{i,3}} \frac{\partial^2}{\partial p_k \partial p_l} f_i(\mathbf{p}) + \sum_{(k, l) \in \mathcal{I}_{i,4}} \frac{\partial^2}{\partial p_k \partial p_l} f_i(\mathbf{p}).
\]
By symmetry, the third and fourth sums are equal to each other. The three sums equal, respectively:

\[
\sum_{(k,l)\in I_{i,1}} \frac{\partial^2}{\partial p_k \partial p_l} f_i(p) = 0
\]  

(156)

\[
\sum_{(k,l)\in I_{i,2}} \frac{\partial^2}{\partial p_k \partial p_l} f_i(p) = \sum_{(k,l)\in I_{i,2}} q_k q_l \left( \frac{f_i(p) - x_i}{(1 - p_k)(1 - p_l)} \right)
\]  

(157)

\[
\sum_{(k,l)\in I_{i,3}} \frac{\partial^2}{\partial p_k \partial p_l} f_i(p) = \sum_{(k,l)\in I_{i,3}} q_k q_l \left( \frac{f_i(p) - x_i}{p_l(1 - p_l)} \right) = \sum_{l \neq i} q_k q_l \left( -\frac{f_i(p) - x_i}{p_l(1 - p_l)} \right)
\]  

(158)

The third sum can be further simplified as

\[
\sum_{(k,l)\in I_{i,3}} \frac{\partial^2}{\partial p_k \partial p_l} f_i(p) = q_i \frac{1}{p_i} \sum_{k \neq i} q_k \left( -\frac{f_i(p) - x_i}{1 - p_k} \right)
\]

\[
\overset{(a)}{=} q_i \frac{1}{p_i} \left( -q_i \frac{f_i(p) - x_i}{p_i} \right)
\]

\[
= -\left( \frac{q_i}{p_i} \right)^2 (f_i(p) - x_i)
\]

\[
= \left( \frac{q_i}{p_i} \right)^2 p_i \prod_{j \neq i} (1 - p_j),
\]  

(159)

where \((a)\) is due to (152). Next, the second sum can be written as:

\[
\sum_{(k,l)\in I_{i,2}} \frac{\partial^2}{\partial p_k \partial p_l} f_i(p) = \sum_{(k,l)\in I_{i,2}} q_k q_l \left( -p_i \prod_{j \neq k,l,i} (1 - p_j) \right) = -\sum_{(k,l)\in I_{i,2}} q_k q_l p_i \prod_{j \neq i} (1 - p_j) \prod_{j \neq i} (1 - p_l).
\]  

(160)

Combining the above results, we have

\[
\sum_{k,l} q_k q_l \frac{\partial^2}{\partial p_k \partial p_l} f_i(p) = -\left( \sum_{k \neq i} q_k p_i \prod_{j \neq i} (1 - p_j) \right) + 2 \left( \frac{q_i}{p_i} \right)^2 p_i \prod_{j \neq i} (1 - p_j)
\]

\[
= p_i \prod_{j \neq i} (1 - p_j) \left( -\sum_{k \neq i} q_k q_l \prod_{j \neq i} \frac{1 - p_j}{1 - p_l} + 2 \left( \frac{q_i}{p_i} \right)^2 \right).
\]  

(161)

Then, the sign of the overall sum is determined by the sign of the term in parentheses, above. This term can be written as

\[
- \sum_{(k,l)\in I_{i,2}} q_k q_l \left( \frac{1}{1 - p_k}(1 - p_l) + 2 \left( \frac{q_i}{p_i} \right)^2 \right) = -\left( \sum_{k \neq i} q_k \frac{1}{1 - p_k} \sum_{l \neq i} q_l \frac{1}{1 - p_l} - \sum_{k \neq i} q_k \frac{q_l}{1 - p_k} \frac{1}{1 - p_l} \right) + 2 \left( \frac{q_i}{p_i} \right)^2
\]

\[
\overset{(b)}{=} -\left( \left( \frac{q_i}{p_i} \right)^2 - \sum_{k \neq i} \left( \frac{q_k}{1 - p_l} \right)^2 \right) + 2 \left( \frac{q_i}{p_i} \right)^2
\]

\[
= \left( \frac{q_i}{p_i} \right)^2 + \sum_{k \neq i} \left( \frac{q_k}{1 - p_k} \right)^2,
\]  

(162)
where \((b)\) is due to (154), and the last expression is clearly positive. This establishes the pseudoconvexity of the excess rate function \(f_i(p)\) on \(p \in (0, 1)^n\).

**Proposition 25:** The excess rate function is invex on \((0, 1)^n\) for all \(i \in [n]\).

**Proof:** For differentiable \(f\) with open convex domain, \(f\) is invex if and only if every stationary point is a global minimizer (see e.g., Thm. 4.9.1 of Cambini and Martein [27]). Next, Thm. 2.27 of Mishra and Giorgi [28] says if \(f\) is differentiable and quasiconvex with open convex domain, then \(f\) is pseudoconvex if and only if every stationary point is a global minimizer. These two results mean that under the assumption of quasiconvexity, invexity and pseudoconvexity coincide. Thus the invexity of our excess rate functions follows from Props. 23 and 24.

VIII. CONCLUSION

This paper has established some new properties of the set \(\Lambda\), with a focus on establishing inner and outer bounds induced by simple polyhedra, spheres, and ellipsoids. A natural extension of this work would be to identify different classes of \(E(c, a_1, a_2)\) ellipsoids, besides the particular \(E_{\text{in}}\) and \(E_{\text{out}}\) ones we have constructed, that induce tighter bounds on \(\Lambda\). A second extension is to seek a combinatorial expression for the volume of \(\Lambda\) that is simpler and easier to compute than the one we have provided, or at least to provide a more accurate approximation of how the volume varies with \(n\).

IX. ACKNOWLEDGEMENT

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X. APPENDIX

A. Proof of Prop. 3

We first show a supporting lemma and its corollary. We define a univariate function \( g(t_{\pi}) = g(t_{\pi}, \mathbf{p}) \), as

\[
g(t_{\pi}, \mathbf{p}) = \prod_{i=1}^{n} (1 + p_{i} t_{\pi} - (1 + t_{\pi}), \quad \mathbf{p} \in [0, 1]^{n}.
\]

**Lemma 17:** For all \( n \geq 2 \), \( g(t_{\pi}, \mathbf{p}) \) can only have one or two real roots on \((-1, \infty)\). More specifically:

- \( t_{\pi} = 0 \) is always a root, and is the unique root iff \( \sum_{i=1}^{n} p_{i} = 1 \), i.e., \( \mathbf{p} \) is a probability vector;
- besides \( t_{\pi} = 0 \), the other root is on \((0, \infty)\) iff \( \sum_{i=1}^{n} p_{i} < 1 \);
- besides \( t_{\pi} = 0 \), the other root is on \((-1, 0)\) iff \( \sum_{i=1}^{n} p_{i} > 1 \).

**Proof:** Applying the chain rule of differentiation, we have:

\[
g'(t_{\pi}) = \sum_{i=1}^{n} p_{i} \prod_{j \neq i} (1 + p_{j} t_{\pi} - 1), \quad g''(t_{\pi}) = \sum_{i=1}^{n} p_{i} \sum_{j \neq i} p_{j} \prod_{k \neq j, i} (1 + p_{k} t_{\pi}).
\]

Here are some simple yet important observations: \( g(0) = 0, g(-1) = \pi(\mathbf{p}) > 0, g'(0) = \sum_{i=1}^{n} p_{i} - 1 \), and \( g'(-1) = \sum_{i=1}^{n} p_{i} \prod_{j \neq i} (1 - p_{j}) - 1 \leq 0 \). The last inequality is justified since we can construct a vector \( \mathbf{x}(\mathbf{p}) \) according to (9) in Def. 2, and then apply the fact \( \Lambda_{eq} = \Lambda \subseteq S \). Furthermore, \( g''(0) \geq 0 \) and in fact \( g''(t_{\pi}) \geq 0 \).
for all \( t_\pi > -1 \) which means \( g'(t_\pi) \) is monotone increasing on \((-1, \infty)\). In the following we first show the forward part, i.e., how to go from the condition on \( \sum_{i=1}^n p_i \) to the properties of the roots.

- **case 1:** \( \sum_{i=1}^n p_i = 1 \). In this case, since \( g'(0) = 0 \) and \( g''(0) \geq 0 \), the stationary point 0 is a local minimizer. As \( g(-1) = \pi(p) \), \( g'(-1) \leq 0 \), \( g'(t_\pi) \) is monotone increasing on \((-1, \infty)\), so what happens on \((-1, \infty)\) is: \( g(t_\pi) \) is monotone decreasing from \( \pi(p) \) \( (t_\pi = -1) \) to 0 \( (t_\pi = 0) \), and then monotone increasing from 0 to \( \infty \) (as \( t_\pi \to \infty \)). Thus the only root on \((-1, \infty)\) is 0.

- **case 2:** \( \sum_{i=1}^n p_i < 1 \). In this case, \( g'(0) < 0 \). Thus \( g(t_\pi) \) is decreasing from \( \pi(p) \) \( (t_\pi = -1) \) to 0 \( (t_\pi = 0) \), then keeps decreasing until some stationary point \( t_{\pi,2}^* > 0 \) such that \( g'(t_{\pi,2}^*) = 0 \), after which \( g(t_\pi) \) keeps increasing as \( t_\pi \to \infty \). Note \( g(t_{\pi,2}^*) < 0 \), so the only other root \( \hat{t}_{\pi,2} \) is on \((0, \infty)\).

- **case 3:** \( \sum_{i=1}^n p_i > 1 \). In this case, \( g'(0) > 0 \). Thus \( g(t_\pi) \) is decreasing from \( \pi(p) \) \( (t_\pi = -1) \) to 0 (at some \( \hat{t}_{\pi,3} \)), and keeps decreasing until at some stationary point \( t_{\pi,3}^* \) such that \( g'(t_{\pi,3}^*) = 0 \), after which \( g(t_\pi) \) keeps increasing as \( t_\pi \to \infty \). Since \( g'(t_\pi) > 0 \) for all \( t_\pi > t_{\pi,3}^* \) and recall \( g'(t_\pi) \) itself is monotone increasing, so \( t_{\pi,3}^* \in (-1, 0) \) which further implies the other root i.e., \( \hat{t}_{\pi,3} \) has to be on \((-1, 0)\).

The converses are clear (proof by contradiction) and are omitted.

**Corollary 4:** Fix \( n \geq 2 \) and \( x \in \mathbb{R}^n_+ \). i) The total number of positive roots of \( f(\delta, x) \) is at most two. Furthermore, ii) if there exists a compatible stabilizing control \( p \) with \( x \) in the sense of \( \Lambda_{eq} \), namely the \((x, p)\) pair satisfies (9) in Def. 2, then \( f(\delta, x) \) has a positive root \( \delta_t \) iff \( g(t_\pi, p) \) has a root \( t_{\pi, p} \in (-1, \infty) \), and the roots of \( f, g \) can be related by \( \delta_t = \frac{1}{\pi(p)}(1 + t_{\pi, p}) \). More specifically \( f(\delta, x) \) has either one or two positive roots:

- \( \delta_t = \frac{1}{\pi(p)} \) is always a positive root, and is the unique root iff \( \sum_{i=1}^n p_i = 1 \), i.e., \( p \) is a probability vector;
- besides \( \delta_t = \frac{1}{\pi(p)} \), \( f(\delta, x) \) also has a larger positive root iff \( \sum_{i=1}^n p_i < 1 \);
- besides \( \delta_t = \frac{1}{\pi(p)} \), \( f(\delta, x) \) also has a smaller positive root iff \( \sum_{i=1}^n p_i > 1 \).

**Proof:** We first show ii). Substituting \( \delta_t , \pi(p) \) and \( x_i(p) = \frac{p_i}{1-p_i} \pi(p) \) into the definition of \( f(\delta, x) \), we have

\[
f(\delta_t, x) = \prod_{i=1}^n \left( 1 + \frac{p_i}{1-p_i} \pi(p) \frac{1}{\pi(p)}(1 + t_{\pi, p}) \right) - \frac{1}{\pi(p)}(1 + t_{\pi, p})
\]

\[
= \frac{1}{\pi(p)} \prod_{i=1}^n (1 + p_i t_{\pi, p}) - (1 + t_{\pi, p}) = \frac{1}{\pi(p)} g(t_{\pi, p}, p) .
\]

Therefore, given \( x \) and its compatible \( p \) in the sense of \( \Lambda_{eq} \), \( \delta_t \) is a root of \( f(\delta, x) \) iff \( t_{\pi, p} \) is a root of \( g(t_{\pi, p}, p) \).

Since \( \delta_t \) is positive iff \( t_{\pi, p} \in (-1, \infty) \), the statement for the three cases then follows from Lem. 17.

We next show i). Recall from the proof of Prop. 1 that if \( f(\delta, x) \) ever has a positive root \( \hat{\delta} \), then we can construct \( p = p(\hat{\delta}, x) \) according to (7) in Def. 2. Since this \( p \) is compatible with \( x \) in the sense of \( \Lambda_{eq} \) meaning \((x, p(\hat{\delta}, x))\)
satisfies (9) in Def. 2, the assertion that \( f(\delta, x) \) can have at most two positive roots follows from \( ii \) just proved.

We now provide the proof of Prop. 3.

**Proof of part 1**

\( \Rightarrow \):

Given \( x \in \partial \Lambda \), from the (preliminary) root testing Prop. 1 we know there exists a positive root \( \delta_u \) for \( f(\delta, x) \). Form a vector of probabilities \( p_u = p_u(\delta_u, x) \) according to (7) in Def. 2; it can be verified \((x, p_u)\) satisfies (9) in Def. 2 namely \( p_u \) is compatible with \( x \) in the sense of \( \Lambda_{eq} \). Massey and Mathys [14] established the one-to-one correspondence (i.e., bijection) between \( \partial S \) and \( \partial \Lambda \), so \( p_u \in \partial S \) and is the only (critical) stabilizing control for \( x \). It can also be verified that \( \frac{1}{\pi(p_u)} \) is a positive root for \( f(\delta, x) \). That the root is unique follows from case 1 in Cor. 4.

\( \Leftarrow \):

If \( f(\delta, x) \) has a unique positive root denoted \( \delta_u \), again form a vector of probabilities \( p_u = p_u(\delta_u, x) \) according to (7), which is compatible with \( x \) in the sense of \( \Lambda_{eq} \). It follows from Cor. 4 that \( g(t_\pi, p_u) \) has a unique root on \((-1, \infty)\) denoted \( t_{\pi p_u} = 0 \), and is related to \( \delta_u \) by \( \delta_u = \frac{1}{\pi(p_u)} (1 + t_{\pi p_u}) = \frac{1}{\pi(p_u)} \). Furthermore \( p_u \) is a probability vector (Lem. 17), which implies \( x \in \partial \Lambda \) [14].

**Proof of part 2**

Given \( x \in \Lambda \setminus \partial \Lambda \), there must exist (Prop. 1) a positive root \( \delta \) for \( f(\delta, x) \). We use this \( \delta \) to construct a vector of probabilities \( p = p(\delta, x) \) as in (7). Recall then the root can be expressed as \( \delta = \frac{1}{\pi(p)} \), and furthermore \((x, p)\) satisfies (9) in Def. 2. Now we use \( p \) to form \( g(t_\pi, p) \) and solve for roots on \((-1, \infty)\). From part 1 of this proposition and Cor. 4 we know there must exist a root (denoted \( t''_\pi \)) other than 0 on \((-1, \infty)\). Define \( \delta' = \frac{1}{\pi(p)} (1 + t''_\pi) \), with which we further define \( p' = p'(\delta', x), x' = x'(p') \) as in Def. 2. First observe \( \delta' \) is a positive root of \( f(\delta', x) \) due to Cor. 4 (since \( t''_\pi \) solves \( g(t_\pi, p) = 0 \)). Second we claim \( x' = x \), because

\[
\pi(p') = \prod_{i=1}^{n} (1 - p'_i) = \prod_{i=1}^{n} \left( 1 - \frac{\delta'x_i}{1 + \delta'x_i} \right) = \prod_{i=1}^{n} \frac{1}{1 + \delta'x_i} = \frac{1}{\delta'}. \tag{166}
\]

where the last equality follows again from Cor. 4. It can then be verified that \( x'_i = \frac{p'_i}{1-p'_i} \pi(p') = x_i \) for all \( i \).

Note \( \delta' \neq \delta \) (as \( t''_\pi \neq 0 \)), and as such we can repeat the above procedure starting from this different positive root \( \delta' \). More specifically, define \( p''_\pi = p''_\pi(\delta', x') \) as in (7). Then the root satisfies \( \delta'' = \frac{1}{\pi(p''_\pi)} \) and furthermore \((x', p''_\pi)\) satisfies (9) in Def. 2. We now use \( p''_\pi \) to form \( g(t_\pi, p''_\pi) \) and solve for the root other than 0 on \((-1, \infty)\). We claim this root has to be such that it allows us to reconstruct \( p \). To see this, denote this root as \( t''''_\pi \in (-1, 0) \cup (0, \infty) \).
Define $\delta'' = \frac{1}{\pi(p)} (1 + t''_\pi)$, with which we further define $p''_i = p'_i(\delta'', x')$, $x''_i = x''(p''_i)$ as in Def. 2. According to Cor. 4, $f(\delta', x') = \frac{1}{\pi(p)} g(t'_{\pi}, p')$, then $\delta''$ is a positive root for $f(\delta, x') = 0$. Now since $x' = x$ (so $f(\delta, x')$ and $f(\delta, x)$ are the same) and furthermore $f$ has exactly two positive roots (since Cor. 4 says $f$ can have at most two), it then has to hold that $\delta'' = \delta$ (as $t''_\pi \neq 0$ implies $\delta'' \neq \delta$), which further gives $p''_i = p$, $\pi(p''_i) = \pi(p)$ and $x''_i = x$. This proves the claim. Effectively this says the above procedure (as illustrated in (167) below) can be reversed.

Furthermore, if $p$ is such that $\sum_{i=1}^n p_i < 1$, then $p'$ is such that $\sum_{i=1}^n p'_i > 1$, and vice versa. To show this, assume wlog $p$ is such that $\sum_{i=1}^n p_i < 1$. Now for $\delta = \frac{1}{\pi(p)}$, $\delta' = \frac{1}{\pi(p)} (1 + t''_\pi)$, Lem. 17 says if $\sum_{i=1}^n p_i < 1$ then $t''_\pi > 0$ and hence $\delta' > \delta$. From (166) $\delta'$ can also be expressed as $\frac{1}{\pi(p')}$ (so $\pi(p') < \pi(p)$). Now let us repeat the above procedure as illustrated in diagram (167) starting from $\delta'$ (rather than $\delta$), we will then get $\delta'' = \frac{1}{\pi(p''_i)} (1 + t''_\pi)$ where $t''_\pi$ is a root on $(-1, 0) \cup (0, \infty)$ solved from $g(t_{\pi}, p') = 0$. Since it has to hold that $\delta'' = \delta = \frac{1}{\pi(p)}$, it then follows $t''_\pi < 0$ which in turn implies (Lem. 17) $\sum_{i=1}^n p'_i > 1$. This shows, as a result of the above procedure one of the two critical stabilizing controls is in $S \setminus \partial S$, the other in $[0, 1] \setminus S$.

Finally we show there cannot be more than two critical stabilizing controls for a given $x$. We prove by contradiction. Assume wlog there are two critical stabilizing controls $p_s$ and $\hat{p}_s$ both in $S$ (for the case of $S^c$ the proof is similar), since both $p_s$ and $\hat{p}_s$ are critical stabilizing controls for the same $x$ it has to hold that $\pi(p_s) \neq \pi(\hat{p}_s)$ (as otherwise $p_s$ would not be distinct from $\hat{p}_s$). As we have just shown above for both $p_s$ and $\hat{p}_s$ there is a corresponding vector of probabilities in $[0, 1] \setminus S$ that critically stabilizes $x$, denoted as $p_s^c$ and $\hat{p}_s^c$ respectively. From the previous parts of the proof we see it has to hold that $\frac{1}{\pi(p_s)} \neq \frac{1}{\pi(p^c_s)}$ and $\frac{1}{\pi(p_s)} \neq \frac{1}{\pi(p^c_s)}$. This means $f(\delta, x)$ already has more than two positive roots, which is impossible according to Cor. 4 (recall with the exceptions of $e_i$’s any critical stabilizing control $p$ gives a positive root of $f$ as $\frac{1}{\pi(p)}$).

\[
\text{given } x \in A \setminus \partial A \rightarrow \text{solve } f(\delta, x) = 0 \rightarrow \text{root } \delta > 0 \rightarrow \text{set } p = p(\delta, x) \text{ as in Def. 2} \rightarrow \text{observe } \delta = \frac{1}{\pi(p)} \rightarrow \text{set } p' = p'(\delta', x') \text{ as in Def. 2} \rightarrow \text{observe } x' = x \rightarrow \delta' = \frac{1}{\pi(p')} (1 + t'_\pi) \rightarrow \text{root } \delta' > 0
\]

We use the following example to demonstrate the above process in both directions.

**Example 2:** For $n = 2$, let $x = (1/4, 1/5)$. Solving $f(\delta, x) = 0$ gives two positive roots $\delta = (11 - \sqrt{41})/2 \approx 2.29844$, $\delta' = (11 + \sqrt{41})/2 \approx 8.70156$. These two roots are also shown in Fig. 2 (the green curve).

- If we start from $\delta$, then $p = p(\delta, x) = \left(\frac{1}{19} (21 - \sqrt{41}), \frac{1}{19} (19 - \sqrt{41})\right) \approx (0.364922, 0.314922)$. Solving $g(t_{\pi}, p) = 0$ yields the non-zero root as $t'_{\pi} = \frac{1}{40} (41 + 11\sqrt{41}) \approx 2.78586$ with which it can be verified that

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\[ \delta_i' = \frac{1}{\pi(p)} (1 + t''_n) \text{ equals } \delta'. \] We can also verify \[ \delta = \frac{1}{\pi(p)}. \]

- Now if we start from \( \delta' \), then \( p' = p(\delta', x) = \left( \frac{2n}{3n} (21 + \sqrt{41}) \right), \frac{1}{3n} (19 + \sqrt{41}) \approx (0.685078, 0.635078). \)

Solving \( g(t''_n, p') = 0 \) yields the non-zero root as \( t''_n = \frac{1}{40} (41 - 11\sqrt{41}) \approx -0.735859 \) with which it can be verified that \( \delta_i' = \frac{1}{\pi(p')} (1 + t''_n) \) equals \( \delta \). We can also verify \( \delta' = \frac{1}{\pi(p')} \).

**B. Proof of Lemma 6**

Since the hyperplane passes through \( c \), the center of the ellipsoid, we can make the translation so that the ellipsoid is centered at the origin and the hyperplane also passes through the origin. Then the ellipsoid has the form \( E = \{ x : x^T R^{-1} x < 1 \} \), where \( Q = [q_1, \ldots, q_n] \) is orthonormal and holds the eigenvectors of \( R \), and \( D = \text{diag}(\lambda_1, \ldots, \lambda_n) \) holds the eigenvalues of \( R \). We use \( \text{Ref}_{\mathcal{H}(n, d)}(v) \) to denote the reflection of point \( v \) w.r.t. hyperplane \( \mathcal{H}(n, d) \).

\[ \Rightarrow: \]

The forward part of this lemma requires us to verify:

\[ R q_i = \lambda_i q_i, \forall i \in [n] \Rightarrow \text{Ref}_{\mathcal{H}(q_i, 0)}(v) \in \partial E \text{ for all } v \in \partial E. \] (168)

Since \( R \) is symmetric and has the aforementioned decomposition \( R = QDQ^T \), it is easy to verify that \( R^{-1} \) is symmetric and, if \( \lambda_i \) is an eigenvalue of \( R \) with associated eigenvector \( q_i \), then \( \lambda_i^{-1} \) is an eigenvalue of \( R^{-1} \) with associated eigenvector \( q_i \), namely:

\[ R^{-1} q_i = \lambda_i^{-1} q_i. \] (169)

Recall the reflecting point w.r.t. \( \mathcal{H}(q_i, 0) \) can be determined by \( \text{Ref}_{\mathcal{H}(q_i, 0)}(v) = v - 2 \frac{v^T q_i}{q_i^T q_i} q_i. \) Therefore \( \text{Ref}_{\mathcal{H}(q_i, 0)}(v) \in \partial E \) for all \( v \in \partial E \) means:

\[ \left( v - 2 \frac{v^T q_i}{q_i^T q_i} q_i \right)^T R^{-1} \left( v - 2 \frac{v^T q_i}{q_i^T q_i} q_i \right) = 1, \text{ for all } v \text{ satisfying } v^T R^{-1} v = 1, \] (170)

which is equivalent to verifying

\[ \frac{v^T q_i}{q_i^T q_i} \left( q_i^T R^{-1} v + v^T R^{-1} q_i - 2 \frac{v^T q_i}{q_i^T q_i} q_i^T R^{-1} q_i \right) = 0, \text{ for all } v \in \partial E \] (171)

Applying (169) (after transpose), the terms in the above parenthesis equals \( \lambda_i^{-1} q_i^T v + v^T \lambda_i^{-1} q_i - 2 \frac{v^T q_i}{q_i^T q_i} q_i^T \lambda_i^{-1} q_i = 0. \)

\[ \Leftarrow: \]

The converse part asks us to show for any vector \( q \) such that \( \mathcal{H}(q, 0) \) is a reflecting hyperplane meaning \( \text{Ref}_{\mathcal{H}(q, 0)}(v) \in \partial E \text{ for all } v \in \partial E \), it has to be an eigenvector of \( R \) meaning there exists some \( i \in [n] \) so that \( R q = \lambda_i q. \)
We prove by contradiction. Suppose for all \( i \in [n] \) it holds true that \( Rq \neq \lambda_i q \), or equivalently \( R^{-1}q \neq \lambda_i^{-1}q \). Recall the qualification (170) or equivalently (171) holds, which reduces to the following (because we can choose \( v \) such that it is not orthogonal to \( q \): \( v^Tq \neq 0 \)) where we also apply the fact that \( R^{-1} \) is symmetric:

\[
(R^{-1}q)^T v + v^T(R^{-1}q) - 2\frac{v^Tq}{q^Tq} q^T(R^{-1}q) = 0. \tag{172}
\]

On the other hand, the LHS of the above equation can be viewed as a function of \( R^{-1}q \), which implies: if \( q \) is not an eigenvector meaning \( R^{-1}q \neq \lambda_i^{-1}q \) for all \( i \in [n] \), we have:

\[
\text{LHS of (172)} \neq (\lambda_i^{-1}q)^Tv + v^T(\lambda_i^{-1}q) - 2\frac{v^Tq}{q^Tq} q^T(\lambda_i^{-1}q) = \lambda_i^{-1}q^Tv + v^T\lambda_i^{-1}q - 2\lambda_i^{-1}v^Tq = 0, \tag{173}
\]

which is a contradiction.

C. Proof of Prop. 17

We classify \( \partial \mathcal{S} \) into two categories: \( p \) with \( |V(p)| = 1 \) (quasi-uniform points) and \( p \) with \( |V(p)| > 1 \). There are two steps in this proof: step 1 is to show all the points with \( |V(p)| > 1 \) cannot be global extremizers, and step 2 is to show for points with \( |V(p)| = 1 \) the global extremizers are \( \{e_i\}_{i=1}^n \). Finally, it remains to evaluate the objective function at each \( e_i \).

**Step 1:**

Fix \( p \) such that \( |V(p)| > 1 \); we will show such a \( p \) cannot be a global extremizer. Prop. 16 implies that if a potential extremizer has \( |V(p)| > 1 \), then exactly two distinct non-zero component values namely \( |V(p)| = 2 \).

Then, suppose \( p \) has \( n' \) non-zero components, taking some value \( p_s > 0 \) for \( k \) of those \( n' \) components, and some value \( p_l > p_s \) for the remaining \( n' - k \) components. Note again \( s \) stands for small and \( l \) for large, and do not denote indices. Correspondingly \( \pi_s = \pi(p)/(1 - p_s) \), \( \pi_l = \pi(p)/(1 - p_l) \). Since \( p \in \partial \mathcal{S} \), we have:

\[
k p_s + (n' - k) p_l = 1, \tag{174}
\]

where \( 0 < p_s < \frac{1}{n'} < p_l < 1 \).

Recall (112) in the proof of Prop. 16 needs to be satisfied. Therefore we specialize the first equality in (112) to \( \mathcal{E}_{\text{out}} \) with such a \( p \) and get:

\[
n c - (k p_s \pi_s + (n' - k) p_l \pi_l) = \frac{n(\pi_s + p_l \pi_l) - (k p_s \pi_s + (n' - k) p_l \pi_l)}{(n-1)c} \tag{175}
\]
After some algebra, we have:

\[
nc(n - 1) = n\pi_s (nc - 1 + kp_s(1 - c)) + np_l\pi_l ((n' - k)(1 - c) + nc - 1)
\]

\[
c(n - 1) = \frac{\pi(p)}{1 - p_s} (nc - 1 + kp_s(1 - c)) + \frac{p_l}{1 - p_l}\pi(p) ((n' - k)(1 - c) + nc - 1)
\]

\[
\frac{c(n - 1)(1 - p_s)(1 - p_l)}{\pi(p)} = \frac{(1 - p_l) (nc - 1 + kp_s(1 - c)) + p_l(1 - p_s) ((n' - k)(1 - c) + nc - 1)}{\pi(p)}
\]

The RHS can be expanded and simplified using (174) and becomes \((n - 1)(c - p_sp_l)\), so the above equality after canceling \((n - 1)\) becomes:

\[
\frac{c}{\pi(p)/(1 - p_s)(1 - p_l)} = c - p_sp_l,
\]

which does not hold, because the LHS is greater than \(c\) while the RHS is less than \(c\). So we have shown a potential candidate extremizer \(p\) with \(|\mathcal{V}(p)| > 1\) does not exist because of the unsatisfiability of (175).

**Step 2:**

Fix \(p\) such that \(|\mathcal{V}(p)| = 1\). Recall for all \(p \in \partial S\) the objective function is initially derived (without any additional assumptions) as \(f_{obj} = \frac{1}{na_1^2} (nc - \Sigma)^2 + \frac{1}{a_2^2} (S - \frac{1}{n}\Sigma)^2\), where \(\Sigma = \sum_{i=1}^{n} x_i, S = \sum_{i=1}^{n} x_i^2\). A point \(p\) with \(|\mathcal{V}(p)| = 1\) is parameterized by integer \(k \in [1, n]\), meaning \(p\) has exactly \(k\) non-zero components. Since \(p \in \partial S\) so each non-zero component equals \(1/k\), furthermore, \(S(k) = \Sigma(k)^2/k\) and when \(k \geq 2\) we can write \(\Sigma(k) = (1 - \frac{1}{k})^{k-1}\).

Observe for both \(E_{in}\) and \(E_{out}\), \(a_2^2\) and \(a_1^2\) can be related by:

\[
a_2^2 = \frac{(n - 1)a_1^2}{na_1^2 - (nc - 1)^2} = \frac{(n - 1)a_1^2}{v},
\]

where the corresponding denominators (for \(E_{in}\) and \(E_{out}\) respectively)

\[
v_{in} = na_1^2_{in} - (nc - 1)^2 = (2nc - 1 - nm)(1 - nm), \quad v_{out} = na_1^2_{out} - (nc - 1)^2 = nc - 1.
\]

A scaled version of the objective function can then be rewritten as

\[
na_1^2 \cdot f_{obj} = (nc - \Sigma(k))^2 + \frac{n/k - 1}{n - 1} \cdot v \cdot \Sigma(k)^2.
\]

We shall show that for both \(E_{in}\) (in the proof of Prop. 18) and \(E_{out}\) (in this proof), the RHS of (178) is monotone increasing in \(k\) for \(k \in [2, n]\) (this assertion is not true for \(k \in [1, n]\)). Consequently, for \(E_{out}\) we only need to verify the objective function evaluated at \(k = 1\) as well as at \(k = 2\) is no smaller than \(1\), for \(E_{in}\) we only need to verify the objective function evaluated at \(k = 1\) as well as at \(k = n\) is no larger than \(1\).
Towards this, we take derivative of the RHS of (178) w.r.t. $k$ and normalize it by $\Sigma(k)^2$, we get

$$-2 \left( \frac{nc}{\Sigma(k)} - 1 \right) h(k) - \frac{n}{n-1} \frac{1}{k^2} v + 2 \frac{n/k - 1}{n-1} v \cdot h(k) \equiv f_d(k), \quad (179)$$

where $h(k) \equiv \frac{1}{k} + \log \left( 1 - \frac{1}{k} \right) < 0$. Note $\frac{d}{dk} \Sigma(k) = \Sigma(k) \cdot h(k)$ for $k \geq 2$. We need to show $f_d(k) \geq 0$.

Recall $\Sigma(k) = (1 - \frac{1}{k})^{k-1}$ is monotone decreasing in $k \in [2, \infty)$ from $1/2$ to $1/e$, it suffices to show a lower bound of $f_d(k)$ is nonnegative, i.e.,

$$f_d(k) \equiv -2 (2nc - 1) h(k) - \frac{n}{n-1} \frac{1}{k^2} v + 2 \frac{n/k - 1}{n-1} v \cdot h(k) \geq 0, \quad (180)$$

or equivalently,

$$2h(k) \left[ -(2nc - 1) + \frac{n/k - 1}{n-1} v \right] \geq \frac{n}{n-1} \frac{1}{k^2} v. \quad (181)$$

It can be verified (by possibly using an upper bound on $v$) that for both $E_{\text{in}}$ and $E_{\text{out}}$ the above bracket term is negative. As will turn out, a convenient and sufficiently tight upper bound on $h(k)$ is crucial for analytical tractability. For this, recall the Taylor expansion $\log(1 + x) = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{x^n}{n}$ for all $x \in (-1, 1)$. If $x < 0$ then any truncation of this series yields an upper bound. In particular, we have $\log(1 + x) < -x^2 + \frac{x^3}{3}$ for $x < 0$. Now setting $x = -\frac{1}{2}$ gives a strict upper bound i.e., $h(k) < -\frac{1}{4} (\frac{1}{2} + \frac{1}{3k})$. We next show (181) for $E_{\text{out}}$.

Applying the upper bound on $h(k)$ and substituting $v_{\text{out}} = nc - 1$, to show (181) it suffices to verify

$$-2 \frac{1}{k^2} \left( \frac{1}{2} + \frac{1}{3k} \right) \left[ -(2nc - 1) + \frac{n/k - 1}{n-1} (nc - 1) \right] \geq \frac{n}{n-1} \frac{1}{k^2} (nc - 1), \quad (182)$$

which can be shown to be equivalent to verify (when $c > 1/n$)

$$\left( \frac{1}{2} + \frac{1}{3k} \right) \left( 1 - \frac{1}{2} \frac{c - 1}{2c - 1} \right) \geq \frac{1}{4}. \quad (183)$$

For $k \in [2, n]$, $\frac{1}{2} + \frac{1}{3k} \geq \frac{1}{2} + \frac{1}{3n} > 0$, $1 - \frac{1}{2} - \frac{1}{2} \frac{c - 1}{2c - 1} \geq \frac{3}{4} - \frac{1}{2} \frac{c - 1}{2c - 1}$. So it suffices to show

$$\left( \frac{1}{2} + \frac{1}{3n} \right) \left( \frac{3}{4} - \frac{1}{2} \frac{c - 1}{2c - 1} \right) \geq \frac{1}{4}. \quad (184)$$

or equivalently $\frac{(3n^2 - 4) + 3n - 2}{24n(nc-1)^2} \geq 0$, which holds true for $c > 1/n$.

So far we have shown for $E_{\text{out}}$ the objective function expressed as $f_{\text{obj}} = \frac{1}{nc^2} (nc - \Sigma)^2 + \frac{1}{n^2} (S - \frac{1}{n} \Sigma^2)$ is monotone increasing in $k$ for $k \in [2, n]$. Now that for $E_{\text{out}}$ we want to show the global minimum of the objective function is no smaller than 1, it only requires us to verify $f_{\text{obj}} \geq 1$ when $k = 1$ and 2. When $k = 1$ i.e., at $e_1$, by construction it is tight so $f_{\text{obj}}|_{k=1} = 1$. When $k = 2$, we need to verify

$$f_{\text{obj}}|_{k=2} = \frac{1}{nc(nc-1)} \left( nc - \frac{1}{2} \right)^2 + \frac{1}{(n-1)c} \left( \frac{1}{8} - \frac{1}{4} \frac{1}{n} \right) \geq 1. \quad (185)$$

The partial derivative w.r.t. $c$ is negative for all $c > 1/n$. Since $\lim_{c \to \infty} f_{\text{obj}}|_{k=2} = 1$, this verifies (185).
D. Proof of Prop. 18

The proof of $\Lambda_{\text{cl}}$ is similar to but more involved than that of $\Lambda_{\text{co}}$. In the following we will omit the parts that are common to both proofs. The general strategies are the same. Step 1 is to show all points $p$ with $|V(p)| > 1$ cannot be global extremizers. Step 2 is to show that among the points $p$ with $|V(p)| = 1$, the global extremizers are $e_i$ as well as $m$. Finally, it remains to evaluate the objective function at $e_i$ or $m$.

**Step 1:**

We first recall again a result that is used a few times during the rest of the proof: the function $(1 - 1/n)^{n-1}$ is monotone decreasing in $n \in [2, \infty)$ from $1/2$ to $1/e$. Its proof is by taking its derivative and applying the inequality $\log(1 + x) \leq x$ for all $x > -1$.

Similar to what has been done for $E_{\text{out}}$, Specializing the first equality in (112) to $E_{\text{in}}$ with such a $p$ satisfying (174), we have:

$$nc - (kp_s \pi_s + (n' - k)p_l \pi_l) = \frac{n(\pi_s + p_l \pi_l) - (kp_s \pi_s + (n' - k)p_l \pi_l)}{v_{1,\text{in}}},$$

where $v_{1,\text{in}} = na_{1,\text{in}}^2 - (nc - 1)^2 = (2nc - 1 - nm)(1 - nm)$. Simplifying using (174), we have:

$$nc(1 - p_s)(1 - p_l) = 1 + v_{1,\text{in}} - n'p_s p_l - v_{1,\text{in}} \frac{n - n'}{n - 1} p_s p_l. \tag{186}$$

In order to show all those $p$ cannot be global maximizers, we need to show the associated $f_{\text{obj}}$ is less than 1. Recall from the proof of Prop. 16 this objective function assuming (112) is given in (114).

Applying our knowledge of $p$ and using (174), we have

$$f_{\text{obj}} = \frac{\pi(s, l, n')}{a_{2,\text{in}}^2} (-\pi(s, l, n') + c(n - 1) - c(n - n')p_s p_l),$$

where $\pi(s, l, n') \equiv (1 - p_s)^k(1 - p_l)^{n' - k}$ for $p_s, p_l$ satisfying (174).

Substituting $a_{2,\text{in}}^2 = \frac{(n-1)a_{1,\text{in}}^2}{v_{1,\text{in}}}$, $a_{1,\text{in}}^2 = n(c - m)^2$, and (186), we see $f_{\text{obj}} < 1$ is equivalent to

$$\left(c - \frac{\pi(s, l, n')}{(n - 1)(1 - \frac{n - n'}{n - 1} p_s p_l)} \right) \left(c - \frac{\pi(s, l, n')}{(1 - p_s)(1 - p_l)} \frac{1}{n - n'p_s p_l} \right) < (c - m)^2. \tag{187}$$

Note $c > 1/n$ gives $c > \frac{\pi(s, l, n')}{(1 - p_s)(1 - p_l)} \frac{1}{n - \frac{n'}{n} p_s p_l}$. We now verify it also ensures $c > \frac{\pi(s, l, n')}{(n - 1)(1 - \frac{n - n'}{n} p_s p_l)}$. Namely we need to show $\pi(s, l, n') < 1 - \frac{1+(n-n')p_s p_l}{n}$, for which we apply AM-GM inequality to $\pi(s, l, n')$

$$\pi(s, l, n') = (1 - p_s)^k(1 - p_l)^{n' - k} \leq \left(\frac{k(1 - p_s) + (n' - k)(1 - p_l)}{n'}\right)^{n'} = \left(1 - \frac{1}{n'}\right)^{n'}. \tag{188}$$

So it suffices to show

$$\left(1 - \frac{1}{n'}\right)^{n'} < 1 - \frac{1+(n-n')p_s p_l}{n}. \tag{189}$$
When \( n' = n \), (189) holds true. When \( n' < n \), it suffices to show \( \frac{1}{n'} > \frac{1 + (n - n') p_s p_l}{n} \), or equivalently, \( \frac{1}{n'} > p_s p_l \), which holds true as well (as \( 0 < p_s < \frac{1}{n'} < p_l < 1 \)).

Therefore we can apply the AM-GM inequality to the LHS of (187), for which it suffices to show:

\[
\left( c - \frac{1}{2} \frac{\pi(s,l,n')}{(n-1)(1 - \frac{n-n'}{n-1} p_s p_l)} + \frac{\pi(s,l,n')}{(1-p_s)(1-p_l)} \left( \frac{1}{n} - \frac{n'}{n} p_s p_l \right) \right)^2 < (c-m)^2. \tag{190}
\]

Clearly \( c > m \) too. So next we need to show for those \( p \)'s that do satisfy (186):

\[
f_r(k, p_s, n') \equiv \frac{1}{2} \left( \frac{\pi(s,l,n')}{(n-1)(1 - \frac{n-n'}{n-1} p_s p_l)} + \frac{\pi(s,l,n')}{(1-p_s)(1-p_l)} \left( \frac{1}{n} - \frac{n'}{n} p_s p_l \right) - \frac{1}{n} (1 - \frac{1}{n})^{n-1} > 0. \tag{191}
\]

Similar to what has been done in the proof of the spherical inner bound \( \Lambda_{\text{ai}} \) (Prop. 9), we show (191) by working with an enlarged feasible set, meaning although (191) is derived assuming (186) (resulted from (112) and (174)), when we optimize the LHS of (191) we do not enforce (186), namely the feasible set is enlarged to be all the points \( p \) with \(|\mathcal{V}(p)| > 1\).

First consider the scenario where \( p \) does not have zero component(s), then the scenario where \( p \) has zero component(s).

Case 1: \( p \) does not have zero component(s), namely \( n' = n \).

When \( n' = n \), (186) simplifies to be

\[
\frac{nc}{\pi(s,l,n)/(1-p_s)(1-p_l)} = 1 + v_{\text{in}} - n p_s p_l. \tag{192}
\]

For fixed \( p_s \in (0, 1/n) \), we take the derivative of the denominator of the above LHS w.r.t. \( k \):

\[
\frac{\partial}{\partial k} \left( \frac{(1-p_s)^k(1-p_l)^{n-k}}{(1-p_s)(1-p_l)} \right) =
\]

\[
(1-p_s)^{k-1} \left( 1 - \frac{1-kp_s}{n-k} \right)^{n-k-1} (n-k) \left( 1 - \frac{1-kp_s}{n-k} \right)^{n-k-1} + \log(1-p_s) - \log \left( 1 - \frac{1-kp_s}{n-k} \right),
\]

where \( p_l \) is solved from (174). Denote \( g_1(k, p_s) = (n-k) \left( 1 - \frac{1-kp_s}{n-k} \right) + \log(1-p_s) - \log \left( 1 - \frac{1-kp_s}{n-k} \right) \), note \( g_1(k, p_s) \) determines the sign of the above derivative. Taking partial derivative of \( g_1(k, p_s) \) w.r.t. \( k \), we get

\[
\frac{\partial}{\partial k} g_1(k, p_s) = \frac{(n-p_k - 1)(n-2)p_s + k - (n-1)(np_s + 1))}{(n-k)^2 (k(p_s - 1) + n-1)^2}, \tag{193}
\]

which can be verified to be positive for all \( k \in (0, n) \) and \( p_s \in (0, 1/n) \). We then evaluate

\[
g_1(0, p_s) = \log \left( 1 + \frac{1}{n} - p_s \right) - \frac{1}{1 - \frac{1}{n}} - \frac{1}{1 - \frac{1}{n}} - \frac{1}{2} \left( \frac{1}{1 - \frac{1}{n}} \right)^2 - \frac{1}{1 - \frac{1}{n}} > 0 \text{ for all } n \geq 2. \tag{194}
\]
where in (a) we apply the inequality \( \log(1 + x) > x - \frac{1}{2}x^2 \) for all \( x > 0 \). So this implies \( g_1(k, p_s) \) itself is positive for all \( k \in (0, n) \), and hence this means for fixed \( p_s \in (0, 1/n) \) the LHS of (192) is monotone decreasing in \( k \) (as its denominator is increasing in \( k \)).

Recall \( nm = (1 - 1/n)^{n-1} \) is monotone decreasing from 1/2 to 1/e, so an upper bound on RHS of (192) is

\[
1 + \left(2nc - 1 - \frac{1}{e}\right)\left(1 - \frac{1}{e}\right) - np_sp_l = \frac{1}{e^2} - np_sp_l + 2 \left(1 - \frac{1}{e}\right) \frac{1}{e^2} + 2 \left(1 - \frac{1}{e}\right) nc.
\]

(195)

Recall \( k \)'s actual support consists of integers from (0, \( n \)). So in order to show (192) is possibly satisfiable only when \( k = n - 1 \), due to the monotone decreasing property (w.r.t. \( k \)) of its LHS, it suffices to show at \( k = n - 2 \), (192) still cannot be satisfied, i.e.,

\[
\frac{nc}{\pi(s, l, n)/((1 - p_s)(1 - p_l))} > \frac{1}{e^2} + 2 \left(1 - \frac{1}{e}\right) nc, \text{ for } k = n - 2,
\]

(196)

or equivalently,

\[
(1 - p_s)^{n-3} \left(\frac{1}{2} + \frac{n - 2}{2} p_s\right) = \pi(s, l, n)/((1 - p_s)(1 - p_l)) < \frac{nc}{\frac{1}{e^2} + 2 \left(1 - \frac{1}{e}\right) nc}.
\]

(197)

The derivative of the LHS w.r.t. \( p_s \) is \(-\frac{1}{2}(1-p_s)^{n-4}(-1 + (n - 2)^2 p_s)\), meaning there exists a single stationary point \( p_s^* = 1/(n - 2)^2 \in (0, 1/n) \) if \( n \geq 5 \) and in fact this stationary point is the unique maximizer (by verifying the second derivative to be negative at \( p_s^* \)). So we will need to show (197) holds at \( p_s^* \) for \( n \geq 5 \), i.e.,

\[
\left(1 - \frac{1}{(n - 2)^2}\right)^{n-3} \left(1 + \frac{1}{n - 2}\right) < \frac{2}{\frac{1}{e^2} + 2 \left(1 - \frac{1}{e}\right) nc}.
\]

(198)

Since \( c > 1/n, n \geq 5, 1 - \frac{1}{(n-2)^2} \in (0, 1) \), it suffices to show

\[
\left(1 - \frac{1}{(n - 2)^2}\right)^{n-3} \left(1 + \frac{1}{n - 2}\right) < \frac{2}{\frac{1}{e^2} + 2 \left(1 - \frac{1}{e}\right) nc} \approx 1.429,
\]

(199)

which can be verified to be true for all \( n \geq 5 \). For \( n = 3 \) or 4, (197) can also be verified to be true (in both cases the LHS maximizes when \( p_s = 1/n \)). \( n = 2 \) case can be skipped since \( k \) has to be a positive integer.

Hence (192) is possibly satisfiable only when \( k = n - 1 \), for which \( \pi(s, l, n) = (1-p_s)^{n-1}(n-1)p_s \) and \( f_r \) in (191) becomes (for \( n' = n \))

\[
f_r(k, p_s, n)|_{k=n-1} = \frac{1}{2} (1-p_s)^{n-2} \left((n-2)p_s^2 + \frac{1}{n}\right) - \frac{1}{n} \left(1 - \frac{1}{n}\right)^{n-1}.
\]

(200)

Since its derivative w.r.t. \( p_s \) can be verified to be negative for \( p_s \in (0, 1/n) \) meaning it is monotone decreasing in \( p_s \), so \( f_r(k, p_s, n)|_{k=n-1} > f_r(k, p_s, n)|_{k=n-1}, p_s=1/n = 0 \). This shows (191) holds true, and concludes the case when a potential extremizer \( p \) does not have zero component(s).
Case 2: \( p \) has zero component(s), namely \( n' < n \).

We first assert that when \( n' < n \), it also holds true that (186) is satisfiable only by those \( p \) such that \( k = n' - 1 \). The proof builds upon results from the previous case (i.e., when \( n' = n \)). Recall there we show for fixed \( p_s \in (0, 1/n) \) the LHS of (192) is monotone decreasing in \( k \), and when \( k = n - 2 \) it is still above the RHS. Note (186) can be rewritten as:

\[
\frac{n'}{n}(1 - n'p_sp_l + v_{in}(1 - \frac{n - n'}{n - 1}p_sp_l)) = \frac{1}{e^2} + 2 \left(1 - \frac{1}{e}\right)n'c. \quad (201)
\]

Note its LHS is the same as that of (192) by reparameterizing \( n \) in (192) with \( n' \), and this allows us to claim that the LHS of (201) is monotone decreasing in \( k < n' \), and furthermore, it suffices to show (201)'s RHS is no larger than \( \frac{1}{e^2} + 2 \left(1 - \frac{1}{e}\right)n'c \), because we can reparameterize (196) using \( n' \). Namely, we want to show:

\[
\frac{n'}{n}(1 - n'p_sp_l + v_{in}(1 - \frac{n - n'}{n - 1}p_sp_l)) \leq \frac{1}{e^2} + 2 \left(1 - \frac{1}{e}\right)n'c. \quad (202)
\]

Applying the upper bound on \( v_{in} \) and recognizing \( 1 - \frac{n - n'}{n - 1}p_sp_l \in (0, 1) \), it suffices to show:

\[
\frac{n'}{n}(1 - n'p_sp_l + \left(2nc - \frac{1}{e}\right)\left(1 - \frac{1}{e}\right)) \leq \frac{1}{e^2} + 2 \left(1 - \frac{1}{e}\right)n'c
\]

\[
\frac{n'}{n}(\frac{1}{e^2} - n'p_sp_l) \leq \frac{1}{e^2},
\]

which is true. Thus we have shown (201) is possibly satisfiable only when \( k = n' - 1 \).

So we investigate \( f_r \) when \( k = n' - 1 \) (or equivalently \( n' = k + 1 \)). In the following we show \( f_r(k, p_s, n')|_{n'=k+1} \) is monotone decreasing in \( p_s \) for fixed \( k \). Taking derivative

\[
\frac{\partial}{\partial p_s} f_r(k, p_s, k + 1) = -\frac{k(1 - p_s)^{k-2}((k + 1)p_s^2(-k + n - 1) + 3p_s(k - n + 1) + n - 2)}{2n(kp_s^2(-k + n - 1) + p_s(k - n + 1) + n - 1)^2} \cdot g_2(k, p_s). \quad (203)
\]

where \( g_2(k, p_s) \equiv n(p_s(k((k + 1)kp_s^2 - 2(k + 1)p_s + k + 4) - 2) + p_s - 2) + 1 - ((k + 1)p_s(kp_s - 1))^2. \)

Since one can show for \( 0 < p_s < \frac{1}{n'} < 1 \) and \( k = n' - 1 \) and \( n' < n \) and \( n > 2 \) (note if \( n = 2 \) there is no need to consider \( n' < n \) case, as the minimum of possible value for \( k \) is 1 and \( k \) also needs to satisfy \( k = n' - 1 < n - 1 \) strictly), we have

\[
(k + 1)p_s^2(-k + n - 1) + 3p_s(k - n + 1) + n - 2 \geq 0.
\]

We then need to show the positiveness of \( g_2(k, p_s) \). We rearrange terms viewing \( g_2(k, p_s) \) as a polynomial of \( p_s \).
and split the coefficient of the quadratic term:

\[ g_2(k, p) = (k^2(k + 1)(n - k - 1)p_s^2 - 2k(k + 1)(n - k - 1)p_s^3 + (k + 1)(n - k - 1)p_s^2 + \]

\[ ((nk(k + 3) - 2k(k + 1)p_s^2 - 2k + 1)(n - 1)p_s + n - 1) \]

\[ = (k + 1)(n - k - 1)p_s^2 (kp_s - 1)^2 + ((nk(k + 3) - 2k(k + 1)p_s^2 - 2k + 1)(n - 1)p_s + n - 1) . \]

It then suffices to show \((nk(k + 3) - 2k(k + 1)p_s^2 - 2k + 1)(n - 1)p_s + n - 1 \geq 0\), which can be verified to be true, since its discriminant is always negative and the coefficient of \(p_s^2\) is positive.

Now showing (191) amounts to showing \(f_r(k, p_s, n')|_{n'=k+1, \; p_s=1/n'} > 0\).

First we show it is monotone decreasing in \(k\). Towards this, we take derivative:

\[
\frac{d}{dk} f_r(k, 1/(k + 1), k + 1) = \frac{k^k(k + 1)^{-k-1}}{2\left((k + 1)^2 - k\right)^2} \cdot g_3(k),
\]

where \(g_3(k) \equiv (2(k + 4)k + 7)n^2 - (3k + 5)(k + 1)n + (k + 1)(k(3k + 4) + 1 + (k + 1)(n - 1) + 3n - 1) \log(k + 1) + (k + 1)^2 \). We need to show \(g_3(k)\) is negative, for which it suffices to show (using the inequality \(\log(1+x) < x - \frac{1}{2}x^2\), \(\forall x \in (-1, 0)\)) a strict upper bound of it is nonpositive. e.g.,

\[
(2(k+4)k+7)n^2-(3k+5)(k+1)n+(k+1)(k(3k+4)+1+2n-1)(k(2n-1)+3n-1) \left(-\frac{1}{k+1} - \frac{1}{2}\left(-\frac{1}{k+1}\right)^2\right) + (k+1)^2 \leq 0.
\]

The above LHS can be simplified as \(\frac{(k-(n-1))(k(3n-1)+4n-1)}{2(k+1)}\), which is nonpositive for all positive \(k \leq n - 1\).

Second, since \(f_r(k, p_s, n')|_{n'=k+1, \; p_s=1/n'}\) is monotone decreasing in \(k\) for all positive \(k \leq n - 1\), it is lower bounded by \(f_r(k, p_s, n')|_{n'=k+1, \; p_s=1/n'}\) \(\forall k = n-1\). Therefore, we have shown the desired inequality (191) holds true, and this concludes the case when a potential extremizer \(p\) has zero component(s).

**Step 2:** This step follows exactly Step 2 of the proof of \(\Lambda_{\infty}\), up to the paragraph right below (181). Applying the upper bound on \(h(k)\), to show (181) it suffices to show

\[
-2 \frac{1}{k^2} \left( \frac{1}{2} + \frac{1}{3k} \right) \left[ -(2nc - 1) + \frac{n/k - 1}{n - 1} v_{in} \right] \geq \frac{n}{n - 1} \frac{1}{k^2} v_{in},
\]

which after rearranging terms becomes:

\[
\left( 1 + \frac{2}{3k} \right) (n - 1) (2nc - 1) \geq \left( n + \left( 1 + \frac{2}{3k} \right) \left( \frac{n}{k} - 1 \right) \right) v_{in},
\]

for which we apply an upper bond on \(v_{in}\), multiply both sides by \(k^2\), and seek to show

\[
k^2 \left( 1 + \frac{2}{3k} \right) (n - 1) (2nc - 1) - k^2 \left( n + \left( 1 + \frac{2}{3k} \right) \left( \frac{n}{k} - 1 \right) \right) \left( 2nc - 1 - \frac{1}{e} \right) \left( 1 - \frac{1}{e} \right) \geq 0.
\]
Denote the above LHS by $g_4(k)$, to show $g_4(k) \geq 0$ for all $k \in [2,n]$ it suffices to show $\frac{d}{dk} g_4(k) \geq 0$ and $g_4(k)|_{k=2} \geq 0$.

$$\frac{d}{dk} g_4(k) = \frac{6k(n-1)(2ecn-1) + n (-2ec(e-3)n + 2) + e^2 - 3) + 2}{3e^2}. \quad (209)$$

The numerator can be rewritten as

$$12eckn^2 - 12eckn - 2e^2cn^2 + 6ecn^2 - 4ecn - 6kn + 6k + e^2n - 3n + 2,$$

or equivalently,

$$6(n-1)(2ecn - 1) - 2e^2cn^2 + 6ecn^2 - 4ecn + e^2n - 3n + 2,$$

which viewed as a linear function of $k$ is increasing in $k$, so to show $\frac{d}{dk} g_4(k) \geq 0$ we need to show it is positive when $k = 2$, i.e., $-2e^2cn^2 + 30ecn - 28ecn + e^2n - 15n + 14 \geq 0$. Since the coefficient of $c$ is $-28en + 30en^2 - 2e^2n^2 > 0$ namely this function is increasing in $c$, it then suffices to show it is positive when $c$ is the minimum possible (i.e., $c = 1/n$), namely, $(30e - 15 - e^2)n + 14(1 - 2e) \geq 0$, which is true for $n \geq 2$.

Having shown $g_4(k)$ is monotone increasing in $k$, we now only need to show $g_4(k)|_{k=2} \geq 0$, i.e.,

$$-4 \left(2(e-5)ecn^2 + (8ec - e^2 + 5)n - 4 \right) \geq 0,$$

or equivalently,

$$2(e-5)ecn^2 + (8ec - e^2 + 5)n - 4 \leq 0. \quad (210)$$

Since for fixed $n$ the LHS is monotone decreasing in $c$ (we can check that $\frac{d\text{LHS}}{dc} = 2en(4 - (5 - e)n) < 0$ for $n \geq 2$). It suffices to show (210) holds when $c$ is the minimum possible (i.e., $c = 1/n$). Setting $c = 1/n$ in (210), after some algebra it gives $\frac{4(2e-1)}{10e-e^2-5} \leq n$ which holds true for $n \geq 2$, since $\frac{4(2e-1)}{10e-e^2-5} \approx 1.199577$.

Thus we have shown the desired inequality (181) for $E_{in}$.

So far we have shown for $E_{in}$ the objective function expressed as $f_{obj} = \frac{1}{na_1} (nc - \Sigma)^2 + \frac{1}{a_2^2} \left(S - \frac{1}{n} \Sigma^2 \right)$ is monotone increasing in $k$ for $k \in [2,n]$. Now that for $E_{in}$ we need to show the global maximum of the objective function is no larger than 1, we only need to verify $f_{obj} \leq 1$ when $k = 1$ and $n$, both of which are true as by construction the objective function is tight at $e_i$ (i.e., $k = 1$) and $m$ (i.e., $k = n$).