Guaranteed Tensor Decomposition: A Moment Approach

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Abstract

We develop a theoretical and computational framework to perform guaranteed tensor decomposition, which also has the potential to accomplish other tensor tasks such as tensor completion and denoising. We formulate tensor decomposition as a problem of measure estimation from moments. By constructing a dual polynomial, we demonstrate that the measure optimization returns the correct CP decomposition under an incoherent condition on the rank-one factors. To address the computational challenge, we present a hierarchy of semidefinite programs based on the sum-of-squares relaxation to approximate the measure optimization. By showing that the constructed dual polynomial is a sum-of-squares modulo the sphere, we prove that the smallest SDP in the relaxation hierarchy is exact and the decomposition can be extracted from the semidefinite program solutions under the same incoherent condition. One implication is that the tensor nuclear norm can be computed exactly using the smallest SDP as long as the rank-one factors of the tensor are incoherent. Numerical experiments are conducted to test the performance of the moment approach.

1. Introduction

Tensor provides a compact and natural representation for high-dimensional, multi-view datasets encountered in fields such as communication, signal processing, large-scale data analysis, and computational neuroscience, to name a few. In many data analysis tasks, tensor-based approaches outperform matrix-based ones due to the ability to identify non-orthogonal components, a property derived from having access to higher order moments (Landsberg, 2009). In this work, we investigate the problem of decomposing a tensor into a linear combination of a small number of rank one tensors, also known as the CP decomposition or the PARAFAC decomposition. Such low-rank tensor decomposition extends the idea of singular value decomposition for matrices and finds numerous applications in data analysis (Papalexakis et al., 2013; Anandkumar et al., 2013; 2012; Cichocki et al., 2014; Comon, 2009; Kolda & Bader, 2009; Lim & Comon, 2010).

We approach tensor decomposition from the point of view of measure estimation from moments. To illustrate the idea, consider determining the CP decomposition of a third order symmetric tensor $A = \sum_{p=1}^{r} \lambda_p x^p \otimes x^p \otimes x^p$, which can be viewed as estimating a discrete measure $\mu^\star = \sum_{p=1}^{r} \lambda_p \delta(x - x^p)$ supported on the unit sphere from its 3rd order moments $A_{ijl} = \int_{\mathbb{S}^{n-1}} x_i x_j x_l d\mu^\star$. This formulation offers several advantages. First, it provides a natural way to enforce a low-rank decomposition by minimizing an infinite-dimensional generalization of the ℓ_1 norm, the total variation norm of the measure. Second, the optimal value of the total variation norm minimization, which is a convex optimization in the space of measures, defines a norm for tensors. This norm, termed as tensor nuclear norm, is an instance of atomic norms, which, as argued by the authors of (Chandrasekaran et al., 2012), is the best possible convex proxy for recovering simple models. Just like the matrix nuclear norm, the tensor nuclear norm can be used to enforce low-rankness in tensor completion, robust tensor principal component analysis, and stable tensor recovery. Finally, finite computational schemes developed for atomic tensor decomposition can be readily modified to accomplish these more complex tensor tasks.

The theoretical analysis of atomic tensor decomposition is fundamental in understanding the regularization and estimation power of the tensor nuclear norm in solving other tensor problems. For one thing, it tells us what types of rank-one tensor combinations are identifiable given full, noise-free data. For another, the dual polynomial constructed to certify a particular decomposition is useful in investigating the performance of tensor nuclear norm minimization for data corrupted by missing observations, noise, and outliers. When the same measure estimation idea was

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applied to line spectral estimation in signal processing, the dual polynomial constructed in (Candès & Fernandez-Granda, 2014) was later utilized to analyze the ability of frequency estimation from incomplete, noisy, and grossly corrupted data (Tang et al., 2014b;a; 2013; Chi & Chen, 2014). We expect that the tensor decomposition results will find similar uses in the corresponding tensor tasks.

Our contributions in this work are three folds. First of all, we formulate atomic tensor decomposition as a moment problem and apply the Lasserre sum-of-squares (SOS) relaxation hierarchy to obtain a series semidefinite programs (SDPs) to approximately solve the moment problem. Secondly, we explicitly construct a dual polynomial to certify that a decomposition with *incoherent* components $\{x^p, p = 1, \ldots, r\}$ is the unique atomic tensor decomposition. The incoherence condition requires that the matrix formed by the vectors $\{x^p\}$ is well-conditioned. Last but not least, by showing that the constructed dual polynomial is an SOS modulo the sphere, we establish that the *smallest* SDP in the Lasserre hierarchy *exactly* solves the atomic decomposition under the *same* incoherent assumption. Such a result is different from existing approximation results for the Lasserre hierarchy, where there is no guarantee on the size of the SDP at which exact relaxation occurs (Nie, 2014). The effectiveness of the lowest order relaxations has enormous consequences for computation, as the Lasserre hierarchy is considered impractical due to the rapid increase of the sizes of SDPs in the hierarchy.

2. Connections to Prior Art

Add comparison with Barak & Moitra (2015); Expand the comparison with Anandkumar as mentioned in the review.

CP tensor decomposition is a classical tensor problem that has been studied by many authors (cf. (Comon, 2009; Kolda & Bader, 2009)). Most tensor decomposition approaches are based on alternating minimization, which typically do not offer any global convergence guarantees (Bro, 1997; Harshman, 1970; Kolda & Bader, 2009; Papalexakis et al., 2013; Comon et al., 2009). However, recent work that combines the idea of alternating minimization and power iteration has yielded guaranteed tensor decomposition in a probabilistic setting (Anandkumar et al., 2013; 2014). In contrast, the theoretical guarantee of our moment approach is deterministic, which is more natural since there is no randomness in the problem formulation.

Another closely related line of work is matrix completion and tensor completion. Low-rank matrix completion and recovery based on the idea of nuclear norm minimization has received a great deal of attention in recent years (Candès & Recht, 2009; Recht et al., 2010; Recht, 2011). A direct generalization of this approach to tensors would be using tensor nuclear norm to perform low-rank tensor completion and recovery. However, this approach was not pursued due to the NP-hardness of computing the tensor nuclear norm (Hillar & Lim, 2013). The mainstream tensor completion approaches are based on various forms of matricization and application of matrix completion to the flattened tensor (Gandy et al., 2011; Liu et al., 2013; Mu et al., 2013; Yuan & Zhang, 2014). Alternating minimization can also be applied to tensor completion and recovery with performance guarantees established in recent work (Huang et al., 2014). Neither matricization nor alternating minimization approaches yields optimal bounds on the number of measurements needed for tensor completion.

In contrast, we expect that the atomic norm, when specialized to tensors, will achieve the information theoretical limit for tensor completion as it does for compressive sensing, matrix completion (Recht, 2011), and line spectral estimation with missing data (Tang et al., 2013). Given a set of simple models or atoms, the atomic norm is an abstraction of ℓ_1-type regularization that favors models composed of fewer atoms.Using the notion of descent cones, the authors of (Chandrasekaran et al., 2012) argued that the atomic norm is the best possible convex proxy for recovering simple models. Particularly, atomic norms were shown in many problems beyond compressive sensing and matrix completion to be able to recover simple models from minimal number of linear measurements. For example, when specialized to the atomic set formed by complex exponentials, the atomic norm can recover signals having sparse representations in the continuous frequency domain with the number of measurements approaching the information theoretic limit without noise (Tang et al., 2013), as well as achieving near minimax denoising performance (Tang et al., 2014a). Continuous frequency estimation using the atomic norm is also an instance of measure estimation from (trigonometric) moments.

The tensor decomposition considered in this work is a special case of atomic decompositions, *i.e.*, decompositions that achieve the atomic norm. Due to the fundamental role of atomic decomposition in understanding the power and limitations of and in developing further theories for atomic norm regularization, sufficient conditions characterizing such decompositions have been developed by explicitly constructing a dual polynomial. This dual polynomial played an instrumental role in establishing the information-theoretic optimality of atomic norms in performing completion and denoising tasks. For finite atomic sets, it is now well-known that if the atoms satisfy certain incoherence conditions such as the restricted isometry property, then a sparse decomposition achieves the atomic norm (Candes, 2008). For the set of rank-one, unit-norm matrices, the atomic norm (*i.e.*, the matrix nuclear norm), is achieved by orthogonal decompositions (Recht et al., 2010). When

the atoms are complex sinusoids parametrized by the frequency, Candès and Fernandez-Granda showed that atomic decomposition is solved by atoms with well-separated frequencies (Candès & Fernandez-Granda, 2014). Similar separation conditions also show up when the atoms are translations of a known waveform (Tang & Recht; Bendory et al., 2014b), spherical harmonics (Bendory et al., 2014a), and radar signals parametrized by translations and modulations (Heckel et al., 2014). The incoherence requirement for our tensor decomposition is also one form of separation condition. In (Tang, 2015), the author showed that such separation conditions are necessary as a consequence of Markov-Bernstein type inequalities. We cite such a resolution limit result in Theorem 2 to complement our sufficient decomposition result.

The computational foundation of our moment approach is based on SOS relaxations, particularly the Lasserre hierarchy for moment problems (Parrilo, 2000; Lasserre, 2001). After more than a decade's developments, SOS relaxations have produced a large body of literature (cf. the monographs (Blekherman et al., 2013), (Lasserre, 2009) and references therein). The Lasserre hierarchy provides a series of SDPs that can approximate moment problems increasingly tight (Lasserre, 2001; Parrilo, 2000; Lasserre, 2008). Indeed, it has been shown that as one moves up the hierarchy, the solutions of the SDP relaxations converge to the infinite-dimensional measure optimization (Nie, 2014). In many cases, finite convergence is also possible, though it is typically hard to determine the sizes of those exact relaxations (Nie, 2014). We show that for the tensor decomposition problem, exact relaxation occurs for the smallest SDP in the hierarchy under certain incoherence conditions. Combining with the necessary condition in Theorem 2, we can roughly say that when the atomic tensor decomposition is solvable by the total variation norm minimization, it is also solvable by a small SDP; when the lowest order SDP relaxation does not work, the original infinite-dimensional measure optimization is also unlikely to work.

3. Model and Algorithm

3.1. Model for tensor decomposition

We focus on third order, symmetric tensors in this work. Given such a tensor $A = [A_{ijl}]_{i,j,l=1}^n \in S^3(\mathbb{R}^n)$, we are interested in decompositions of the form

$$A = \sum_{p=1}^{r} \lambda_p x^p \otimes x^p \otimes x^p \tag{1}$$

where $\|x^p\| = 1$ and $\lambda_p > 0$. The decomposition expressing a tensor as the sum of a finite number of rank-one tensors is called the CP decomposition (Canonical Polyadic Decomposition), which also goes by the name of CANDECOMP (Canonical Decomposition) (Carroll & Chang, 1970) and PARAFAC (Parallel Factors Decomposition) (Harshman, 1970). The positive coefficient assumption does not reduce the generality of the model since the sign of λ_p can be absorbed into the vector x^p. The smallest r that allows such a decomposition is called the symmetric rank of A, denoted by $\mathrm{srank}(A)$. A decomposition with $\mathrm{srank}(A)$ terms is always possible, though like many other tensor problems, determining the symmetric rank of a general 3rd-order, symmetric tensor is NP-hard (Hillar & Lim, 2013).

Denote the unit sphere of $\mathbb{R}^n$ as $\mathbb{S}^{n-1}$, and the set of (non-negative) Borel measures on $\mathbb{S}^{n-1}$ as $\mathcal{M}_+(\mathbb{S}^{n-1})$. We write the CP decomposition in (1) as

$$A = \int_{\mathbb{S}^{n-1}} x \otimes x \otimes x d\mu^\star \tag{2}$$

where the decomposition measure $\mu^\star = \sum_{p=1}^r \lambda_p \delta(x - x^p) \in \mathcal{M}_+(\mathbb{S}^{n-1})$. Hereafter, we use a superscript $\star$ to indicate that the measure is the "true", unknown decomposition measure to be identified from the tensor A. Since the entries of A are 3rd order moments of the measure $\mu^\star$, tensor decomposition is an instance of measure estimation from moments. Model (2) is more general than (1) in the sense that it allows decompositions involving infinite number of rank-one tensors. However, in most cases the decompositions of interest involve finite terms. In particular, we restate the problem of determining $\mathrm{srank}(A)$ as

$$\underset{\mu \in \mathcal{M}_+(\mathbb{S}^{n-1})}{\text{minimize}} \|\mu\|_0 \text{ subject to } A = \int_{\mathbb{S}^{n-1}} x \otimes x \otimes x d\mu \tag{3}$$

where $\|\mu\|_0$ is the support size of μ. This is a generalization of the ℓ_0 "norm" minimization problem to the infinite-dimensional measure space.

Following the idea of using the ℓ_1 norm as a convex proxy for the ℓ_0 "norm" and recognizing "$\|\mu\|_{\ell_1} = \mu(\mathbb{S}^{n-1})$", we formulate symmetric tensor decomposition as the following optimization

$$\begin{aligned} &\underset{\mu \in \mathcal{M}_+(\mathbb{S}^{n-1})}{\text{minimize}} \ \mu(\mathbb{S}^{n-1}) \\ &\text{subject to } A = \int_{\mathbb{S}^{n-1}} x \otimes x \otimes x d\mu \end{aligned} \tag{4}$$

Note the total mass $\mu(\mathbb{S}^{n-1})$ is the restriction of the total variation norm to the set of (non-negative) Borel measures. For any third order symmetric tensor A, the optimal value of (4) defines the tensor nuclear norm $\|A\|_*$, which is a special case of the more general atomic norms. According to the Caratheodory's convex hull theorem (Barvinok, 2002), there always exists optimal solutions with finite supports. We call a decomposition corresponding to an optimal, finite measure solving (4) an *atomic tensor decomposition*.

The optimization (4) is an instance of the problem of mo-

ments (Lasserre, 2008), whose dual is

$$\begin{aligned} &\underset{Q\in S^3(\mathbb{R}^n)}{\text{maximize}} \ \langle Q, A\rangle \\ &\text{subject to } \langle Q, x\otimes x\otimes x\rangle \le 1, \forall x\in \mathbb{S}^{n-1}. \end{aligned} \tag{5}$$

We have used $\langle A, B\rangle = \sum_{i,j,l} A_{ijl}B_{ijl}$ to denote the inner product of two 3rd order tensors. The homogeneous polynomial $q(x) := \langle Q, x\otimes x\otimes x\rangle = \sum_{i,j,k} Q_{ijk}x_ix_jx_k$ corresponding to a dual feasible solution is called a dual polynomial. We will see that the dual polynomial associated with the optimal dual solution can be used to certify the optimality of a particular decomposition.

3.2. Moment Relaxation

The tensor decomposition problem (4) is a special truncated moment problem (Nie, 2012), where we observe only third order moments of a measure $\mu^\star$ supported on the unit sphere. Therefore, we can apply the Lasserre SDP hierarchy (Lasserre, 2001) to approximate the infinite dimensional linear program (4). We first introduce a few notations in order to describe the SDP hierarchy. We use $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}^n$ to denote a multi-integer index. The notation x^α represents the monomial $x_1^{\alpha_1}x_2^{\alpha_2}\cdots x_n^{\alpha_n}$. The size of α, $|\alpha| = \sum \alpha_i$, is the degree of x^α. The set $\mathbb{N}_k^n = \{\alpha : |\alpha| \le k\} \subset \mathbb{N}^n$ consists of indices with sizes less than of equal to k. The notation $\mathbb{R}^{\mathbb{N}_k^n}$ ($\mathbb{R}^{\mathbb{N}_k^n\times\mathbb{N}_k^n}$, resp.) represents the set of real vectors (matrices, resp.) whose entries are indexed by elements in $\mathbb{N}_k^n$ ($\mathbb{N}_k^n \times \mathbb{N}_k^n$, resp.).

For $k = 2, 3, 4, \cdots$ and a vector $z \in \mathbb{R}^{\mathbb{N}_{2k}^n}$, we use the matrix $M_k(z) \in \mathbb{R}^{\mathbb{N}_k^n\times\mathbb{N}_k^n}$ to denote the moment matrix associated with the vector $z \in \mathbb{R}^{\mathbb{N}_{2k}^n}$, whose (α, β)th entry is $z_{\alpha+\beta}$ for $\alpha, \beta \in \mathbb{N}_k^n$. The notation $L_{k-1}(z) \in \mathbb{R}^{\mathbb{N}_{k-1}^n\times\mathbb{N}_{k-1}^n}$ is reserved for the localizing matrix of the polynomial $p(x) := \|x\|_2^2 - 1$, whose (α, β)th entry is

$$[L_{k-1}(z)]_{\alpha,\beta} \quad = \quad \sum_{|\gamma|\le 2} p_\gamma z_{\alpha+\beta+\gamma}, \alpha, \beta \in \mathbb{N}_{k-1}^n \tag{6}$$

with p_γ the coefficient for the monomial x^γ in $p(x)$.

Each measure μ supported on $\mathbb{S}^{n-1}$ is associated with an infinite sequence $\bar{y} \in \mathbb{R}^{\mathbb{N}^n}$, called the moment sequence, via $\bar{y}_\alpha := \int_{\mathbb{S}^{n-1}} x^\alpha d\mu, \alpha \in \mathbb{N}^n$. When $\alpha = (0, 0, \ldots, 0)$, we use $\bar{y}_0 = \int_{\mathbb{S}^{n-1}} 1 d\mu = \mu(\mathbb{S}^{n-1})$ to denote the total mass of the measure μ. Denote by $\mathfrak{M}(\mathbb{S}^{n-1}) \subset \mathbb{R}^{\mathbb{N}^n}$ the set of all such moment sequences. Instead of optimizing with respect to a measure μ in (4), we can equivalently optimize with respect to a moment sequence:

$$\underset{\bar{y}\in\mathfrak{M}(\mathbb{S}^{n-1})}{\text{minimize}} \ \bar{y}_0 \text{ subject to } \bar{y}_\alpha = A_{ijk} \text{ if } x^\alpha = x_ix_jx_k \tag{7}$$

The constraint that $\bar{y} \in \mathfrak{M}(\mathbb{S}^{n-1})$ involves an infinite sequence. To obtain a finite optimization, we relax (7) by replacing $\bar{y}$ with its $2k$-truncation $y \in \mathbb{R}^{\mathbb{N}_{2k}^n}$ and replacing the constraint $\bar{y} \in \mathfrak{M}(\mathbb{S}^{n-1})$ with the following easy-to-enforce conditions for y to be the finite truncation of a moment sequence (Lasserre, 2009):

$$M_k(y) \succcurlyeq 0, L_{k-1}(y) = 0. \tag{8}$$

Both the linear matrix inequality and equality can be proved by considering their quadratic forms and using the fact that μ is a Borel (hence nonnegative) measure on $\mathbb{S}^{n-1}$ and $p(x) = \|x\|_2^2 - 1 \equiv 0$ on $\mathbb{S}^{n-1}$.

Hence, we obtain a finite-dimensional relaxation for (7):

$$\begin{aligned} &\underset{y\in\mathbb{R}^{\mathbb{N}_{2k}^n}}{\text{minimize}} \ y_0 \text{ subject to } \ y_\alpha = A_{ijl} \text{ if } x^\alpha = x_ix_jx_l \\ &\qquad\qquad M_k(y) \succcurlyeq 0, L_{k-1}(y) = 0. \end{aligned} \tag{9}$$

Denote by $\|A\|_{k,*}$ the optimal value of (9). One can verify that $\|\cdot\|_{k,*}$ indeed defines a norm in the space of symmetric tensors. Clearly $\|A\|_{k,2}$ is smaller than $\|A\|_*$ for all symmetric tensors A and increasing k (*i.e.,* using longer truncation) allows us to get better approximatations. In a more general setting, it has been shown that the optimal value of (9) converges to that of (4) as $k \to \infty$ even in finite steps (Nie, 2014). Furthermore, if the moment matrix $M_k(\hat{y})$ associated with the optimal solution $\hat{y}$ of (9) satisfies the flat extension condition, *i.e.*, $\text{rank}(M_k(\hat{y}) = \text{rank}(M_{k-1}(\hat{y}))$, then we can apply an algebraic procedure to recover the measure $\hat{\mu}$ from the moment matrix (Curto & Fialkow, 1996; Henrion & Lasserre, 2005). Our goal is to show that under reasonable conditions on the true decomposition measure $\mu^\star$ that generates observations in A, the smallest relaxation with $k = 2$ is exact, *i.e.*, $\|A\|_{2,*} = \|A\|_*$, and is sufficient for the recovery of $\mu^\star$. The facial structures of the norm $\|\cdot\|_{2,*}$ at these tensors are the same as the facial structures of the tensor nuclear norm $\|\cdot\|_*$.

By following a standard procedure of deriving the Lagrange dual, we get the following dual problem of (9):

$$\begin{aligned} &\underset{Q\in S^3(\mathbb{R}^n),H,G}{\text{maximize}} \ \langle Q, A\rangle \\ &\text{subject to } \ e_0 - 1_\Omega(\text{vec}(Q)) = M_k^*(H) + L_{k-1}^*(G) \\ &\qquad\qquad H \succcurlyeq 0 \end{aligned} \tag{10}$$

Here $*$ represents the adjoint operator; $e_0 \in \mathbb{R}^{\mathbb{N}_{2k}^n}$ denotes the first canonical basis vector; and the operation $\text{vec}(Q)$ takes the unique entries in the symmetric tensor Q to form a vector, which is then embedded by 1_Ω into the third order moment vector space $\mathbb{R}^{\mathbb{N}_3^n}$.

We show that (9) is an SOS relaxation by rewriting its dual (10) as an SOS optimization. For this purpose, we denote the vector consisting of all monomials of x of degrees up to k by $\nu_k(x)$, also known as the Veronese map. For example, when $k = 2$, $\nu_2(x)$ has the following form:

$$\nu_2(x) = \begin{bmatrix} 1 & x_1 & \cdots & x_n & x_1^2 & x_1x_2 & \cdots & x_n^2 \end{bmatrix}^T \tag{11}$$

Define two polynomials $\sigma(x) := \nu_k(x)'H\nu_k(x)$ and

$s(x) := \nu_{k-1}(x)'G\nu_{k-1}(x)$ for feasible solutions H and G of (10). Since $H \succcurlyeq 0$, the polynomial $\sigma(x)$ is the Gram matrix representation of an SOS polynomial and $s(x)$ is an arbitrary polynomial of degree $2k-2$. We now rewrite the optimization (10) as an SOS optimization:

$$\begin{aligned} &\underset{Q \in S^3(\mathbb{R}^n)}{\text{maximize}} \ \langle Q, A \rangle \\ &\text{subject to } 1 - q(x) = s(x)(\|x\|^2 - 1) + \sigma(x) \\ &\qquad \deg(s(x)) \leq 2k-2 \\ &\qquad \sigma(x) \text{ is an SOS with } \deg(\sigma(x)) \leq 2k \end{aligned} \tag{12}$$

where $q(x) = \langle Q, x \otimes x \otimes x \rangle$ is the dual polynomial defined before. Compared with the dual polynomial in (5), the one here $q(x) = 1 - \sigma(x) - s(x)(\|x\|^2 - 1)$ has a more structured form. We call $1 - q(x)$ an SOS modulo the sphere.

4. Main Results

The main theorem of this work relies on the construction of dual polynomials that certify the optimality of the decomposition measure $\mu^\star$. Due to space limitation, the detailed construction of the dual polynomials are deferred to the supplemental materials. The constructed dual polynomials are also essential to the development of noise performance and tensor completion results using the moment approach. We record the following proposition, which forms the basis of the dual polynomial proof technique.

Proposition 1. Suppose $\text{supp}(\mu^\star) = \{x^p, p = 1, \ldots, r\}$ is such that $\{x^p \otimes x^p \otimes x^p, p = 1, \ldots, r\}$ forms a linearly independent set.
1. If there exists a $Q \in S^3(\mathbb{R}^n)$ such that the associated dual polynomial $q(x)$ satisfies

$$q(x^p) = 1, p = 1, \ldots, r \tag{13}$$

$$q(x) < 1, x \neq x^p, \forall p, \tag{14}$$

then $\mu^\star = \sum_{p=1}^r \lambda_p \delta(x - x^p)$ is the unique solution of the moment problem (4).
2. If in addition to part 1, the dual polynomial $q(x)$ also has the form $1 - \sigma(x) - s(x)(\|x\|^2 - 1)$, where $\sigma(x)$ is an SOS with $\deg(\sigma(x)) \leq 2k$, and $\deg(s(x)) \leq 2(k-1)$, then the optimization (9) is an exact relaxation of (4), *i.e.,* $\|A\|_{k,*} = \|A\|_*$. Furthermore, $y^\star$, the $2k$-truncation of the moment sequence for $\mu^\star$ is an optimal solution to (9).
3. Suppose $\{x^p, p = 1, \ldots, r\}$ are linearly independent. (So $r \leq n$.) In addition to the conditions in parts 1 and 2, if the Gram matrix H for the SOS $\sigma(x)$ in part 2 has rank $|\mathbb{N}_k^n| - r$, then $y^\star$, the $2k$-truncation of the moment sequence for $\mu^\star$, is the unique solution to (9) and we can extract the measure $\mu^\star$ from the moment matrix $M_k(y^\star)$.

A dual polynomial satisfying the interpolation and boundedness conditions (13) and (14) is used frequently as the starting point to derive several atomic decomposition and super-resolution results (Candès & Fernandez-Granda, 2014; Tang & Recht; Bendory et al., 2014b;a; Heckel et al., 2014). The second part of Proposition 1, which additionally requires the polynomial to be an SOS modulo the sphere to certify the exact relaxation of the SDP (9), is a contribution of this work. Part 3 is a consequence of the flat extension condition (Curto & Fialkow, 1998; 1996). We remark that there is a version of part 3 that allows $r > n$ under additional assumptions, which we did not present here. Constructing a structured dual polynomial satisfying conditions in parts 2 and 3 allows us to identify the class of polynomial-time solvable instances of the tensor decomposition problem, which are NP hard in the worst case.

We are now ready to state our major theorem:

Theorem 1. *For a symmetric tensor $A = \sum_{p=1}^r \lambda_p x^p \otimes x^p \otimes x^p$, if the vectors $\{x^p\}$ are incoherent, that is, the matrix $X = [x^1, x^2, \ldots, x^r]$ satisfies*

$$\|X^T X - I_r\| \leq 0.0016, \tag{15}$$

then there exists a dual symmetric tensor Q such that the dual polynomial $q(x) = \langle Q, x \otimes x \otimes x \rangle$ satisfies the conditions in all three parts of Proposition 1 with $k = 2$. Thus, $A = \sum_{p=1}^r \lambda_p x^p \otimes x^p \otimes x^p$ is the unique decomposition that achieves both the tensor nuclear norm $\|A\|_*$ and its relaxation $\|A\|_{2,*}$. Furthermore, this unique decomposition can be also found by solving (9) of the smallest size.

A few remarks follow. The constant 0.0016 in the incoherent condition (15) is not material and is not optimized.

The condition (15) requires $r \leq n$, which seems weak considering that the generic rank of a 3rd order symmetric tensor is at least $\frac{(n+2)(n+1)}{6}$ for all n except $n = 5$ (Comon et al., 2008). Furthermore, the Kruskal's sufficient condition states that a decomposition $A = \sum_{p=1}^r \lambda_p x^p \otimes x^p \otimes x^p$ is unique as long as $r \leq \frac{3k_X - 2}{2}$ where k_X is the Kruskal rank, or the maximum value of k such that any k columns of the matrix $X = [x^1, \cdots, x^r]$ are linearly independent (Landsberg, 2009). Since $k_X \leq n$, the Kruskal rank condition is valid for r as large as $\frac{3n-2}{2}$.

There are two reasons for the requirement of $r \leq n$. The first one is technical: we used a perturbation analysis of the orthogonal symmetric tensor decomposition, which prevents $r > n$ in the first place. The second reason is due to the use of $k = 2$ in the relaxation (9) and is more fundamental. In order to extract the decomposition, we apply the flat extension condition $M_1(y) = M_2(y)$ and the procedure developed in (Henrion & Lasserre, 2005). Since the size of $M_1(y)$ is $n + 1$, there is no way to identify more than $n + 1$ components from the moment matrix $M_2(y)$. If the goal is extract the decomposition from the moment matrix, as addressed in this paper, we will need to increase the relaxation to $k \geq 3$ to recover decompositions with more

than $n+1$ components. However, if the goal is denoising or tensor completion, it is still possible to achieve optimal noise performance and exact completion using $k=2$ even if $r > n+1$. Indeed, numerical experiments in Section 6.2 show that the smallest SDP of (9) can recover all moments up to order 4 correctly for r as large as $2n$.

To complement the sufficient condition in Theorem 1, we cite a theorem of (Tang, 2015) which demonstrates that a separation or incoherence condition on $\{x^p\}$ is necessary.

Theorem 2. *(Tang, 2015) Consider a set of vectors $S = \{x^p, p = 1, \ldots, r\} \subset \mathbb{S}^{n-1}$. If any signed measure supported on S is the unique solution to the optimization*

$$\underset{\mu \in \mathcal{M}(\mathbb{S}^{n-1})}{\text{minimize}} \|\mu\|_{\text{TV}} \text{ subject to } A = \int_{\mathbb{S}^{n-1}} x^{m\otimes} d\mu \quad (16)$$

then the maximal incoherence of points in S satisfies

$$\max_{i \neq j} (|\langle x^i, x^j \rangle|) \leq \cos(2/m). \quad (17)$$

Here $\mathcal{M}(\mathbb{S}^{n-1})$ is the set of all signed measures on $\mathbb{S}^{n-1}$ and $\|\cdot\|_{\text{TV}}$ denotes the total variation norm of a measure.

The incoherence condition (17) is a separation condition on points on $\mathbb{S}^{n-1}$ as it is equivalent to that the angle between any two points x^i and x^j is greater than $2/m$. The upper bound in (17) further confirms that knowledge of higher moments reduces the incoherence requirement. Note that when m is odd, we can again focus on Borel (non-negative) measures supported on $S = \{\pm x^p, p = 1, \ldots, r\}$, and the total variation norm $\|\mu\|_{\text{TV}}$ can be replaced by the total mass $\mu(\mathbb{S}^{n-1})$. We also observe that the incoherence condition (15) in Theorem 1 for 3rd order symmetric tensor implies $\max_{i \neq j}(|\langle x_i, x_j \rangle|) \leq 0.0016 < \cos(2/3) \approx 0.7859$, which is stronger than the necessary condition (17).

5. Extensions

5.1. Tensor completion and denoising

Since the optimal value of (4) defines the tensor nuclear norm $\|\cdot\|_*$, the results developed for tensor decomposition will form the foundation for tensor completion and stable low-rank tensor recovery. Similar to its matrix counterpart, the tensor nuclear norm favors low-rank solutions when the observations are corrupted by noise, missing data, and outliers. For example, when a low-rank tensor $A^\star$ is partially observed on an index set Ω, we can fill in the missing entries by solving a tensor nuclear norm minimization problem (Jain & Oh, 2014; Acar et al., 2011; Yuan & Zhang, 2014; Huang et al., 2014; Gandy et al., 2011):

$$\underset{A}{\text{minimize}} \|A\|_* \text{ subject to } A_\Omega = A^\star_\Omega. \quad (18)$$

This line of thinking was previously considered infeasible due to the intractability of the tensor nuclear norm. However, we can use the relaxed norm $\|\cdot\|_{k,*}$ to approximate (18):

$$\underset{A}{\text{minimize}} \|A\|_{k,*} \text{ subject to } A_\Omega = A^\star_\Omega. \quad (19)$$

which is equivalent to the SDP:

$$\begin{aligned} &\underset{y \in \mathbb{R}^{\mathbb{N}^n_{2k}}}{\text{minimize}}\ y_0 \\ &\text{subject to } y_\alpha = A_{ijl} \text{ when } x^\alpha = x_i x_j x_l \text{ and } (i,j,l) \in \Omega \\ &\qquad M_k(y) \succcurlyeq 0, L_{k-1}(y) = 0. \end{aligned} \quad (20)$$

Building on the dual polynomial of Theorem 1, we expect to show that $\|\cdot\|_{2,*}$ can be used to perform completion with a minimal number of tensor measurements, given that the tensor factors are incoherent.

Gaussian-type noise, which is unavoidable in practical scenarios, can also be handled using the tensor nuclear norm:

$$\underset{A}{\text{minimize}} \frac{1}{2}\|A - B\|_2^2 + \gamma \|A\|_*, \quad (21)$$

where B is the observed noisy entries of the tensor and γ is a regularization parameter. Replacing $\|\cdot\|_*$ with $\|\cdot\|_{k,*}$ gives rise to a hierarchy of SDP relaxations for (21):

$$\begin{aligned} &\underset{y \in \mathbb{R}^{\mathbb{N}^n_{2k}}}{\text{minimize}} \frac{1}{2}\|A - B\|_2^2 + \gamma y_0 \\ &\text{subject to } y_\alpha = A_{ijl} \text{ when } x^\alpha = x_i x_j x_l \\ &\qquad M_k(y) \succcurlyeq 0, L_{k-1}(y) = 0. \end{aligned} \quad (22)$$

We conducted numerical experiments to demonstrate the performance of tensor completion and denoising using the smallest SDP relaxations in (20) and (22).

5.2. Non-symmetric and high-order tensors

We briefly discuss extensions to non-symmetric and high-order tensor problems. Consider decomposing a non-symmetric tensor $A = [A_{ijk}] \in \mathbb{R}^{n_1 \times n_2 \times n_3}$ into the form $A = \sum_{p=1}^r \lambda_p x^p \otimes y^p \otimes z^p$, where $\|x^p\| = \|y^p\| = \|z^p\| = 1$ and $\lambda_p > 0$. Similar to (4), we formulate the non-symmetric tensor decomposition again as estimating a measure μ supported on $K = \mathbb{S}^{n_1} \times \mathbb{S}^{n_2} \times \mathbb{S}^{n_3}$:

$$\underset{\mu \in \mathcal{M}_+(K)}{\text{minimize}} \mu(K) \text{ subject to } A = \int_K x \otimes y \otimes z d\mu. \quad (23)$$

Optimization (23) admits a similar SDP relaxation hierarchy for $k = 2, 3, \cdots$:

$$\begin{aligned} &\underset{m \in \mathbb{R}^{\mathbb{N}^n_{2k}}}{\text{minimize}}\ m_0 \\ &\text{subject to } m_\alpha = A_{ijl} \text{ when } \xi^\alpha = x_i y_j z_l \\ &\qquad M_k(m) \succcurlyeq 0, L^{h_1}_{k-1}(m), L^{h_2}_{k-1}(m), L^{h_3}_{k-1}(m) = 0, \end{aligned} \quad (24)$$

where $\xi = (x, y, z)$, and $\{L^{h_i}_{k-1}\}$ are localizing matrices corresponding to the constraints $h_1(\xi) = \|x\|_2^2 - 1 = 0, h_2(\xi) = \|y\|_2^2 - 1 = 0$ and $h_3(\xi) = \|z\|_2^2 - 1 = 0$.

The SDPs in (24) can be modified to solve tensor completion and denoising problems.

The measure formulation extends easily to higher-order tensors. For the SDP relaxation hierarchy, we just need to fill in the moment vector with the observed, high-order moments, and add more constraints corresponding to the constraints defining the measure domain K. However, theoretical treatment might be more challenging, especially if we would like to allow the rank r to go beyond the individual tensor dimensions.

6. Numerical Experiments

We performed a series of experiments to illustrate the performance of the SDP relaxations (9) in solving the tensor decomposition and other related problems. All the SDPs are solved using the CVX package.

6.1. Phase transitions with full data

Figure 1 shows the phase transitions for the success rate of the SDP relaxation (9) with $k = 2$ when we vary the rank r, the incoherence $\Delta = \max_{i \neq j} |\langle x^i, x^j \rangle|$, and the dimension n. The purpose is to figure out the critical incoherence value. In preparing the upper plot in Figure 1, we took $n = 10$, $r \in \{2, 4, \ldots, 20\}$, and $\Delta \in \{0.38, 0.39, \ldots, 0.52\}$. We choose the maximal incoherence Δ instead of the quantity in condition (15) because in the experiments the rank r goes beyond n, in which case condition (15) is always violated. To compute the success rate, we produced $T = 10$ instances for each (r, Δ) configuration. We used the acceptance-rejection method to generate an instance with r vectors such that $\max_{i \neq j} |\langle x^i, x^j \rangle| \leq \Delta$. This method becomes inefficient when $\Delta < 0.38$, forcing us to test Δs in the chosen range. After being passed through the SDP (9), an instance is declared success if the difference between the recovered moment vector and the true moment vector has an ℓ_2 norm less than 10^{-4}. Again, we choose this success criterion instead of correct identification of the decomposition because the rank r goes beyond n, in which case we can not identify the decomposition from the moment matrix. It is easy to see that when $r \leq n$ and the 4th order moment matrix is recovered correctly, the flat extension condition is satisfied and the decomposition can be extracted from the moment matrix.

We observe from the upper plot of Figure 1 that the incoherence condition can be relaxed for smaller tensors with smaller ranks. For rank $r \leq n = 10$, a critical separation of $\Delta = 0.45$ is sufficient for exact recovery. Though the figure does not show the transition for $\Delta < 0.38$ due to the difficulty of generating vectors maintaining such a small incoherence, by extrapolation we expect that when $\Delta \leq 0.38$, the relaxation (9) can recover instances with

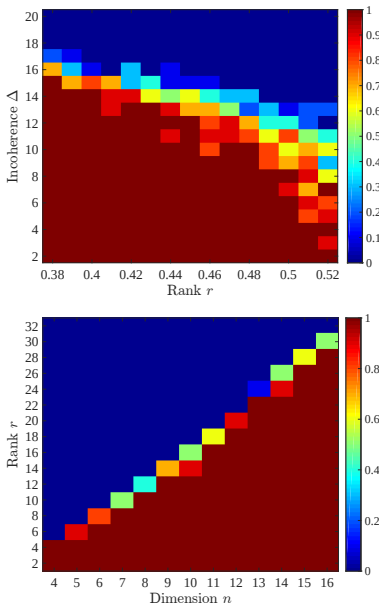

Figure 1. Color coded success rates of the lowest order SDP in recovering the 4th order moment vector: rank r vs incoherence Δ (Upper) for $n = 10$ and rank r vs dimension n for $\Delta = 0.38$.

rank up to $r = 15 = \frac{3n}{2}$. We comment that the limitation to the range $\Delta \leq 0.38$ is due to the inefficiency of our rejection sampling methods to generate vectors with maximal incoherence smaller than 0.38. There are many vector configurations with a far smaller incoherence (Rankin, 1955), but we are not aware of an efficient algorithms to generate them (except for the orthogonal ones).

In the next experiment, we examine the phase transition when the dimension n and the rank r are varied while the incoherence Δ is fixed to 0.38. The purpose is to determine the critical rank r when the vectors $\{x^p\}$ are well-separated. We observe a clear phase transition, whose boundary is roughly $r = 2.1n - 6.4$.

6.2. Phase transition for completion

In this set of experiments, we test the power of the SDP relaxation (20) in performing symmetric tensor completion. In figure 2, we plot the success rates for tensors with *orthogonal* components when the number of observations, the rank r, and the dimension n are varied. To compute the success rate, the following procedure was repeated 10 times for each (m, r) or (m, n) configuration, where m is the number of measurements. A set of r random, orthonormal vectors $\{x^p\}$ together with a vector $\lambda \in \mathbb{R}^r$ following the uniform distribution on $[0, 1]$ were generated to produce the tensor $A = \sum_{p=1}^{r} \lambda_p x^p \otimes x^p \otimes x^p$. A uniform random subset of the tensor entries were sampled to form the observations. Since symmetric tensors have duplicated

entries, we made sure only the unique entries were sampled and counted towards the measurements. The optimization (20) was then run to complete the tensor as well as estimating all the moments up to order 4. The optimization was successful if the ℓ_2 norm between the recovered 4th order moment vector and the true moment vector is less than 10^{-4}. We applied the same procedure to prepare the phase transition plots in Figure 3 except that the vectors $\{x^p\}$ are not orthogonal, but rather maintain an incoherence $\max_{i \neq j} |\langle x^i, x^j \rangle \geq 0.38$.

For orthogonal tensor completions shown in Figure 2, we observe clear phase transitions for both the number of measurements versus the rank r, and versus the dimension n. Even though the degree of freedom for a dimension n, rank r, third-order symmetric tensor is rn, which is linear in both r and n, the boundaries in both plots of Figure 2 are curved. This phenomenon is seen in other completion tasks such as matrix completion (Candès & Recht, 2009) and compressed sensing off the grid (Tang et al., 2013). For non-orthogonal tensor completion, the phase transition boundaries are more blurred as seen from Figure 3. We believe this is because our selected value for the incoherence, 0.38, is still too large.

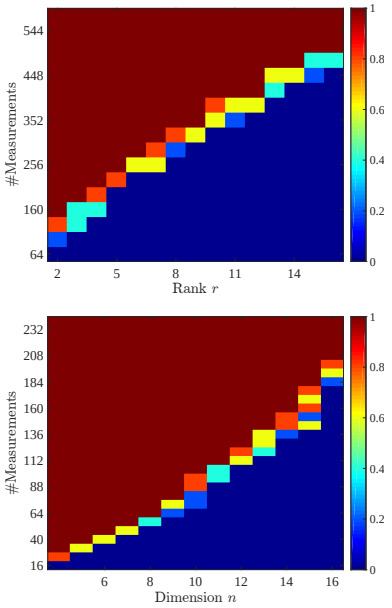

Figure 2. Color coded success rate of the lowest order SDP for *orthogonal* symmetric tensor completion: the number of measurements vs. rank r for fixed $n = 16$ (Upper), and the number of measurements vs. dimension n for fixed $r = 4$ (Lower).

6.3. Noise robustness

In the last experiment, we show one example to demonstrate that the moment approach for tensor recovery is robust to Gaussian type noise. For $n = 5$, we generated a

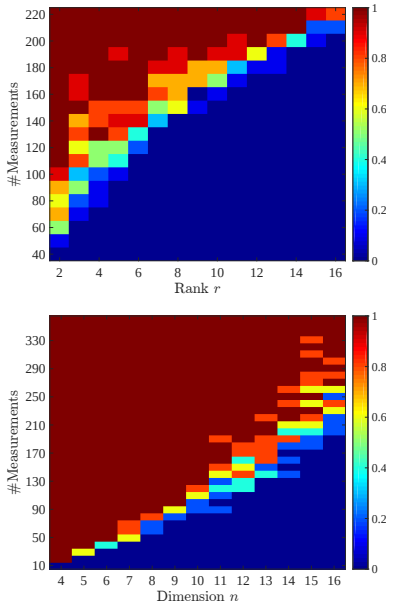

Figure 3. Color coded success rate of the lowest order SDP for non-orthogonal, symmetric tensor completion: the number of measurements vs. rank r for fixed $n = 10$ (Upper), and the number of measurements vs. dimension n for fixed $r = 4$ (Lower).

tensor with $r = 6$ random rank-one factors maintaining an incoherence less than 0.38. Gaussian noise of standard deviation σ equal to half the average magnitude of the tensor elements was added to all the unique entries of the tensor. We then ran the optimization (22) with $k = 2$ to perform denoising. The penalization parameter γ is set to equal σ. The noise-free and recovered 4th order moment vectors (except for the 0th order moments), and the observations are plotted in Figure 4. Note only 3rd order moments are observed while the algorithm returns all moments up to order 4. We chose to remove the 0th order moments because they are large and including them makes the plot less discernible. We see from Figure 4 that in addition to denoise the observed 3rd moments, which are entries of the tensor, the algorithm can also interpolates 0th to 2nd order moments and extrapolates the 4th order moments.

7. Conclusions

In this work, we formulated tensor decomposition as a measure estimation problem from observed moments, and used the total mass minimization to seek for a low-rank CP decomposition. We approximate this infinite-dimensional measure optimization using a hierarchy of SDPs. For third order symmetric tensors, by explicitly constructing an interpolation dual polynomial, we established that tensor decomposition is possible using the moment approach under an incoherence condition. Furthermore, by showing that

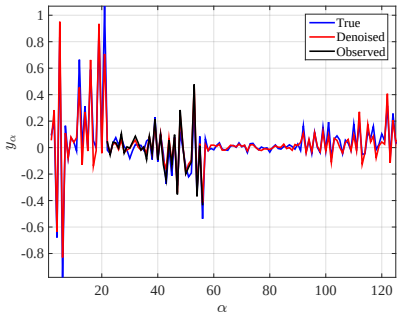

Figure 4. Tensor denoising using (22). Best viewed in color.

the constructed dual polynomial is a sum-of-square modulo the sphere, we demonstrated that the smallest SDP in the relaxation hierarchy is exact, and the CP tensor decomposition can be identified from the recovered, truncated moment matrix. A complimentary resolution limit result was cited to show that certain incoherent condition was necessary. We discussed possible extensions to non-symmetric, and higher-order tenors, as well as generalizations to tensor completion and denoising. Numerical experiments were performed to test the power of the moment approach in tensor decomposition, completion, and denoising.

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Supplementary Material

7.1. Proof of Proposition 1

Proof. 1. Any symmetric tensor Q that satisfies the conditions in part 1 of Proposition 1 is dual feasible. The decomposition measure $\mu^\star$ is clearly primal feasible. We also have

$$\begin{aligned}\langle Q, A\rangle &= \sum_{p=1}^{r} \lambda_p \langle Q, x^p \otimes x^p \otimes x^p\rangle \\ &= \sum_{p=1}^{r} \lambda_p q(x^p) = \sum_{p=1}^{r} \lambda_p = \mu^\star(\mathbb{S}^{n-1}),\end{aligned}$$

establishing a zero duality gap at the primal-dual feasible solution pair $(\mu^\star, Q)$. Therefore, $\mu^\star$ is primal optimal and Q is dual optimal.

For uniqueness, suppose $\hat{\mu}$ is another optimal solution. We then have

$$\begin{aligned}\mu^\star(\mathbb{S}^{n-1}) &= \langle Q, A\rangle \\ &= \left\langle Q, \int_{\mathbb{S}^{n-1}} x\otimes x\otimes x d\hat{\mu}\right\rangle \\ &= \sum_{x\in \operatorname{supp}(\mu^\star)} \hat{\mu}(x) q(x) \\ &+ \int_{\mathbb{S}^{n-1}/\operatorname{supp}(\mu^\star)} q(x) d\hat{\mu} \\ &< \sum_{\hat{x}_p \in \operatorname{supp}(\mu^\star)} \hat{\lambda}_p + \int_{\mathbb{S}^{n-1}/\operatorname{supp}(\mu^\star)} 1 d\hat{\mu} \\ &= \hat{\mu}(\mathbb{S}^{n-1})\end{aligned}$$

due to condition (14) if $\hat{\mu}(\mathbb{S}^{n-1}/\operatorname{supp}(\mu^\star)) > 0$, contradicting the optimality of $\hat{\mu}$. So all optimal solutions are supported on $\operatorname{supp}(\mu^\star)$. Since the tensors $\{x^p \otimes x^p \otimes x^p\}$ for $x^p \in \operatorname{supp}(\mu^\star)$ are linearly independent, the coefficients are also uniquely determined.

2. Denote by p_0 and d_0 the optimal values for the primal problem (4) and the dual problem (5), respectively; and denote by p_1 and d_1 the optimal values for the primal-dual problems (9) and (12) (or (10)), respectively. We next argue that these four quantities are equal. First, part 1 establishes $p_0 = d_0$. Second, weak duality and the construction of relaxations (9) and (12) imply that $d_1 \le p_1 \le p_0 = d_0$. Also the feasible set of (12) projected onto the Q space is a subset of the feasible set of (5). Since the conditions of part 2 states that the optimal dual solution Q to (5) is also feasible to (12), we hence conclude that Q is also an optimal solution to (12) and obtain $d_1 = d_0$. Therefore, $p_0 = d_0 = d_1 = p_1$, and the relaxations (9) and (12) are tight.

To show the optimality of $y^\star$, the $2k$-truncation of the (infinite) moment vector $\bar{y}^\star$ corresponding to the measure $\mu^\star$. We first note that $y^\star$ is feasible to (9). Then zero duality gap, as verified below

$$y_0^\star = \mu^\star(\mathbb{S}^{n-1}) = p_0 = d_1 = \langle Q, A\rangle,$$

establishes the optimality of $y^\star$.

3. Denote by $\sigma(x) = \nu_k(x)' H \nu_k(x)$ the SOS polynomial associated with H. Note $\nu_k(x^p)' H \nu_k(x^p) = \sigma(x^p) = 1 - q(x^p) = 0$ for $p = 1, \ldots, r$, implying $H\nu_k(x^p) = 0, p = 1, \ldots, r$ due to $H \succcurlyeq 0$. Since $\operatorname{rank}(H) = |\mathbb{N}_k^n| - r$ by the assumption, the null space of H is $\operatorname{span}\{\nu_k(x^p), p = 1, \ldots, r\}$.

For any optimal solution $\hat{y}$ of (9), complementary slackness implies that

$$HM_k(\hat{y})) = 0.$$

So the eigen-space of $M_k(\hat{y})$ is a subspace of $\operatorname{span}\{\nu_k(x^p), p = 1, \ldots, r\}$. We hence write

$$M_k(\hat{y}) = VDV'$$

where $V = \left[\nu_k(x^1) \cdots \nu_k(x^r)\right]$ and D is an $r \times r$ semidefinite matrix (not necessarily diagonal at this point). Note that $M_k(y^\star) = V\Lambda V'$. We next argue that $D = \Lambda$.

The moment matrix $M_k(\hat{y})$ contains a submatrix specified by the third order moments in the tensor A, and hence is equal to the corresponding submatrix in $M_k(y^\star)$. More precisely, $M_k(\hat{y})$ contains the block (at the location indicated by the orange color in Figure 5):

$$\begin{aligned}&\int_{\mathbb{S}^{n-1}} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \begin{bmatrix} x_1^2 & x_1x_2 & \cdots & x_{n-1}x_n & x_n^2 \end{bmatrix} d\mu^\star \\ =& X\Lambda V_2'\end{aligned}$$

where $X = \left[x^1 \cdots x^p\right]$, V_2 is the submatrix of V whose rows correspond to the second-order monomials in $\nu_k(x)$, and $\Lambda = \operatorname{diag}([\lambda_1, \ldots, \lambda_r])$. Therefore, we have

$$X\Lambda V_2' = XDV_2' \tag{25}$$

Due to Lemma 3.1 (ii) of (De Lathauwer, 2008), $\operatorname{rank}(X) = r$ implies that $\operatorname{rank}(V_2) = r$. Multiplying both sides of (25) by the pseudo-inverse matrices $X^\dagger$ from left and $(V_2')^\dagger$ from right yield $D = \Lambda$. So $M_k(\hat{y}) = M_k(y^\star)$, and $\hat{y} = y^\star$ is the unique solution of (9).

To see that we can extract the measure $\mu^\star$ from $M_k(\hat{y}) = M_k(y^\star)$, we note that the matrix $M_k(y^\star) = V\Lambda V'$ has rank r for all $k \ge 1$. Hence the flat extension condition $\operatorname{rank}(M_{k-1}(y^\star) = M_k(y^\star))$ is satisfied for all $k \ge 2$. Therefore, according to (Curto & Fialkow, 1996; Henrion & Lasserre, 2005), we could recover the measure from the moment matrix $M_k(y^\star)$. □

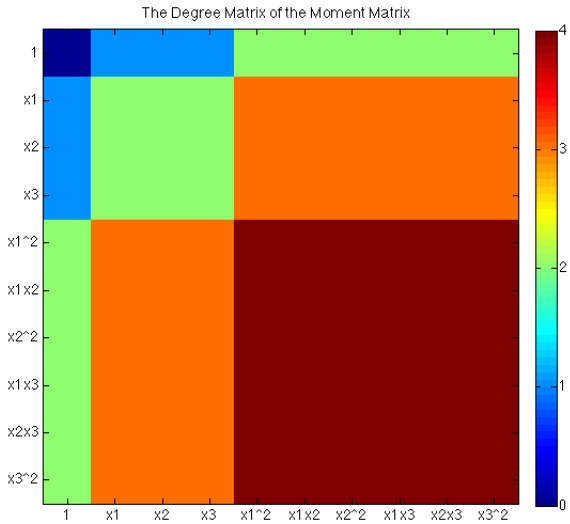

Figure 5. The colors code the degrees of the entries in the moment matrix for an instance with $n = 3, k = 2$.

7.2. Dual Certificate: the Orthonormal Case

The proof of Theorem 1 is based on a perturbation analysis of the orthogonal case. In this and the next sections, we focus on constructing a dual polynomial for orthogonal decompositions. Hereafter, the relaxation order is fixed to $k = 2$.

When the vectors $\{x^p, p = 1, \ldots, r\}$ are orthonormal, we verify that the symmetric tensor

$$Q = \sum_{p=1}^{r} x^p \otimes x^p \otimes x^p$$

satisfies the conditions in part 1 of Proposition 1. To see this, note

$$q(x^p) = \langle Q, x^p \otimes x^p \otimes x^p \rangle = \sum_{p'=1}^{r} \langle x^{p'}, x^p \rangle^3 = 1.$$

In addition, for any fixed $x \in \mathbb{S}^{n-1}$ we have

$$\begin{aligned} q(x) = \langle Q, x \otimes x \otimes x \rangle &= \sum_{p=1}^{r} \langle x^p, x \rangle^3 \\ &\leq \max_p \langle x^p, x \rangle \sum_{p=1}^{r} \langle x^p, x \rangle^2 \\ &\leq \|X^T x\|^2 \end{aligned}$$

where we used $\max_p \langle x^p, x \rangle \leq \max_p \|x^p\| \|x\| = 1$ for all p. Due to the orthogonality of the columns of $X = [x^1 \cdots x^r]$, we clearly have $\|X^T x\|^2 \leq \|x\|^2 = 1$. For $q(x) = 1$, all the involved inequalities must be equalities. For $\max_p \langle x^p, x \rangle = 1$, we need $x = x^p$ for some p, which is the only possible case that $q(x) = 1$. For all other cases, $q(x) < 1$. Therefore, $Q = \sum_p x^p \otimes x^p \otimes x^p$ satisfies the conditions of part 1 in Proposition 1. This argument combined with part 1 of Proposition 1 lead to

Theorem 3. *If the vectors in* $\mathrm{supp}(\mu^\star)$ *are orthonormal, then* $\mu^\star$ *is the unique optimal solution to* (4).

7.3. SOS Dual Certificate: the Orthonormal Case

In the following, we show that for $q(x) = \sum_{p=1}^{r} \langle x, x^p \rangle^3$, we could find an SOS $\sigma(x)$ and a polynomial $s(x)$ with degrees 4 and 2 respectively, such that

$$1 - q(x) = \sigma(x) + s(x)(\|x\|_2^2 - 1)$$

We start with assuming $x^p = e_p$, the pth canonical basis vector, for $p = 1, 2, \ldots, r$, in which case $q(x)$ becomes $\sum_{p=1}^{r} x_p^3$. Later on we will apply a rotation to derive the general case from this special case.

We take $s(x) = -\frac{3}{2}\left(\sum_{p=1}^{r} x_p^2\right) - \frac{3}{2}\left(\sum_{p=r+1}^{n} x_p^2\right) = \nu_1(x)' G_0 \nu_1(x)$ with

$$G_0 = \begin{bmatrix} 0 & \\ & -\frac{3}{2} I_n \end{bmatrix}. \tag{26}$$

Consider

$$\begin{aligned} & 1 - q(x) - s(x)(\|x\|_2^2 - 1) \\ =& 1 - \sum_{p=1}^{r} x_p^3 + \frac{3}{2}\left(\sum_{p=1}^{r} x_p^2\right)\left(\sum_{p=1}^{n} x_p^2 - 1\right) \\ & + \frac{3}{2}\left(\sum_{p=r+1}^{n} x_p^2\right)\left(\sum_{p=1}^{n} x_p^2 - 1\right) \\ =& 1 - \frac{3}{2}\left(\sum_{p=1}^{r} x_p^2\right) - \frac{3}{2}\left(\sum_{p=r+1}^{n} x_p^2\right) - \sum_{p=1}^{r} x_p^3 \\ & + \frac{3}{2}\sum_{p=1}^{r} x_p^4 + \frac{3}{2}\sum_{p=r+1}^{n} x_p^4 \\ & + 3\sum_{p<p'=1}^{r} x_p^2 x_{p'}^2 + 3\sum_{p<p'=r+1}^{n} x_p^2 x_{p'}^2 + 3\sum_{p=1}^{r}\sum_{p'=1}^{n} x_p^2 x_{p'}^2. \end{aligned} \tag{27}$$

We show that this polynomial is an SOS $\sigma(x)$ with Gram matrix H_0 defined on top of the next page. Here the row partition of H_0 corresponds to the partition of the Veronese

$$H_0 = \begin{bmatrix} 1 & & & & & & & -\mathbf{1}_r' & f\mathbf{1}_{n-r}' \\ & \frac{1}{2}I_r & & & & & & -\frac{1}{2}I_r & \\ & & aI_{n-r} & & & & & & \\ & & & I_{C_2^r} & & & & & \\ & & & & bI_{r(n-r)} & & & & \\ & & & & & cI_{C_2^{n-r}} & & & \\ -\mathbf{1}_r & -\frac{1}{2}I_r & & & & & & \frac{1}{2}I_r + \mathbf{1}_r\mathbf{1}_r' & d\mathbf{1}_r\mathbf{1}_{n-r}' \\ f\mathbf{1}_{n-r} & & & & & & & d\mathbf{1}_{n-r}\mathbf{1}_r' & \left(\frac{3}{2} - e\right) I_{n-r} + e\mathbf{1}_{n-r}\mathbf{1}_{n-r}' \end{bmatrix} \tag{28}$$

map $\nu_2(x)$ given in the following

$$\nu_2(x) = \begin{bmatrix} 1 \\ \begin{bmatrix} x_1 \\ \vdots \\ x_r \end{bmatrix} \\ \begin{bmatrix} x_{r+1} \\ \vdots \\ x_n \end{bmatrix} \\ \begin{bmatrix} x_1x_2 \\ x_1x_3 \\ \vdots \\ x_{r-1}x_r \end{bmatrix} \\ \begin{bmatrix} x_1x_{r+1} \\ \vdots \\ x_rx_n \end{bmatrix} \\ \begin{bmatrix} x_{r+1}x_{r+2} \\ \vdots \\ x_{n-1}x_n \end{bmatrix} \\ \begin{bmatrix} x_1^2 \\ \vdots \\ x_r^2 \end{bmatrix} \\ \begin{bmatrix} x_{r+1}^2 \\ \vdots \\ x_n^2 \end{bmatrix} \end{bmatrix} := \begin{bmatrix} \nu_2^0(x) \\ \nu_2^1(x) \\ \nu_2^2(x) \\ \nu_2^3(x) \\ \nu_2^4(x) \\ \nu_2^5(x) \\ \nu_2^6(x) \\ \nu_2^7(x) \end{bmatrix} \tag{29}$$

and a, b, c, d, e, f are parameters to be determined later.

Since

$$\begin{aligned} &\nu_2(x)' H_0 \nu_2(x) \\ =& 1 - \frac{3}{2}\sum_{p=1}^{r} x_p^2 + (a+2f)\sum_{p=r+1}^{n} x_p^2 - \sum_{p=1}^{r} x_p^3 \\ &+ \frac{3}{2}\sum_{p=1}^{r} x_p^4 + \frac{3}{2}\sum_{p=r+1}^{n} x_p^4 \\ &+ 3\sum_{p<p'=1}^{r} x_p^2 x_{p'}^2 + (c+2e)\sum_{p<p'=r+1}^{n} x_p^2 x_{p'}^2 \\ &+ (b+2d)\sum_{p=1}^{r}\sum_{p'=1}^{n} x_p^2 x_{p'}^2 \end{aligned}$$

comparison of coefficients with those of $1 - q(x) - s(x)(\|x\|_2^2 - 1)$ in (27) gives

$$\begin{aligned} a + 2f &= -\frac{3}{2} \\ c + 2e &= 3 \\ b + 2d &= 3 \end{aligned}$$

We will judiciously choose the parameters so that H_0 is PSD. Note that H_0 must have r zero eigenvalues with eigenvectors $\{\nu_2(e^p) : p = 1, \ldots, r\}$. For later analysis, we also need H_0 to have precisely r zero eigenvalues, and the smallest non-zero eigenvalue of H_0 to be lower bounded by a numerical constant regardless of n and r.

For that purpose, we next find all the eigenvalues of H_0. The obvious ones include $a, 1, b$ and c of multiplicities $n-r, C_2^r, r(n-r)$ and C_2^{n-r}, respectively. The rest of eigenvalues are those of E defined as

$$\begin{bmatrix} 1 & & -\mathbf{1}_r' & f\mathbf{1}_{n-r}' \\ & \frac{1}{2}I_r & -\frac{1}{2}I_r & \\ -\mathbf{1}_r & -\frac{1}{2}I_r & \frac{1}{2}I_r + \mathbf{1}_r\mathbf{1}_r' & d\mathbf{1}_r\mathbf{1}_{n-r}' \\ f\mathbf{1}_{n-r} & & d\mathbf{1}_{n-r}\mathbf{1}_r' & \left(\frac{3}{2} - e\right) I_{n-r} + e\mathbf{1}_{n-r}\mathbf{1}_{n-r}' \end{bmatrix}$$

We choose $e + a = \frac{3}{2}$ and decompose E as $A + B$ such that A is

$$\begin{bmatrix} 1 & & -\mathbf{1}_r' & f\mathbf{1}_{n-r}' \\ & \frac{1}{2r}\mathbf{1}_r\mathbf{1}_r' & -\frac{1}{2r}\mathbf{1}_r\mathbf{1}_r' & \\ -\mathbf{1}_r & -\frac{1}{2r}\mathbf{1}_r\mathbf{1}_r' & \left(1 + \frac{1}{2r}\right)\mathbf{1}_r\mathbf{1}_r' & d\mathbf{1}_r\mathbf{1}_{n-r}' \\ f\mathbf{1}_{n-r} & & d\mathbf{1}_{n-r}\mathbf{1}_r' & (e + \frac{a}{(n-r)})\mathbf{1}_{n-r}\mathbf{1}_{n-r}' \end{bmatrix}$$

and B is

$$\begin{bmatrix} 0 & & \\ & \frac{1}{2}\left(I_r - \frac{1}{r}\mathbf{1}_r\mathbf{1}_r'\right) & -\frac{1}{2}\left(I_r - \frac{1}{r}\mathbf{1}_r\mathbf{1}_r'\right) & \\ & -\frac{1}{2}\left(I_r - \frac{1}{r}\mathbf{1}_r\mathbf{1}_r'\right) & \frac{1}{2}\left(I_r - \frac{1}{r}\mathbf{1}_r\mathbf{1}_r'\right) & \\ & & & * \end{bmatrix}$$

where the right-bottom block of B occupied by $*$ is $a\left(I_{n-r} - \frac{1}{n-r}\mathbf{1}_{n-r}\mathbf{1}_{n-r}'\right)$. It is easy to verify that $AB = BA = 0$. Hence the eigenvalues of E consist of those of A and B. The eigenvalues of B are 0, 1, and a of multiplicities $r+3, r-1, n-r-1$, respectively.

Next we choose the parameters such that the eigenvalues of A are easy to compute. We first ensure that A has rank 3, which requires the matrix, by rank invariance of Gaussian elimination,

$$\begin{bmatrix} 1 & & & \\ & \frac{1}{2r}\mathbf{1}_r\mathbf{1}_r' & & \\ & & \mathbf{0}_r & (d+f)\mathbf{1}_r\mathbf{1}_{n-r}' \\ & & (d+f)\mathbf{1}_{n-r}\mathbf{1}_r' & * \end{bmatrix}$$

whose bottom-right block is $\left(e + \frac{a}{(n-r)} - f^2\right)\mathbf{1}_{n-r}\mathbf{1}_{n-r}'$, to have rank 3, or equivalently, $d + f = 0$.

Multiplying A with a vector of the form $v := \begin{bmatrix} \alpha \\ \beta\mathbf{1}_r \\ \gamma\mathbf{1}_r \\ \delta\mathbf{1}_{n-r} \end{bmatrix}$ shows that the eigenvectors of A are of the form v. Consequently, the non-zero eigenvalues of A can be computed by solving a smaller set of eigenvalue equations

$$\begin{bmatrix} 1 & 0 & -r & f(n-r) \\ 0 & 1/2 & -1/2 & 0 \\ -1 & -1/2 & r+1/2 & -f(n-r) \\ f & 0 & -fr & (n-r)e+a \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{bmatrix} = \lambda \begin{bmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{bmatrix} \tag{30}$$

We already have five equations on a, b, c, d, e, f:

$$\begin{aligned} a + 2f &= -\frac{3}{2} \\ c + 2e &= 3 \\ b + 2d &= 3 \\ e + a &= \frac{3}{2} \\ d + f &= 0 \end{aligned}$$

or,

$$\begin{aligned} b &= 3 - 2d = 3 - \frac{3}{2} - a = \frac{3}{2} - a \\ c &= 3 - 2e = 2a \\ d &= \frac{3}{4} + \frac{a}{2} \\ e &= \frac{3}{2} - a \\ f &= -\frac{3}{4} - \frac{a}{2} \end{aligned}$$

Plugging these into the matrix in (30) leads to a matrix involving a single parameter a:

$$\begin{bmatrix} 1 & 0 & -r & -\left(\frac{3}{4}+\frac{a}{2}\right)(n-r) \\ 0 & 1/2 & -1/2 & 0 \\ -1 & -1/2 & r+1/2 & \left(\frac{3}{4}+\frac{a}{2}\right)(n-r) \\ -\left(\frac{3}{4}+\frac{a}{2}\right) & 0 & \left(\frac{3}{4}+\frac{a}{2}\right)r & (n-r)\left(\frac{3}{2}-a\right)+a \end{bmatrix}$$

Symbolic calculation shows the non-zero eigenvalues of this matrix are zeros of the polynomial

$$\begin{aligned} &h(\lambda; r, n, a) = (2+r)(15(-n+r) \\ &+ 4a(-4 + (7+a)n - (7+a)r)) \\ &+ 2(16 + 39n - 31r + 15(n-r)r \\ &- 4a^2(n-r)(1+r) + 4a((1+r)(8+7r) - n(11+7r)))\lambda \\ &+ 16(-4 - 3n + 2a(-1+n-r) + r)\lambda^2 + 32\lambda^3 \end{aligned}$$

We want to make sure $\lambda = a \neq 0$ is one non-zero eigenvalue, which means $h(a; r, n, a) = 0$, or after simplification:

$$\begin{aligned} &a^3(r-3) + 15(r+2) + 4a^2(13r+32) - 2a(29r+67) \\ &= 0 \end{aligned}$$

We pick the smallest positive root branch $a = a(r)$, which is an increasing function of r with limit $a(+\infty) = \frac{1}{2}$, and $a(1) > 0.3387$. We next argue that, after plugging $a = a(r)$, $h(\lambda; r, n, a(r))$ has two other zeros that are larger than $\frac{1}{2}$ (hence larger than $a(r)$), which means the other two non-zero eigenvalues of A are greater than $a(r) \in (0.3387, 0.5)$. The argument is based on median value theorem by showing $h(1/2; r, n, a(r)) > 0$, $h(n/2; r, n, a(r)) < 0$ combined with the obvious fact $\lim_{\lambda\to\infty} h(\lambda; r, n, a(r)) = +\infty$.

We first show $h(1/2; r, n, a) > 0$ for $1 \leq r \leq n$ and $a \in [0.2, 0.5)$. As a function of r with parameter n and a, the function

$$\begin{aligned} h(1/2; r, n, a) &= 4 - 8a - 3n + 20an + 4a^2n \\ &\quad + (3 - 20a - 4a^2)r \end{aligned}$$

is linear in r and is decreasing since $3 - 20a - 4a^2 < 0$ for

$a \in [0.2, 0.5)$. Therefore, we obtain

$$\begin{aligned} h(1/2; r, n, a) &\geq h(1/2; n, n, a) \\ &= 4 - 8a \\ &> 0. \end{aligned}$$

Second, we show that $h(n/2; r, n, a) < 0$ for $a \in [0.2, 0.5)$ and $r \in [0, n]$:

$$\begin{aligned} & h(n/2; r, n, a) \\ =& (-2+n)(16a + (7 - 4a(9+a))n + 8(-1+a)n^2) \\ & + (30 - 8a(9+a) - 46n + 8a(11+a)n \\ & + (19 - 4a(9+a))n^2)r + (-1+2a)(15+2a)(-1+n)r^2 \\ \leq& (-2+n)(16a + (7 - 4a(9+a))n \\ & + 8(-1+a)n^2) + 2(1-2a)(15+2a)(-1+n)nr \\ & + (-1+2a)(15+2a)(-1+n)r^2. \end{aligned}$$

We used the fact that

$$\begin{aligned} & 30 - 8a(9+a) - 46n + 8a(11+a)n + (19 - 4a(9+a))n^2 \\ & \leq 2(1-2a)(15+2a)(n-1)n \end{aligned}$$

which can be proved by observing that

$$\begin{aligned} & 2(1-2a)(15+2a)(n-1)n - (30 - 8a(9+a) - 46n \\ & + 8a(11+a)n + (19 - 4a(9+a))n^2) \\ & = -30 + 8a(9+a) \\ & + (46 - 8a(11+a) - 2(1-2a)(15+2a))n \\ & + (-19 + 4a(9+a) + 2(1-2a)(15+2a))n^2 \end{aligned}$$

is an increasing function of n (since $(46 - 8a(11+a) - 2(1-2a)(15+2a)) > 0$ for $a \in [0.2, 0.5)$), and its value at $n = 1$ is $-3 + 12a(9+a) - 8a(11+a) \geq 1$.

Now the upper bound on $h(n/2; r, n, a)$ is an increasing function of r for $r \in [1, n]$. We therefore further bound $h(n/2; r, n, a)$ by setting $r = n$ in its upper bound:

$$\begin{aligned} h(n/2; r, n, a) \leq& -32a - 14n + 8a(11+a)n \\ & + 8(1-3a)n^2 + (7 - 4a(5+a))n^3 \\ :=& u(n; a) \end{aligned}$$

Since $\frac{d}{dn} u(n; a)$ is

$$-14 + 8a(11+a) + 16(1-3a)n + 3(7 - 4a(5+a))n^2$$

is decreasing for $n \geq 0$ due to $3(7 - 4a(5+a)) < 0$ and $16(1-3a) < 0$ when $a \in (0.3387, 0.5)$, we have

$$\begin{aligned} \frac{d}{dn} u(n; a) \leq& \frac{d}{dn} u(8; a) \\ =& 1458 - 8a(517 + 95a) \\ <& 0 \end{aligned}$$

for $n \geq 8$ and $a \in (0.3387, .5)$. Therefore, $u(n; a)$ is further upper bounded by its value at $n = 8$ for $n \geq 8$:

$$\begin{aligned} h(n/2; r, n, a) \leq& u(8; a) = -16(-249 + 2a(347 + 62a)) \\ <& 0 \end{aligned}$$

for $a \in (0.3387, .5)$.

To sum, we showed that $h(\lambda; r, n, a(r))$, whose zeros are eigenvalues of A, has the property that $\lambda_1 = a(r) \in (0.3387, 1/2)$ is a zero, and $h(1/2; r, n, a(r)) > 0, h(n/2; r, n, a(r)) < 0$, and $h(+\infty; r, n, a) > 0$. Therefore, the other two zeros of $h(\lambda; r, n, a(r))$ are greater than $1/2 > a(r)$.

In sum, the matrix H_0 has rank $|\mathbb{N}_2^n| - r$ and the minimal non-zero eigenvalue for H_0 is

$$\min\left\{a(r), \frac{3}{2} - a(r), 2a(r), \frac{1}{2}, 1\right\} = a(r)$$

since $a(r) \in (0.3387, 1/2)$. This shows that H_0 is PSD.

When $\mathrm{supp}(\mu^\star)$ is orthonormal, but not canonical basis vectors, we augment the matrix $X = \begin{bmatrix} x^1 & \cdots & x^r \end{bmatrix}$ to an orthonormal matrix $P = \begin{bmatrix} X & P_1 \end{bmatrix}$ and transform the variable x to $z = P'x = P^{-1}x$. Then the tensor $A = \sum_p x^p \otimes x^p \otimes x^p$ is transformed to $\sum_p e_p \otimes e_p \otimes e_p$. Then the dual polynomial

$$q_0(z) = 1 - \nu_2(z)' H_0 \nu_2(z) + \frac{3}{2}\|z\|_2^2(\|z\|_2^2 - 1)$$

with H_0 constructed above satisfies the conditions in Proposition 1, and certifies the optimality of the decomposition $\sum_p e_p \otimes e_p \otimes e_p$. We transform this polynomial back to the x-domain to obtain

$$q(x) := q_0(P'x) = 1 - \nu_2(P'x)' H_0 \nu_2(P'x) + \frac{3}{2}\|x\|_2^2(\|x\|_2^2 - 1)$$

where we have used $\|P'x\|_2^2 = \|x\|_2^2$ since P is orthonormal. According to Lemma 1, the polynomial

$$\nu_2(P'x) H_0 \nu_2(P'x) = \nu_2(x)'(J' H_0 J)\nu_2(x)$$

is an SOS with the Gram matrix $J' H_0 J$, whose smallest eigenvalue is greater than $\frac{1}{2} \times 0.3387 > \frac{1}{6}$. One can verify that $q(x)$ satisfies all the conditions in Proposition 1. As a consequence, we obtain:

Theorem 4. *If the vectors in* $\mathrm{supp}(\mu^\star)$ *are orthonormal, then the SDP relaxation* (9) *with* $k = 2$ *gives the exact decomposition. Furthermore, the constructed dual polynomial has the form*

$$q(x) = 1 - \nu_2(x)' H \nu_2(x) + \frac{3}{2}\|x\|_2^2(\|x\|_2^2 - 1)$$

where H *has* r *zero eigenvalues, and the* $(r+1)$*th smallest eigenvalue is greater than* $\frac{1}{6}$*. When the support are formed by a subset of canonical basis vectors, the lower bound on eigenvalues can be chosen as* $\frac{1}{3}$*.*

The SOS matrix decomposition is verified by Matlab. With

$n = 7$ and $r = 3$, we have the following plot for H_0:

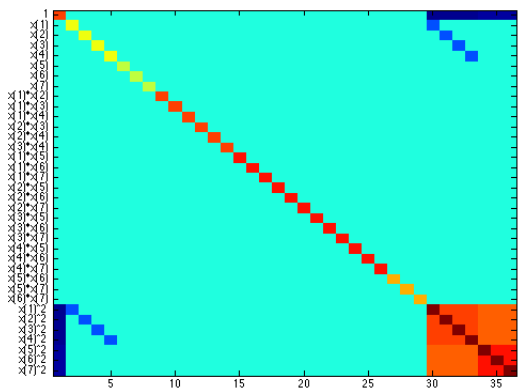

Figure 6. H_0 has $r = 4$ zero eigenvalues and the 5th smallest is $a(4) = 0.3789$.

7.4. Dual Certificate: The Non-Orthonormal Case

We now proceed to apply a perturbation analysis to construct a dual polynomial for the non-orthonormal case.

Suppose the measure $\mu^\star = \sum_{k=1}^r \lambda_k \delta(x - x^k)$ where $\{x^k, k = 1, \ldots, r\}$ are not orthogonal. Define $X = [x^1, \cdots, x^r]$ and find $N \in \mathbb{R}^{n\times(n-r)}$ which has orthonormal columns and is orthogonal to X. Further define $P = \begin{bmatrix} X & N \end{bmatrix}$. Then the transformation $x \mapsto z = P^{-1}x$ maps x^k to the kth canonical basis vector e_k. The unit sphere is mapped to an ellipsoid $E^{n-1} = \{z : z'P'Pz = 1\}$.

If we could construct a polynomial $q(z) = \langle Q, z \otimes z \otimes z\rangle$ with symmetric Q such that

$$q(e_k) = 1, k = 1, \ldots, r \tag{31}$$

$$|q(z)| < 1, z \in E^{n-1}, z \neq e_k \tag{32}$$

then the polynomial $q_1(x) := q(P^{-1}x) = \langle Q, P^{-1}x \otimes P^{-1}x \otimes P^{-1}x\rangle$ would satisfy

$$q_1(x^k) = q(e_k) = 1, k = 1, \ldots, r$$
$$|q_1(x)| = |q(P^{-1}x)| < 1, x \in S^{n-1}, x \neq x^k.$$

To construct $q(z)$, we note that it must satisfy $q(e_k) = 1$ and $q(z)$ achieves maximum at $z = e_k$ for $k = 1, \ldots, r$. Denote $L(z; \nu) = q(z) - \nu(z'P'Pz - 1)$ as the Lagrangian. A necessary condition for $q(z)$ to achieve maximum at e_k is given by the KKT condition:

$$\begin{aligned}\frac{\partial L(z)}{\partial z}|_{z=e_k} =& \frac{\partial q(z)}{\partial z}|_{z=e_k} - \nu\frac{\partial}{\partial z}(z'P'Pz - 1)|_{z=e_k}\\ =& 3\sum_{i=1}^n \langle Q, e_k \otimes e_k \otimes e_i\rangle e_i - 2\nu P'Pe_k\\ =& 0\end{aligned}$$

Taking inner product with e_k yields

$$3q(e_k) = 3\langle Q, e_k \otimes e_k \otimes e_k\rangle = 2\nu e_k' P'Pe_k = 3,$$

implying $\nu = \frac{3}{2}$. Therefore, the symmetric tensor Q must satisfy

$$\sum_{i=1}^n \langle Q, e_k \otimes e_k \otimes e_i\rangle e_i = P'Pe_k, k = 1, \ldots, r. \tag{33}$$

Note the condition (31) is a consequence of (33). We pick

$$\begin{aligned}Q =& \sum_{k=1}^r e_k \otimes e_k \otimes P'Pe_k + \sum_{k=1}^r e_k \otimes P'Pe_k \otimes e_k\\ &+ \sum_{k=1}^r P'Pe_k \otimes e_k \otimes e_k - 2\sum_{k=1}^r \underbrace{(e_k'P'Pe_k)}_{=1} e_k \otimes e_k \otimes e_k\end{aligned}$$

which actually has minimal energy among all symmetric Q that satisfies (33). The dual polynomial is then given by

$$\begin{aligned}q(z) =& \langle Q, z \otimes z \otimes z\rangle\\ =& \sum_{k=1}^r [3z_k^2(z'P'Pe_k) - 2z_k^3]\\ =& \sum_{k=1}^r [3(z'P'Pe_k) - 2z_k]z_k^2.\end{aligned}$$

Clearly, $q(z)$ satisfies the interpolation condition (31). In the following, we show that $q(z)$ also satisfies the condition (32). The argument is based on partitioning the ellipsoid E^{n-1} into a region that is far from any e_k and a region that is near to some e_k.

First note

$$q(z) \leq \max_k [3(z'P'Pe_k) - 2z_k] \sum_{k=1}^r z_k^2$$

When $z \in E^{n-1}$, due to $\|P'P - I\| \leq \epsilon$, we have $-\epsilon z'z \leq 1 - z'z \leq \epsilon z'z$, implying

$$\frac{1}{1+\epsilon} \leq \quad z'z \quad \leq \frac{1}{1-\epsilon}$$

Therefore, we can further upper bound $q(z)$ as

$$\begin{aligned}q(z) \leq& \max_k [3(z'P'Pe_k) - 2z_k] \sum_{k=1}^r z_k^2\\ \leq& \frac{1}{1-\epsilon} \max_k [3(z'P'Pe_k) - 2z_k]\end{aligned}$$

So, if

$$\max_k [3(z'P'Pe_k) - 2z_k] < 1 - \epsilon$$

then $q(z) < 1$. We showed that $q(z) < 1$ in the "far-away" region.

Define $N_k = \{z : 3(z'P'Pe_k) - 2z_k \geq 1 - \epsilon, z'P'Pz = 1\}$. When $P'P \approx I$, this is saying $z_k \geq 1 - \epsilon$, so $z \in N_k$ is close to e_k. The union of N_ks defines the "near region".

We want to make sure that $q(z)$ is strictly less than 1 in each N_k except when $z = e_k \in N_k$. For that purpose, we perform a Taylor expansion of the Lagrangian $L(z) = L(z; 3/2)$ in N_k around $z = e_k$

$$\begin{aligned} L(z) &= q(z) - \frac{3}{2}(z'P'Pz - 1) \\ &= L(e_k) + (z - e_k)' \frac{\partial L}{\partial z}|_{z=e_k} \\ &+ \frac{1}{2}(z - e_k)' H(\xi_z)(z - e_k) \\ &= 1 + \frac{1}{2}(z - e_k)' H(\xi_z)(z - e_k) \end{aligned}$$

where $H(\xi_z)$ is the Hessian of $L(z)$ evaluated at ξ_z and $\xi_z \in N_k$ depends on $z \in N_k$.

Since $q(z) = L(z)$ on the ellipsoid E^{n-1}, it suffices to show $\frac{1}{2}(z - e_k)' H(\xi_z)(z - e_k) < 0$ for $z \in N_k / \{e_k\}$. For this purpose, we compute the Hessian matrix $H(\xi)$:

$$\begin{aligned} H(\xi) &= \frac{\partial}{\partial z}\left[3\sum_{i=1}^{n}\langle Q, z \otimes z \otimes e_i\rangle e_i - 3P'Pz\right]|_{z=\xi} \\ &= 6\sum_{i,j=1}^{n}\langle Q, \xi \otimes e_j \otimes e_i\rangle e_i \otimes e_j - 3P'P \end{aligned}$$

Plugging in the expression for Q, we get that the Hessian $H(\xi)$ equals

$$\begin{aligned} &6\sum_{i,j=1}^{n}[\xi_j e_i' P'Pe_j + \xi_i e_j' P'Pe_i] e_i \otimes e_j \\ &\quad + 6\sum_{i=1}^{n}[(\xi' P'Pe_i) - 2\xi_i] e_i \otimes e_i - 3P'P \end{aligned}$$

To get a sense why this Hessian guarantees a negative second order term in the Taylor expansion, we set $\xi = e_k$ to get

$$\begin{aligned} H(e_k) &= 6\sum_{i,j=1}^{n}[e_k(j) e_i' P'Pe_j + e_k(i) e_j' P'Pe_i] e_i \otimes e_j \\ &+ 6\sum_{i=1}^{n}[(e_k' P'Pe_i) - 2e_k(i)] e_i \otimes e_i - 3P'P \\ &= 6\left[\sum_i (e_i' P'Pe_k) e_i \otimes e_k + \sum_j (e_j' P'Pe_k) e_k \otimes e_j\right] \\ &+ 6\sum_{i=1}^{n}[(e_k' P'Pe_i) - 2e_k(i)] e_i \otimes e_i - 3P'P \end{aligned}$$

When $P'P \approx I$,

$$\begin{aligned} H(e_k) &\approx 12 e_k \otimes e_k - 6 e_k \otimes e_k - 3I \\ &= 6 e_k \otimes e_k - 3I \end{aligned}$$

which is PSD except in the direction e_k, which is orthogonal to the tangent space of $E^{n-1} \approx S^{n-1}$ at $z = e_k$. Therefore, the Hessian projected onto the tangent space is negative definite, as desired.

Returning to the non-orthogonal case, we bound

$$\begin{aligned} H(\xi) &= 6\sum_{i,j=1}^{n}[\xi_j e_i' P'Pe_j + \xi_i e_j' P'Pe_i] e_i \otimes e_j \\ &+ 6\sum_{i=1}^{n}[(\xi' P'Pe_i) - 2\xi_i] e_i \otimes e_i - 3P'P \end{aligned}$$

for $\xi \in N_k$ with

$$N_k = \{\xi : 3(\xi' P'Pe_k) - 2\xi_k \geq 1 - \epsilon, \xi' P'P\xi = 1\}$$

Note

$$\begin{aligned} \sum_{i,j=1}^{n}(\xi_j e_i' P'Pe_j) e_i \otimes e_j &= P'P\,\mathrm{diag}(\xi) \\ \sum_{i,j=1}^{n}(\xi_i e_j' P'Pe_i) e_i \otimes e_j &= \mathrm{diag}(\xi) P'P \\ \sum_{i=1}^{n}(\xi' P'Pe_i) e_i \otimes e_i &= \mathrm{diag}(P'P\xi) \\ \sum_{i=1}^{n}\xi_i e_i \otimes e_i &= \mathrm{diag}(\xi) \end{aligned}$$

lead to the following concise expression for the Hessian matrix $H(\xi)$:

$$\begin{aligned} &6(P'P\,\mathrm{diag}(\xi) + \mathrm{diag}(\xi)P'P + \mathrm{diag}(P'P\xi) - 2\,\mathrm{diag}(\xi)) \\ &\quad - 3P'P \end{aligned}$$

We want to show that

$$(z - e_k)' H(\xi)(z - e_k) \quad < \quad 0, \forall \xi, z \in N_k.$$

We first argue that $z \in N_k = \{z : 3(z'P'Pe_k) - 2z_k \geq 1 - \epsilon, z'P'Pz = 1\}$ imposes certain restrictions on the size of z, and implies that z is close to e_k. Indeed, $\|I - P'P\| \leq \epsilon$ and $z'P'Pz = 1$ imply that

$$\frac{1}{1+\epsilon} \leq \frac{1}{\lambda_{\max}(P'P)} \leq \|z\|^2 \leq \frac{1}{\lambda_{\min}(P'P)} \leq \frac{1}{1-\epsilon}.$$

To show the closeness of z and e_k, we observe that

$$\begin{aligned} 3z'P'Pe_k - 2z_k &= 3z'(P'P - I)e_k + 3z'e_k - 2z_k \\ &= z_k + 3z'(P'P - I)e_k \end{aligned}$$

Since $|3z'(P'P - I)e_k| \leq 3\|z\|\|P'P - I\| \leq \frac{3\epsilon}{\sqrt{1-\epsilon}}$, z_k is bounded from below as follows:

$$\begin{aligned} z_k &\geq 1 - \epsilon - 3z'(P'P - I)e_k \\ &\geq 1 - \epsilon - \frac{3\epsilon}{\sqrt{1-\epsilon}}. \end{aligned}$$

On the other hand, $z_k \leq \|z\| \leq \frac{1}{\sqrt{1-\epsilon}}$.

A consequence of the sizes of z and z_k is that

$$\begin{aligned}\|z - z_k e_k\|^2 &= \sum_{j\neq k} z_j^2 \\ &= \|z\|^2 - z_k^2 \\ &\leq \frac{1}{1-\epsilon} - \left(1-\epsilon-\frac{3\epsilon}{\sqrt{1-\epsilon}}\right)^2\end{aligned}$$

Therefore, we have

$$\begin{aligned}&\|z - e_k\|_\infty \\ \leq& \max\{\epsilon + \frac{3\epsilon}{\sqrt{1-\epsilon}}, \frac{1}{\sqrt{1-\epsilon}} - 1, \\ &\sqrt{\frac{1}{1-\epsilon} - \left(1-\epsilon-\frac{3\epsilon}{\sqrt{1-\epsilon}}\right)^2}\} \\ :=& c_1(\epsilon) \\ =& O(\epsilon)\end{aligned}$$

and

$$\begin{aligned}&\|z - e_k\|^2 \\ =& \sum_{j\neq k} z_j^2 + (z_k - 1)^2 \leq \|z - z_k e_k\|^2 \\ &+ \max\left\{\epsilon + \frac{3\epsilon}{\sqrt{1-\epsilon}}, \frac{1}{\sqrt{1-\epsilon}} - 1\right\}^2 \\ =& \frac{1}{1-\epsilon} - \left(1-\epsilon-\frac{3\epsilon}{\sqrt{1-\epsilon}}\right)^2 \\ &+ \max\left\{\epsilon + \frac{3\epsilon}{\sqrt{1-\epsilon}}, \frac{1}{\sqrt{1-\epsilon}} - 1\right\}^2 \\ =& c_2(\epsilon)\end{aligned}$$

Next we show that each term in

$$P'P\operatorname{diag}(\xi) + \operatorname{diag}(\xi)P'P + \operatorname{diag}(P'P\xi) - 2\operatorname{diag}(\xi)$$

is close to $e_k e_k'$, except the last term which is close to $2e_k e_k'$. The first term is bounded as follows:

$$\begin{aligned}&\|P'P\operatorname{diag}(\xi) - e_k e_k'\| \\ \leq& \|P'P\operatorname{diag}(\xi) - P'Pe_k e_k'\| + \|P'Pe_k e_k' - e_k e_k'\| \\ \leq& \|P'P\|\|\xi - e_k\|_\infty + \|P'P - I\| \\ \leq& (1+\epsilon)c_1(\epsilon) + \epsilon\end{aligned}$$

Similar bounds hold for the term $\operatorname{diag}(\xi)P'P$.

$$\begin{aligned}&\|\operatorname{diag}(P'P\xi) - e_k e_k'\| \\ =& \|P'P\xi - e_k\|_\infty \\ \leq& \|P'P\xi - \xi\|_\infty + \|\xi - e_k\|_\infty \\ \leq& \|P'P - I\|\|\xi\|_2 + c_1(\epsilon) \\ \leq& \frac{\epsilon}{\sqrt{1-\epsilon}} + c_1(\epsilon)\end{aligned}$$

and the term $\operatorname{diag}(\xi)$

$$\|\operatorname{diag}(\xi) - e_k e_k'\| \leq \|\xi - e_k\|_\infty \leq c_1(\epsilon)$$

These bounds imply that

$$\begin{aligned}&\|P'P\operatorname{diag}(\xi) + \operatorname{diag}(\xi)P'P + \operatorname{diag}(P'P\xi) - 2\operatorname{diag}(\xi) \\ &\qquad - e_k e_k'\| \\ \leq& 2(1+\epsilon)c_1(\epsilon) + 2\epsilon + \frac{\epsilon}{\sqrt{1-\epsilon}} + c_1(\epsilon) + c_1(\epsilon) \\ :=& c_3(\epsilon) \\ =& O(\epsilon)\end{aligned}$$

Furthermore, we have

$$\begin{aligned}&\|P'Pe_k e_k' P'P - e_k e_k\| \\ =& \|P'Pe_k e_k' P'P - P'Pe_k e_k' + P'Pe_k e_k' - e_k e_k'\| \\ \leq& \|P'P\|\|e_k e_k'\|\|P'P - I\| + \|P'P - I\|\|e_k e_k'\| \\ \leq& (1+\epsilon)\epsilon + \epsilon \\ =& O(\epsilon)\end{aligned}$$

Therefore, we get

$$\begin{aligned}&\|H(\xi) - (6P'Pe_k e_k' P'P - 3P'P)\| \\ \leq& 6c_3(\epsilon) + 6\epsilon(2+\epsilon) \\ :=& c_4(\epsilon) \\ =& O(\epsilon)\end{aligned}$$

For any $z \in N_k$, we show $(z - e_k)'P'Pe_k$ is small due to the fact that both z and e_k lie on E^{n-1}:

$$\begin{aligned}1 &= z'P'Pz \\ &= e_k' P'Pe_k + 2(z - e_k)'P'Pe_k + (z - e_k)'P'P(z - e_k) \\ &= 1 + 2(z - e_k)'P'Pe_k + (z - e_k)'P'P(z - e_k)\end{aligned}$$

implying

$$\begin{aligned}|(z - e_k)'P'Pe_k| &= \frac{1}{2}(z - e_k)P'P(z - e_k) \\ &\leq \frac{1}{2}\|P'P\|\|z - e_k\|^2 \\ &\leq \frac{1}{2}(1+\epsilon)\|z - e_k\|^2\end{aligned}$$

The following chain of inequalities

$$\begin{aligned}
&(z-e_k)'H(\xi)(z-e_k)\\
\leq&(z-e_k)'(6P'Pe_ke_k'P'P-3P'P)(z-e_k)\\
&+\|z-e_k\|_2^2c_4(\epsilon)\\
=&6[(z-e_k)'P'Pe_k]^2-3(z-e_k)'P'P(z-e_k)\\
&+\|z-e_k\|^2c_4(\epsilon)\\
=&\frac{3}{2}(1+\epsilon)^2\|z-e_k\|^4-3(z-e_k)'P'P(z-e_k)\\
&+\|z-e_k\|^2c_4(\epsilon)\\
\leq&\frac{3}{2}(1+\epsilon)^2\|z-e_k\|^4-3(1-\epsilon)\|z-e_k\|^2\\
&+\|z-e_k\|^2c_4(\epsilon)\\
=&\frac{3}{2}(1+\epsilon)^2\|z-e_k\|^4-(3-3\epsilon-c_4(\epsilon))\|z-e_k\|^2
\end{aligned}$$

show that the second order term is negative if

$$\frac{3}{2}(1+\epsilon)^2\|z-e_k\|^2<3-3\epsilon-c_4(\epsilon)$$

So it suffices to require

$$c_2(\epsilon)\frac{3}{2}(1+\epsilon)^2<3-3\epsilon-c_4(\epsilon)$$

Numerical computation shows that the above inequality holds if

$$\epsilon\leqslant 0.0016.$$

We summarize the above argument into a theorem:

Theorem 5. *For a symmetric tensor $A=\sum_{p=1}^r\lambda_px^p\otimes x^p\otimes x^p$, if the vectors $\{x^p\}$ are near orthogonal, that is, the matrix $X=[x^1,x^2,\ldots,x^r]$ satisfies*

$$\|X'X-I_r\|\leq 0.0016,$$

then there exists a dual symmetric tensor Q such that the dual polynomial $q(x)=\langle Q,x\otimes x\otimes x\rangle$ satisfies the conditions in part 1 of Proposition 1. Thus, $A=\sum_{p=1}^r\lambda_px^p\otimes x^p\otimes x^p$ is the unique decomposition that achieves the tensor nuclear norm, and can be found by solving (4).

7.5. SOS Dual Certificate: The Non-Orthonormal Case

After rotating to the canonical basis vectors, the dual polynomial we constructed for the orthogonal case is

$$q_0(z)=\sum_{k=1}^r z_k^3$$

while the one for the non-orthogonal case is

$$q(z)=\sum_{k=1}^r[3(z'P'Pe_k)-2z_k]z_k^2.$$

We first show that this $1-q(z)$ is an SOS modulo the ellipsoid E^{n-1}. We know that $q_0(z)$ is an SOS modulo the sphere, that is, there exist symmetric matrices $H\succcurlyeq 0$ and $G\in\mathbb{R}^{r\times r}$ such that

$$1-q_0(z)=\nu_2(z)'H\nu_2(z)+\nu_1(z)'G\nu_1(z)(\|z\|^2-1).$$

In Section 7.3, we constructed $G=G_0$ in (26) and $H=H_0$ in (28). So (H_0,G_0) is in the feasible set of the following two constraints:

$$\begin{aligned}
&\nu_2(z)'H\nu_2(z)+\nu_1(z)'G\nu_1(z)(\|z\|^2-1)=1-q_0(z),\forall z\\
&H\succcurlyeq 0.
\end{aligned}\tag{34}$$

Note that any feasible H must satisfy $\nu_2(e_i)'H\nu_2(e_i)=0$ for $i=1,2,\ldots,r$, implying that $\{\nu_2(e_i):i=1,2,\ldots,r\}$ spans a subspace of the null space of H.

Define matrices B_α and C_α^0 that satisfy

$$\nu_2(z)\nu_2(z)'=\sum_{|\alpha|\leq 4}B_\alpha z^\alpha$$

$$\nu_1(z)\nu_1(z)'(\|z\|^2-1)=\sum_{|\alpha|\leq 4}C_\alpha^0 z^\alpha$$

These notations allow us to write

$$\nu_2(z)'H\nu_2(z)=\langle\nu_2(z)\nu_2(z)',H\rangle=\sum_{|\alpha|\leq 4}\langle B_\alpha,H\rangle z^\alpha$$

$$\begin{aligned}
\nu_1(z)'G\nu_1(z)(\|z\|^2-1)&=\langle\nu_1(z)\nu_1(z)'(\|z\|^2-1),G\rangle\\
&=\sum_{|\alpha|\leq 4}\langle C_\alpha^0,G\rangle z^\alpha
\end{aligned}$$

Denote by b_α^0 the coefficient for z^α in $1-q_0(z)$. We write the polynomial equation $\nu_2(z)'H\nu_2(z)+\nu_1(z)'G\nu_1(z)(\|z\|^2-1)=1-q_0(z)$ equivalently as

$$\langle B_\alpha,H\rangle+\langle C_\alpha^0,G\rangle=b_\alpha,|\alpha|\leq 4$$

Therefore, we obtain the SDP formulation of (34)

$$\begin{aligned}
&\text{find } G,H\\
&\text{subject to } \langle B_\alpha,H\rangle+\langle C_\alpha^0,G\rangle=b_\alpha^0,|\alpha|\leq 4\\
&H\succcurlyeq 0.
\end{aligned}\tag{35}$$

As aforementioned, G_0 and H_0 defined respectively in (26) and (28) form a feasible point for (35).

Now we switch to the non-orthogonal case, and we would like to show that

$$q(z)=\sum_{k=1}^r[3(z'P'Pe_k)-2z_k]z_k^2$$

is an SOS module the ellipsoid E^{n-1}. That is, we want to solve the feasibility problem

$$\begin{aligned}
&\text{find } G \text{ and } H\\
&\text{subject to}\\
&\nu_2(z)'H\nu_2(z)+\nu_1(z)'G\nu_1(z)(z'P'Pz-1)=1-q(z)\\
&H\succcurlyeq 0.
\end{aligned}\tag{36}$$

or equivalently in SDP

$$\begin{aligned} &\text{find } G \text{ and } H \\ \text{subject to} \quad & \\ &\langle B_\alpha, H\rangle + \langle C_\alpha, G\rangle = b_\alpha, |\alpha| \le 4 \\ &H \succcurlyeq 0. \end{aligned} \tag{37}$$

Here B_α is defined as before, while b_α is the coefficient for z^α in $1 - q(z)$ for $|\alpha| \le 4$ and C_α is defined via

$$\nu_1(z)\nu_1(z)'(z'P'Pz - 1) = \sum_{|\alpha|\le 4} C_\alpha z^\alpha$$

We again note that any feasible H must satisfy $\nu_2(e_i)'H\nu_2(e_i) = 0$ for $i = 1, 2, \ldots, r$, implying that $\{\nu_2(e_i) : i = 1, 2, \ldots, r\}$ spans a subspace of the null space of H.

When $\|P'P - I\| \le \epsilon$ with ϵ small, C_α is close to C^0_α and b_α is close to b^0_α. We claim that, when ϵ is sufficiently small, we can always take $G_1 = G_0$ and H_1 in the neighborhood of H_0 that form a feasible point of (37). Denote $\Delta H = H_1 - H_0$ and $e_\alpha = (b_\alpha - b^0_\alpha) - (\langle C_\alpha, G_0\rangle - \langle C^0_\alpha, G_0\rangle)$, then ΔH must satisfy

$$\langle B_\alpha, \Delta H\rangle = e_\alpha, |\alpha| \le 4$$

These set of equality constraints, which are equivalent to

$$\begin{aligned} \nu_2(z)'\Delta H\nu_2(z) &= \sum_{|\alpha|\le 4} e_\alpha z^\alpha \\ &= q(z) - q_0(z) - \nu_1(z)'G_0\nu_1(z)(z'P'Pz - z'z), \end{aligned}$$

also implies that $\nu_2(e_i)'\Delta H\nu_2(e_i) = 0, i = 1, \ldots, r$. Therefore, $\{\nu_2(e_i) : i = 1, 2, \ldots, r\}$ spans a subspace of the null space of H_0, H_1 and ΔH. Since the null space of H_0 is exactly $\mathrm{span}(\{\nu_2(e_i) : i = 1, 2, \ldots, r\})$, and the minimal non-zero eigenvalue of H_0 is strictly greater than $1/3$ according to Theorem 4, it suffices to find a symmetric ΔH that satisfies

$$\langle B_\alpha, \Delta H\rangle = e_\alpha, |\alpha| \le 4$$

and $\|\Delta H\|$ is very small, much smaller than $\frac{1}{3}$.

In the following, we will complete the argument by showing that the solution $\Delta\hat{H}$ to

$$\begin{aligned} &\text{minimize } \|\Delta H\|_F \\ &\text{subject to } \langle B_\alpha, \Delta H\rangle = e_\alpha, |\alpha| \le 4. \end{aligned} \tag{38}$$

satisfies $\|\Delta H\|_F \le 0.0048$ under the conditions of $\|P'P - I\| \le 0.0016$, implying that $\Delta\bar{H} = \frac{1}{2}(\Delta\hat{H} + \Delta\hat{H}')$ is the desired ΔH.

We first estimate $\|e\|_\infty$. Note

$$\begin{aligned} q(z) - q_0(z) &= \sum_{k=1}^r [3(z'P'Pe_k) - 2z_k]z_k^2 - \sum_{k=1}^r z_k^3 \\ &= 3\sum_{k=1}^r [(z'P'Pe_k) - z_k]z_k^2 \end{aligned}$$

which involves only third order monomials of the form $z_k^3, k = 1, \ldots, r$, $z_k^2 z_j : k = 1, \ldots, r; j = r+1, \ldots, n$, and $z_k^2 z_j : j \ne k = 1, \ldots, r$. The coefficient for z_k^3 is $3(1 - e_k'P'Pe_k) = 0$, and the coefficient for $z_k^2 z_j$ is $-3e_j'P'Pe_k$. When $k = 1, \ldots, r; j = r+1, \ldots, n$, $-3e_j'P'Pe_k = 0$ due to the construction of P; when $j \ne k = 1, \ldots, r$, $-3e_j'P'Pe_k$ is non-zero. Therefore, we get

$$\|b - b^0\|_\infty \le 3 \max_{1\le j\ne k\le r} |e_j'P'Pe_k| \le 3\epsilon.$$

We next bound

$$\begin{aligned} |\langle C_\alpha, G_0\rangle - \langle C^0_\alpha, G_0\rangle| &= |\langle C_\alpha - C^0_\alpha, G_0\rangle| \\ &= \frac{3}{2}|\operatorname{trace}(C_\alpha - C_\alpha)| \end{aligned}$$

To control $\operatorname{trace}(C_\alpha - C^0_\alpha)$, we write

$$\sum_{|\alpha|\le 4} (C_\alpha - C^0_\alpha)z^\alpha = \nu_1(z)\nu_1(z)'[z'(P'P - I)z]$$

Taking trace on both sides gives

$$\begin{aligned} &\sum_{|\alpha|\le 4} \operatorname{trace}(C_\alpha - C^0_\alpha)z^\alpha \\ &= \operatorname{trace}(\nu_1(z)\nu_1(z)')[z'(P'P - I)z] \\ &= \left(1 + \sum_{i=1}^r z_i^2\right)[z'(P'P - I)z] \\ &= \left(1 + \sum_{i=1}^r z_i^2\right) \sum_{1\le j\ne k\le r} (P'P - I)_{jk} z_j z_k \end{aligned}$$

Since the diagonal of $P'P - I$ constitutes of zeros, the only monomials that have non-zero coefficients are of the forms $z_i^2 z_j z_k$ with $1 \le i \le r, 1 \le j \ne k \le r$, and $z_j z_k$ with $1 \le j \ne k \le r$. To compute the coefficients for $z_i^2 z_j z_k$, we consider two separate cases. When $j = i$, the coefficient for the term $z_i^3 z_k$ is $(P'P - I)_{ik} + (P'P - I)_{ki}$. When $j \ne i$ and $k \ne i$, the coefficient for the term $z_i^2 z_j z_k$ is $(P'P - I)_{jk} + (P'P - I)_{kj}$. In both cases, we can bound the absolute value of the coefficient by

$$\max_{j\ne k} |(P'P - I)_{jk} + (P'P - I)_{kj}| \le 2\epsilon.$$

A similar argument shows that the coefficients for $z_j z_k$ with $1 \le j \ne k \le r$ are also bounded by 2ϵ. Hence, we get

$$\max_{|\alpha|\le 4} |\operatorname{trace}(C_\alpha - C^0_\alpha)| \le 2\epsilon.$$

Since the components of $b_\alpha - b_\alpha^0$ and $\langle C_\alpha - C_\alpha^0, G_0\rangle$ attain non-zero at different αs, we conclude that

$$\|e\|_\infty \le 3\epsilon.$$

Denote by $S \in \mathbb{R}^{|\mathbb{N}_4^n|\times|\mathbb{N}_2^n|^2}$ the matrix whose αth row is $\mathrm{vec}(B_\alpha)^T$ for $|\alpha| \le 4$. The solution to (38) is given by $\mathrm{vec}(\Delta H) = S^\dagger e$ where we used $\dagger$ to represent pseudo-inverse.

We want to control

$$\|S^\dagger\|_{\infty,2} = \max_\alpha \|[S^\dagger]_\alpha\|_2$$

where $[S^\dagger]_\alpha$ is the αth row of $S^\dagger$. Note S has orthogonal rows, and each $\mathrm{vec}(B_\alpha)$ is composed of zeros and ones, and the ones indicate where the monomial z^α locates in $\nu_2(z)\nu_2(z)'$. As a consequence, we have SS' is a diagonal matrix with the diagonal element d_α counts the number of appearances of z^α in $\nu_2(z)\nu_2(z)'$, which is always greater than or equal to 1. Therefore, we get

$$\begin{aligned}\|S^\dagger\|_{\infty,2} &= \|S'(SS')^{-1}\|_{\infty,2}\\ &\le \max_\beta \|[S']_\beta \,\mathrm{diag}(d^{-1})\|_2\\ &\le \max_\beta \|S^\beta\|_2\end{aligned}$$

where S^β represents that βth column of S. The index β indexes the rows and columns of $\nu_2(z)\nu_2(z)'$. Each column of S consists of zeros and a single one, with the latter representing which z^α is at the entry of $\nu_2(z)\nu_2(z)'$ specified by the column index β. Therefore, we obtain

$$\|S^\dagger\|_{\infty,2} \le \max_\beta \|S^\beta\|_2 \le 1$$

We conclude that

$$\begin{aligned}\|\Delta\bar{H}\|_F &\le \|\Delta\hat{H}\|_F\\ &= \|S^\dagger e\|_2 \le \|S^\dagger\|_{\infty,2}\|e\|_\infty\\ &\le 3\epsilon\\ &\le 0.0048\end{aligned}$$

for $\epsilon \le 0.0016$. Therefore, the minimal non-zero eigenvalue of the Gram matrix $H_1 = H_0 + \Delta\bar{H}$ is lower bounded by $1/3 - 0.0048 > 0$.

So far we have showed that $q(z)$ is a SOS modulo the ellipsoid $\{z : z'P'Pz = 1\}$. To prove Theorem 1, we need to map z back into x, and make sure the after the mapping, the new Gram matrix still have rank $|\mathbb{N}_2^n| - r$. It suffices to show that the change of basis transformation on $\mathbb{R}^n$ that maps x to z induces a well-conditioned transformation between $\nu_2(x)$ and $\nu_2(z)$. This is given in Lemma 1 developed in the next section. Therefore, we have completed the proof of Theorem 1.

7.6. Change of Basis Formula

Consider two n-dimensional variables x and z linked by a change of basis transformation $x = Pz$ or $z = P^{-1}x$. We aim at finding the matrix J that expresses $\nu_2(z)$ in terms of $\nu_2(x)$, *i.e.*,

$$\nu_2(z) = \nu_2(P^{-1}x) = J\nu_2(x).$$

The transform J is well defined since a polynomial of degree k in z is always transformed into a polynomial of degree k in x under $z = P^{-1}x$. It's easy to see J has the form:

$$J = \begin{bmatrix} 1 & & \\ & P^{-1} & \\ & & J_2 \end{bmatrix}$$

where J_2 expresses all quadratic monomials of z in terms of quadratic monomials of x. To find J_2, we rewrite the relationship $zz' = P^{-1}xx'P^{-1'}$ as

$$\mathrm{vec}(zz') = P^{-1} \otimes_K P^{-1}\,\mathrm{vec}(xx')$$

where the subscript in the Kronecker product notation $\otimes_K$ is used to distinguish it from the tensor product notation $\otimes$, and $\mathrm{vec}(\cdot)$ vectorizes a matrix column-wise. Denote by $\bar{\nu}_2(x)$ all unique quadratic monomials in x, and write $\bar{\nu}_2(x) = \Pi\,\mathrm{vec}(xx')$, where Π is the matrix that picks and averages the duplicated quadratic monomials of x in $\mathrm{vec}(xx')$. One can verify that $\mathrm{vec}(xx') = \Pi^\dagger\bar{\nu}_2(x)$, and the smallest and largest singular values of Π are $\frac{1}{\sqrt{2}}$ and 1 respectively. Consequently, we have

$$\bar{\nu}_2(z) = \Pi\,\mathrm{vec}(zz') = \Pi\left(P^{-1} \otimes_K P^{-1}\right)\Pi^\dagger\bar{\nu}_2(x),$$

or equivalently $J_2 = \Pi P^{-1}\otimes_K P^{-1}\Pi^\dagger$. So if $\|PP' - I\| \le \epsilon$, the singular values of J_2 are lower bounded and upper bounded by $\frac{1}{\sqrt{2}}\frac{1}{1+\epsilon}$ and $\frac{\sqrt{2}}{1-\epsilon}$ respectively. The same holds for J. We summarize these results in the following lemma.

Lemma 1. *The change of basis transformation $x = Pz$ induces a linear transformation between $\nu_2(z)$ and $\nu_2(x)$*

$$\nu_2(z) = J\nu_2(x) = \begin{bmatrix} 1 & & \\ & P^{-1} & \\ & & \Pi\left(P^{-1} \otimes_K P^{-1}\right)\Pi^\dagger \end{bmatrix}\nu_2(x)$$

such that the singular values of J fall into the interval $[\frac{1}{\sqrt{2}}\frac{1}{1+\epsilon}, \frac{\sqrt{2}}{1-\epsilon}]$.