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On Optimal Designs for a d-Cube

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Abstract

We show that for the d-cube $K=[-1,1]^d\subset\mathbb{R}^d$, there is for degree 2 a symmetric optimal design supported on the discrete set consisting of the vertices, the edge midpoints and the origin with cardinality $2^d+d2^{d-1}+1$. In general there is a continuum of possible optimal designs with, however, a support of larger cardinality. We also consider numerically the degree three case for the square $[-1,1]\subset\mathbb{R}^2$. Our calculations indicate that there is an optimal measure supported on 16 points but that these do not form a regular grid.

1 Introduction

Optimal Experimental Design has a rich history within Statistics. The interested reader may consult the classical book of Karlin and Studden [5] (especially Chapter X) and the more recent monograph of Dette and Studden [4].

Here we first give a brief introduction to the general theory and then will specialize to the case when the design space is the cube $K=[-1,1]^d\subset\mathbb{R}^d$.

Consider the design space $K\subset\mathbb{R}^d$, compact. We let $\mathcal{P}_s(K)$, denote the set of polynomials of degree s restricted to K and set $n:=\dim(\mathcal{P}_s(K))$.

We may write any $p\in\mathcal{P}_s(K)$ in the form

$$p=\sum_{k=1}^n\theta_k p_k$$

where $\mathcal{B}_s:=\{p_1,p_2,\ldots,p_n\}$ is a basis for $\mathcal{P}_s(K)$.

Suppose now that we observe the values of a particular $p\in\mathcal{P}_s(K)$ at a set of $m\ge n$ points $X:=\{x_j\,:\,1\le j\le m\}\subset K$ with some random errors, i.e., we observe

$$y_j=p(x_j)+\epsilon_j,\quad 1\le j\le m$$

where we assume that the errors $\epsilon_j\sim N(0,\sigma)$ are independent. In matrix form this becomes

$$\mathbf{y}=V_s\boldsymbol{\theta}+\boldsymbol{\epsilon}$$

where $\mathbf{y},\boldsymbol{\epsilon}\in\mathbb{R}^m$, $\boldsymbol{\theta}\in\mathbb{R}^n$, and

$$V_s=\begin{bmatrix} p_1(x_1) & p_2(x_1) & \cdot\ \cdot\ \cdot & p_n(x_1)\\ p_1(x_2) & p_2(x_2) & \cdot\ \cdot\ \cdot & p_n(x_2)\\ \cdot & & & \cdot\\ \cdot & & & \cdot\\ \cdot & & & \cdot\\ \cdot & & & \cdot\\ \cdot & & & \cdot\\ p_1(x_m) & p_2(x_m) & \cdot\ \cdot\ \cdot & p_n(x_m)\end{bmatrix}\in\mathbb{R}^{m\times n}$$

is the associated Vandermonde matrix.

Our assumption on the error vector $\boldsymbol{\epsilon}$ means that

$$\mathrm{cov}(\boldsymbol{\epsilon})=\sigma^2 I_m\in\mathbb{R}^{m\times m}.$$

Now, the least squares estimate of $\boldsymbol{\theta}$ is

$$\widehat{\boldsymbol{\theta}}:=(V_s^tV_s)^{-1}V_s^t\mathbf{y}$$

and we may compute its covariance matrix

$$\mathrm{cov}(\widehat{\boldsymbol{\theta}})=\sigma^2(V_s^tV_s)^{-1}.$$

Hence the confidence region of level t for θ is the set

$$\begin{aligned} &\{\boldsymbol{\theta}\in\mathbb{R}^n\,:\,(\boldsymbol{\theta}-\widehat{\boldsymbol{\theta}})^t[\mathrm{cov}(\widehat{\boldsymbol{\theta}})]^{-1}(\boldsymbol{\theta}-\widehat{\boldsymbol{\theta}})\le t\}\\ = &\{\boldsymbol{\theta}\in\mathbb{R}^n\,:\,\sigma^{-2}(\boldsymbol{\theta}-\widehat{\boldsymbol{\theta}})^t(V_s^tV_s)(\boldsymbol{\theta}-\widehat{\boldsymbol{\theta}})\le t\}.\end{aligned}$$

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The volume of such a set is proportional to $1/\sqrt{\det(V_s^t V_s)}$ and hence maximizing the $\det(V_s^t V_s)$ is equivalent to choosing the observation points $x_i \in K$ so as to have the most "concentrated" confidence region for the parameter to be estimated.

Note however that the entries of $\frac{1}{m} V_s^t V_s$ are the discrete inner products of the p_i with respect to the measure

$$\mu_X = \frac{1}{m}\sum_{k=1}^{m} \delta_{x_k}. \tag{1}$$

More specifically,

$$\frac{1}{m} V_s^t V_s = M_s(\mu_X)$$

where

$$M_s(\mu) := \left[\int_K p_i(x) p_j(x) d\mu\right] \in \mathbb{R}^{n\times n} \tag{2}$$

is the Moment, or Gram, matrix of the polynomials p_i with respect to the measure μ.

In general we may consider arbitrary probability measures on K, setting

$$\mathcal{M}(K) := \{\mu : \mu \text{ is a probability measure on } K\}.$$

Definition 1.1. A probability measure (or design) $\mu \in \mathcal{M}(K)$ is said to be a D–optimal measure of degree s if it has the property that

$$\det(M_s(\mu)) \ge \det(M_s(\xi)),\ \ \forall \xi \in \mathcal{M}(K).$$

There is also a second statistical interpretation of D–optimal measures. If we set

$$\mathbf{p}(x) = \begin{bmatrix} p_1(x) \\ p_2(x) \\ \cdot \\ \cdot \\ p_n(x) \end{bmatrix} \in \mathbb{R}^n \tag{3}$$

then the least squares estimate of the observed polynomial is

$$\mathbf{p}^t(x)\widehat{\boldsymbol{\theta}}.$$

We may compute its variance to be

$$\begin{aligned} \operatorname{var}(\mathbf{p}^t(x)\widehat{\boldsymbol{\theta}}) &= \sigma^2 \mathbf{p}^t(x)(V_s^t V_s)^{-1}\mathbf{p}(x) \\ &= \frac{1}{m}\sigma^2 \mathbf{p}^t(x)(M_s(\mu_X))^{-1}\mathbf{p}(x) \end{aligned} \tag{4}$$

where μ_X is again given by (1).

In the Statistics literature (see e.g. [4]) one usually denotes, for $\mu \in \mathcal{M}(K)$,

$$G_s(\mu) = \max_{x\in K} \mathbf{p}^t(x)(M_s(\mu))^{-1}\mathbf{p}(x).$$

Definition 1.2. A probability measure $\mu \in \mathcal{M}(K)$ is said to be a G–optimal measure of degree n if it has the property that

$$G_s(\mu) \le G_s(\xi),\ \ \forall \xi \in \mathcal{M}(K).$$

It follows from (4) that a G–optimal measure minimizes the maximum variance of the estimate of the observed polynomial.

The remarkable Kiefer-Wolfowitz equivalence theorem states that these two notions of optimality are equivalent.

Theorem 1.3. (Kiefer and Wolfowitz [6]) A measure $\mu \in \mathcal{M}(K)$ with $\det(M_s(\mu)) \neq 0$ is G–optimal of degree s if and only if $G_s(\mu) = n$, if and only if it is D–optimal of degree s.

The G-optimality criterion has also an interpretation in terms of the polynomials orthogonal on K with respect to the measure μ. To see this, suppose that $M_s(\mu)$ is non-singular and note that then the matrix $M_s(\mu)$, being a Gram matrix, is positive definite. It's inverse is then also positive definite and hence has a Cholesky factorization $(M_s(\mu))^{-1} = L_s(\mu)^t L_s(\mu)$ where $L_s(\mu) \in \mathbb{R}^{n\times n}$ is lower triangular. It follows that we may write

$$\begin{aligned} \mathbf{p}^t(x)(M_s(\mu))^{-1}\mathbf{p}(x) &= \mathbf{p}^t(x) L_s(\mu)^t L_s(\mu)\mathbf{p}(x) \\ &= (L_s(\mu)\mathbf{p}(x))^t (L_s(\mu)\mathbf{p}(x)) \\ &= \sum_{j=1}^{n} q_j^2(x) \end{aligned}$$

where

$$\mathbf{q} := \begin{bmatrix} q_1 \\ q_2 \\ \cdot \\ \cdot \\ q_n \end{bmatrix} := L_s(\mu) \begin{bmatrix} p_1 \\ p_2 \\ \cdot \\ \cdot \\ p_n \end{bmatrix}.$$

The polynomials q_j are in fact orthonormal as

$$\begin{aligned}\left[\int_K q_i(x)q_j(x)d\mu(x)\right] &= \int_K \mathbf{q}(x)\mathbf{q}(x)^t d\mu(x)\\ &= \int_K (L_s(\mu)\mathbf{p}(x))(L_s(\mu)\mathbf{p}(x))^t d\mu(x)\\ &= \int_K L_s(\mu)\mathbf{p}(x)\mathbf{p}(x)^t L_s(\mu)^t d\mu(x)\\ &= L_s(\mu)\left(\int_K \mathbf{p}(x)\mathbf{p}(x)^t d\mu(x)\right)L_s(\mu)^t\\ &= (L_s(\mu)M_s(\mu)L_s(\mu)^t)^t\\ &= I.\end{aligned}$$

Indeed, since $L_s(\mu)$ is lower triangular, the q_j are the just the result of applying the Gram-Schmidt orthonormalization procedure to the p_j.

Now note that

$$K_s^\mu(x) := \sum_{j=1}^n q_j^2(x) \tag{5}$$

is the diagonal of the reproducing kernel for $\mathcal{P}_s(K)$ (with respect to the measure μ) and is sometimes also called the (reciprocal of the) Christoffel function. It plays an important role in the theory of Orthogonal Polynomials.

Hence

$$\mathrm{var}(\mathbf{p}^t(x)\widehat{\boldsymbol{\theta}}) = \frac{1}{m}\sigma^2 K_s^\mu(x) \tag{6}$$

and the experiment that minimizes the maximum variance of the estimate of the observed polynomial is exactly the one that minimizes the maximum of K_s^μ. For this optimal measure

$$\max_{x\in K} K_s^\mu(x) = n.$$

We also remark that optimal designs, in the case when the cardinality of the support is equal to the dimension of the space of polynomials $\mathcal{P}_s(K)$, is closely related to near optimal points for polynomial interpolation. Indeed, a D-optimal measure in this case would be supported on a so-called set of Fekete points. G-optimality is equivalent to the Fejér condition of minimizing the maximum of the sum of the squares of the Lagrange polynomials. See [1] and [3], for example, for more details.

2 The Cube $K = [-1,1]^d \subset \mathbb{R}^d$

2.1 The degree $s = 1$ case

This is the simplest case, but it already illustrates some of the complexity of the general problem.

Proposition 2.1. For $K = [-1,1]^d \subset \mathbb{R}^d$ an optimal design of degree $s = 1$ is given by the equally weighted probability measure supported on the vertices of the cube, i.e.,

$$\mu = 2^{-d} \sum_{\mathbf{v}\in\{-1,1\}^d} \delta_{\mathbf{v}}.$$

Proof. It is easy to check that the monomials

$$1, x_1, x_2, \cdots, x_d$$

are orthonormal with respect to μ. Hence

$$K_{s=1}^\mu(\mathbf{x}) = 1 + \sum_{j=1}^d x_j^2 \le 1 + d,\ \forall \mathbf{x} \in [-1,1]^d.$$

Moreover $K_1^\mu(\mathbf{v}) = d + 1$ for each vertex $\mathbf{v}$. Consequently

$$\max_{\mathbf{x}\in[-1,1]^d} K_1^\mu(\mathbf{x}) = d + 1 = \dim(\mathcal{P}_1(K))$$

and μ is G-optimal. ■

2.1.1 Hadamard Matrices and Fekete Points

In dimensions d for which there exists a Hadamard matrix of order $n = d + 1$ there are optimal measures with a much smaller of $d + 1$ Fekete points, albeit these points do *not* have the symmetry of the cube.

Definition 2.2. A matrix $H \in \mathbb{R}^{n\times n}$ with entries $H_{ij} \in \pm 1$ and rows and columns orthogonal, i.e.,

$$H_n H_n^t = nI_n$$

is said to be a Hadamard matrix.

Hadamard matrices maximize the (absolute value of the) determinant among all matrices with ±1 entries and hence also for all matrices with entries $|H_{ij}| \le 1$. Hadamard's famous conjecture is that such matrices exist for all n a multiple of 4. This remains a much studied open problem. In particular, Sylvester's construction gives a Hadamard matrix for all n a power of 2, but the existence for many other values of n is also known.

Now suppose that d is such that a Hadmard matrix, H_{d+1}, of dimension $d + 1$ exists. By multiplying on the left and right by appropriate diagonal matrices, we may assume that the first row and first column of H_{d+1} are all 1*s*. We let $X \in \mathbb{R}^{(d+1)\times d}$ be the matrix obtained by removing the first column of H_{d+1}. The $d + 1$ rows of X give the coordinates of a subset of $d + 1$ vertices of the cube $[-1, 1]^d$, and it is these points that we consider. In particular $V_d := H_{d+1}$ is the Vandermonde matrix for these points and the polynomials of degree at most one with basis

$$\{1, x_1, \cdots, x_d\}.$$

Hence, by the definition of Hadamard matrices the points X are such that their associated Vandermonde matrix has determinant as large as possible (in absolute value). Points with this proerty are known as Fekete points.

The associated fundamental Lagrange polynomials are

$$[\ell_1(\mathbf{x}), \cdots, \ell_{d+1}(\mathbf{x})] = [1, \mathbf{x}^t]V_d^{-1} = \frac{1}{d+1}[1, \mathbf{x}^t]V_d^t.$$

They have the property that

$$\begin{aligned}\sum_{i=1}^{d+1} \ell_i^2(\mathbf{x}) &= [\ell_1(\mathbf{x}), \cdots, \ell_{d+1}(\mathbf{x})] \times \begin{bmatrix} \ell_1(\mathbf{x}) \\ \cdot \\ \cdot \\ \ell_{d+1}(\mathbf{x}) \end{bmatrix} \\ &= \frac{1}{(d+1)^2}[1, \mathbf{x}^t]V_d^t V_d \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix} \\ &= \frac{1 + \|\mathbf{x}\|_2^2}{d+1} \le 1\end{aligned}$$

for all $\underset{\sim}{x} \in [-1, 1]^d$.

As shown in [2] this last condition is also sufficient to prove that the points X are Fekete points.

If we take the equally weighted discrete measure

$$\mu_X := \frac{1}{d+1}\sum_{x\in X} \delta_x$$

then the polynomials $p_i := \sqrt{d+1}\,\ell_i$ are orthonormal with respect to μ_X and

$$K_1(\mathbf{x}) = (d+1)\sum_{i=1}^{d+1} \ell_i^2(\mathbf{x}) \le d+1, \;\; \mathbf{x} \in [-1, 1]^d$$

and hence X is G-optimal.

Remark. Such points X form the vertices of a *regular* simplex. As the Vandermonde determinant is a (dimensional) multiple of the volume of this simplex, it is of maximal volume. Also, as the sum of the Lagrange polynomials squared is bounded by 1 on the circumball $B_d := \mathbf{x} \in \mathbb{R}^d \,:\, \|\mathbf{x}\|_2 \le \sqrt{d}$, X is also a Fekete set and μ an optimal measure for B_d. □

Example. For $d = 3$,

$$H_{d+1} = H_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}$$

so that the four points are

$$(1, 1, 1), (-1, 1, -1), (1, -1, -1), (-1, -1, 1).$$

The simplex with these vertices is shown in Figure 1 below.

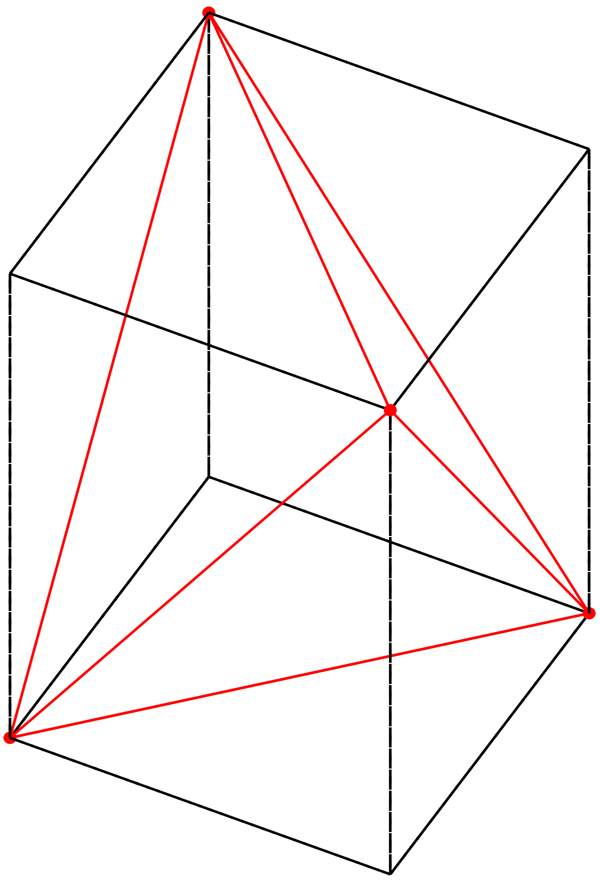

Figure 1: Regular Simplex Inscribed in the Cube

2.2 The degree $s = 2$ case

Consider first the dimension $d = 2$ case, i.e., $K = [-1, 1]^2 \subset \mathbb{R}^2$.

Indeed consider the symmetric measure μ say, supported on the nine points $\{-1, 0, +1\}^2$ with weights

$$\begin{array}{ll} w_2, & \text{at the four vertices, } (\pm 1, \pm 1) \\ w_1, & \text{at the four side midpoints, } (\pm 1, 0), (0, \pm 1) \\ w_0, & \text{at } (0, 0). \end{array}$$

(The index j on w_j counts the number of non-zero components of the corresponding support point). From the symmetry, the Christoffel function at the support points has three different values

$$K_2((1, 1)), K_2((1, -1)), K_2((0, 0)).$$

We proceed to compute these three values. Notice that we may group the monomials of degree at most 2 into three subsets

$$\{1, x_1^2, x_2^2\},\ \{x_1, x_2\}\ \{x_1 x_2\}$$

which are mutually orthogonal., in the sense that a monomial in one set is orthogonal to those of the other sets (but not to those of the same set. Moreover x_1 and x_2 are also mutually orthogonal. Hence to find the orthonormal polynomials of degree 2 we need to only orthonormalize the first group $\{1, x_1^2, x_2^2\}$ and normalize the other three monomials.

Now observe that the required moments

$$\int_K x_1^2 d\mu = \int_K x_2^2 d\mu = \int_K x_1^4 d\mu = \int_K x_2^4 d\mu = a, \text{ say}$$

and let

$$b = \int_K x_1^2 x_2^2 d\mu.$$

With this notation the Gram matrix for $\{1, x_1^2, x_2^2\}$ is

$$G_2 := \begin{bmatrix} 1 & a & a \\ a & a & b \\ a & b & a \end{bmatrix}.$$

It follows that

$$K_2(\mathbf{x}) = [1\ x_1^2\ x_2^2] G_2^{-1} \begin{bmatrix} 1 \\ x_1^2 \\ x_2^2 \end{bmatrix} + \frac{x_1^2}{a} + \frac{x_2^2}{a} + \frac{x_1^2 x_2^2}{b}. \quad (7)$$

In particular, one may calculate

$$K_2((0,0)) = \frac{a+b}{a+b-2a^2}.$$

For an optimal measure it is required that $K_2((0,0)) = 6$, i.e.,

$$\frac{a+b}{a+b-2a^2} = 6 \iff 12a^2 - 5(a+b) = 0.$$

Let us denote

$$p_1(a,b) = 12a^2 - 5(a+b). \quad (8)$$

We may also calculate

$$K_2((1,1)) = \frac{2+b-3a}{a+b-2a^2} + \frac{2}{a} + \frac{1}{b}.$$

Then

$$K_2((1,1)) = 6 \iff 12a^3b - 2a^3 - 13a^2b + a^2 - 5ab^2 + 5ab + 2b^2 = 0$$

We denote

$$p_2(a,b) := 12a^3b - 2a^3 - 13a^2 * b + a^2 - 5ab^2 + 5ab + 2b^2. \quad (9)$$

Finally, we calculate

$$K_2((1,0)) = \frac{a + 2ab - 2a^2 - b^2}{a+b-2a^2} + \frac{1}{a}.$$

It is necessary that also this equals the dimension, 6, i.e.,

$$K_2((1,0)) = 6 \iff 12a^4 - 12a^3b - 10a^3 + 4a^2b + 2a^2 + 5ab^2 - b^2 = 0.$$

We denote

$$p_3(a,b) := 12a^4 - 12a^3b - 10a^3 + 4a^2b + 2a^2 + 5ab^2 - b^2. \quad (10)$$

For an optimal measure it is necessary that $p_1(a,b) = p_2(a,b) = p_3(a,b) = 0$. However, one may verify that

$$p_3 = \frac{1}{2}a(2a-b-1)p_1 - \frac{1}{2}p_2$$

and hence the third equation is redundant.

Then, using Matlab's Symbolic Toolbox system we find that a Groebner basis for the ideal generatted by p_1 and p_2 is

$$\{9216b^3 - 5628b^2 + 65b + 65a,\ 768b^4 - 405b^3 - 25b^2\}.$$

It follows that b is a solution of

$$768b^4 - 405b^3 - 25b^2 = b^2(768b^2 - 405b - 25) = 0,$$

i.e.,

$$b = \frac{405 \pm 65\sqrt{57}}{1536}.$$

But $b = \int_K x_1^2 x_2^2 d\mu$ must be positive and hence

$$b = \frac{405 + 65\sqrt{57}}{1536}.$$

Then, from the first equation of the Groebner basis we obtain

$$a = \frac{9216b^3 - 5628b^2 + 65b}{65} = \frac{105 + 5\sqrt{57}}{192}.$$

Now, in terms of the weights

$$b=\int_K x_1^2x_2^2d\mu=4w_2$$

and

$$a=\int_K x_1^2d\mu=4w_2+2w_1$$

and hence

$$w_2=\frac{b}{4}=\frac{405+65\sqrt{57}}{6144}$$

while

$$w_1=(a-4w_2)/2=(a-b)/2=\frac{435-25\sqrt{57}}{3072}.$$

It turns out that these weights are also sufficient to be an optimal measure. Indeed consider the measure supported on the nine points $\{-1,0,+1\}^2$ with the above weights

$$\begin{aligned} w_2 &= \frac{405+65\sqrt{57}}{6144} \text{ at the four vertices}\\ w_1 &= \frac{435-25\sqrt{57}}{3072} \text{ at the four side midpoints}\\ w_0 &= 1-4w_2-4w_1=\frac{87-5\sqrt{57}}{512} \text{ at } (0,0). \end{aligned}$$

Proposition 2.3. The above discrete measure is an optimal design of degree 2 for the square $[-1,1]^2$.

Proof. With again the aid of Matlab's Symbolic Toolbox one can show that the Christoffel function for this measure is

$$K_2(\mathbf{x})=6-C\{x_1^2(1-x_1^2)+x_2^2(1-x_2^2)\}$$

where

$$C=\frac{42-2\sqrt{57}}{5}>0.$$

Hence

$$K_2(\mathbf{x})\le 6=\dim(\mathcal{P}_2(K)),\ \mathbf{x}\in[-1,1]^2$$

and $K_2(\mathbf{x})=6$ at each of the points of the support of μ. It follows that μ is G-optimal. ■

Remark. The support of the optimal measure is a product set. However, the measure itself is *not* a tensor product measure. Indeed if it were the tensor product of the (symmetric) univariate measure

$$d\nu=\omega_1\delta_{-1}+\omega_0\delta_0+\omega_1\delta_{+1}$$

then necessarily we would have

$$w_2=\omega_1^2,\ w_1=\omega_0\omega_1,\ w_0=\omega_0^2$$

and hence $w_2w_0=w_1^2$, which can be confirmed to *not* be the case. ■

In general dimension d we look for an optimal measure supported on (a subset of) the points

$$X:=\{-1,0,1\}^d$$

with weights w_j, $0\le j\le d$, on

$$X_j:=\{\mathbf{c}\in X\ :\ \sum_{i=1}^d |c_i|=j\}.$$

For example X_d is the set of vertices of the cube, X_{d-1} is the set of edge midpoints, and X_0 is the singleton of the origin. It is a standard fact that

$$\#(X_j)=\binom{d}{j}2^j. \tag{11}$$

Specifically, we consider measures of the form

$$\mu=\sum_{j=0}^d w_j\sum_{\mathbf{c}\in X_j}\delta_{\mathbf{c}}. \tag{12}$$

Again, there are only two possible non-zero moments.

Lemma 2.4. For a measure μ of the form (12) we have for $1 \le k \le d$,

$$\int_K x_k^2 d\mu = \int_K x_k^4 d\mu = \sum_{j=0}^{d-1} \binom{d-1}{j} 2^{j+1} w_{j+1}$$

and for $1 \le i \ne k \le d$,

$$\int_K x_i^2 x_k^2 d\mu = \sum_{j=0}^{d-2} \binom{d-2}{j} 2^{j+2} w_{j+2}.$$

Proof. First note that $\int_K x_k^4 d\mu = \int_K x_k^2 d\mu$ as for each point in the support $\mathbf{x} \in X$, $x_k^2 = x_k^4$. Then, by symmetry,

$$\begin{aligned}
\int_K x_k^2 d\mu &= \frac{1}{d} \int_K \Big(\sum_{k=1}^{d} x_k^2\Big) d\mu \\
&= \frac{1}{d} \sum_{j=0}^{d} \{w_j \times j \times \#(X_j)\} \\
&= \frac{1}{d} \sum_{j=0}^{d} j \binom{d}{j} 2^j w_j \\
&= \frac{1}{d} \sum_{j=1}^{d} j \binom{d}{j} 2^j w_j \\
&= \sum_{j=1}^{d} \frac{(d-1)!}{(d-j)!(j-1)!} 2^j w_j \\
&= \sum_{j=0}^{d-1} \binom{d-1}{j} 2^{j+1} w_{j+1}, \quad (j' := j-1).
\end{aligned}$$

Similarly,

$$\begin{aligned}
\int_K x_i^2 x_k^2 d\mu &= \frac{1}{d(d-1)} \int_K \Big(\sum_{1 \le i \ne k \le d} x_i^2 x_k^2\Big) d\mu \\
&= \frac{1}{d(d-1)} \int_K \Big(\sum_{i=1}^{d} x_i^2\Big)^2 - \sum_{i=1}^{d} x_i^4 \, d\mu \\
&= \frac{1}{d(d-1)} \sum_{j=0}^{d} w_j \times (j^2 - j) \times \#(X_j) \\
&= \frac{1}{d(d-1)} \sum_{j=0}^{d} j(j-1) \binom{d}{j} 2^j w_j \\
&= \sum_{j=0}^{d-2} \binom{d-2}{j} 2^{j+2} w_{j+2}
\end{aligned}$$

after changing indices, $j' := j-2$. ■

Again, for such measures we may divide the monomials in into mutually orthogonal groups

$$\mathcal{P}_2(K) = \{1, x_1^2, \cdots, x_d^2\} \cup \{x_1, x_2, \cdots, x_d\} \cup \{x_i x_k\}_{1 \le i < k \le d}.$$

Moreover, the monomials $\{x_1, x_2, \cdots, x_d\}$ are orthogonal among themselves, as are the monomials $\{x_i x_k\}_{1 \le i < k \le d}$.

To orthogonalize the first group, let G_d be the associated Gram matrix. Setting $a = \int_K x_k^2 d\mu = \int_K x_k^4 d\mu$ and $b = \int_K x_i^2 x_k^2 d\mu$, $i \ne k$, we easily see that

$$G_d = \begin{bmatrix} 1 & a & a & \cdot & \cdot & a \\ a & a & b & \cdot & \cdot & b \\ \cdot & b & a & b & \cdot & b \\ \cdot & b & b & a & b & \cdot \\ \cdot & & & & & b \\ a & b & \cdot & \cdot & b & a \end{bmatrix} \in \mathbb{R}^{(d+1)\times(d+1)}. \tag{13}$$

Then

$$K_2(\mathbf{x}) = [1\, x_1 \cdots x_d] G_d^{-1} \begin{bmatrix} 1 \\ x_1 \\ \cdot \\ \cdot \\ x_d \end{bmatrix} + \frac{1}{a} \sum_{j=1}^{d} x_j^2 + \frac{1}{b} \sum_{i<k} x_i^2 x_k^2. \tag{14}$$

Lemma 2.5. In case $D := (a-b)(a+(d-1)b-da^2) \neq 0$,

$$G_d^{-1} = \frac{1}{D}\begin{bmatrix} Y & A & A & \cdot & \cdot & A \\ A & C & B & \cdot & \cdot & B \\ \cdot & B & C & B & \cdot & B \\ \cdot & B & B & C & B & \cdot \\ \cdot & & & & & B \\ A & B & \cdot & \cdot & B & C \end{bmatrix} \in \mathbb{R}^{(d+1)\times(d+1)}$$

where

$$\begin{array}{rcl} Y &=& (a-b)(a+(d-1)b), \\ A &=& -a(a-b), \\ B &=& a^2-b, \\ C &=& a+(d-2)b-(d-1)a^2. \end{array}$$

Proof. We compute $G_dG_d^{-1}$ and verify that we obtain the identity. For the first row of G_d times the first column of G_d^{-1} we calculate

$$\begin{array}{rcl} [1\ a\ a\ \cdots\ a]\begin{bmatrix} Y \\ A \\ A \\ \cdot \\ \cdot \\ A \end{bmatrix} &=& Y+daA \\ &=& (a-b)(a+(d-1)b)+da(-a(a-b)) \\ &=& (a-b)(a+(d-1)b-da^2) \\ &=& D \end{array}$$

and hence the $(1,1)$ entry of the product is indeed 1.

For the first row of G_d times column j, $j \geq 2$, we calculate

$$\begin{array}{rcl} [1\ a\ a\ \cdots\ a]\begin{bmatrix} A \\ B \\ \cdot \\ B \\ C \\ B \\ \cdot \\ B \end{bmatrix} &=& A+a((d-1)B+C) \\ &=& -a(a-b)+a((d-1)(a^2-b) \\ && \quad +(a+(d-2)b-(d-1)a^2)) \\ &=& -a(a-b)+a(0\times a^2-b+a) \\ &=& 0. \end{array}$$

Further, for the ith row, $i \geq 2$, of G_d times the first column of G_d^{-1},

$$\begin{array}{rl} & [a\ b\ \cdots\ b\ a\ b\ \cdots\ b]\begin{bmatrix} Y \\ A \\ A \\ \cdot \\ \cdot \\ A \end{bmatrix} \\ = & aY+A((d-1)b+a) \\ = & a(a-b)(a+(d-1)b)-a(a-b)((d-1)b+a) \\ = & ((d-a)b+a)(a(a-b)-a(a-b)) \\ = & 0. \end{array}$$

Next, for the ith row, $i \geq 2$, times the ith column

$$\begin{array}{rl} & [a\ b\ \cdots\ b\ a\ b\ \cdots\ b]\begin{bmatrix} A \\ B \\ \cdot \\ B \\ C \\ B \\ \cdot \\ B \end{bmatrix} \\ = & aA+(d-1)bB+aC \end{array}$$

$$
\begin{array}{rl}
= & -a^2(a-b)+(d-1)b(a^2-b)+a(a+(d-2)b-(d-1)a^2) \\
= & -a^2(a-b)+\{(d-1)a^2b-(d-1)b^2+a^2+(d-2)ab-(d-a)a^3\} \\
= & -a^2(a-b)+(a-b)(a-b+d(b-a^2)+a^2) \\
= & (a-b)(a+(d-1)b-da^2) \\
= & D.
\end{array}
$$

Finally, for the ith row, $i\geq 2$, times the jth column, $i\neq j\geq 2$,

$$
\begin{array}{rl}
& [a\ b\ \cdots\ b\ a\ b\ \cdots\ b]\begin{bmatrix} A \\ B \\ \cdot \\ B \\ C \\ B \\ \cdot \\ B \end{bmatrix} \\
= & aA+bC+aB+(d-2)bB \\
= & -a^2(a-b)+b(a+(d-2)b-(d-1)a^2)+a(a^2-b)+(d-2)b(a^-b) \\
= & 0
\end{array}
$$

after expansion. ■

It follows then from (14) that (for $D\neq 0$)

$$
\begin{aligned}
K_2(\mathbf{x}) &= \frac{1}{D}\Big\{Y+2A\sum_{j=1}^d x_j^2+C\sum_{j=1}^d x_j^4+2B\sum_{1\leq j<k\leq d} x_j^2x_k^2\Big\} \\
&\quad +\frac{1}{a}\sum_{j=1}^d x_j^2+\frac{1}{b}\sum_{1\leq j<k\leq d} x_j^2x_k^2. \qquad (15)
\end{aligned}
$$

An optimal measure (12) supported on the set X would be such that

$$K_2(\mathbf{x})=\dim(\mathcal{P}_2(K))=\binom{d+2}{2},\ \forall \mathbf{x}\in X.$$

There being only two moments a,b to be determined, we have a very over determined system of conditions. Based on the $d=2$ experience we first consider the two conditions

$$
\begin{aligned}
K_2((0,\cdots,0)) &= \binom{d+2}{2}, \\
K_2((1,\cdots,1)) &= \binom{d+2}{2}.
\end{aligned}
$$

Now, assuming that $D\neq 0$, from (15) it follows that

$$
\begin{array}{rl}
& K_2((0,\cdots,0))=\binom{d+2}{2} \\
\iff & \dfrac{Y}{D}=\binom{d+2}{2} \\
\iff & \dfrac{a+(d-1)b}{a+(d-1)b-da^2}=\binom{d+2}{2} \\
\iff & a+(d-1)b-\binom{d+2}{2}(a+(d-1)b-da^2)=0 \\
\iff & 2(a+(d-1)b)-(d+2)(d+1)(a+(d-1)b-da^2)=0 \\
\iff & d(d+3)a+d(d-1)(d+3)b-d(d+1)(d+2)a^2=0 \\
\iff & (d+3)a+(d-1)(d+3)b-(d+1)(d+2)a^2=0. \qquad (16)
\end{array}
$$

Secondly, again from (15), while suppressing some of the elementary algebraic details,

$$
\begin{array}{rl}
& K_2((1,\cdots,1))=\binom{d+2}{2} \\
\iff & \dfrac{Y+2dA+dC+2B\binom{d}{2}}{D}+\dfrac{d}{a}+\dfrac{1}{b}\binom{d}{2}=\binom{d+2}{2} \\
\iff & \dfrac{(a-b)(-(2d-1)a+(d-1)b+d)}{(a-b)(a+(d-1)b-da^2)}+\dfrac{d}{a}+\dfrac{1}{b}\binom{d}{2}=\binom{d+2}{2} \\
\iff & \dfrac{-(2d-1)a+(d-1)b+d}{a+(d-1)b-da^2}+\dfrac{d}{a}+\dfrac{1}{b}\binom{d}{2}=\binom{d+2}{2}
\end{array}
$$

$$\iff \quad (-(2d-1)a+(d-1)b+d) \\ +(a+(d-1)b-da^2)\left(\frac{d}{a}+\frac{1}{b}\binom{d}{2}-\binom{d+2}{2}\right)=0. \tag{17}$$

Now (16) is linear in b and hence we may solve

$$b=\frac{(d+1)(d+2)a^2-(d+3)a}{(d-1)(d+3)}. \tag{18}$$

This may be substituted back into (17) to obtain, after some amount of elementary algebra,

$$2(d+1)(d+2)^2a^2-(d+3)(2d^2+3d+7)a+(d+3)^2=0 \tag{19}$$

from which we obtain

$$a=\frac{(d+3)}{4(d+1)(d+2)^2}\left((2d^2+3d+7)+(d-1)\sqrt{4d^2+12d+17}\right) \tag{20}$$

where we take the $+$ in the quadratic equation as the $-$ results in a negative value for b.

Substituing the vallue of a (20) into (18) results in (after some elementary algebra)

$$b=\frac{d+3}{8(d+1)(d+2)^3}\left((4d^3+8d^2+11d-5)+(2d^2+d+3)\sqrt{4d^2+12d+17}\right). \tag{21}$$

Lemma 2.6. For a,b given by (20) and (21), respectively, the value of $D=(a-b)(a+(d-1)b-da^2)>0$.

Proof. In fact, we will show that both $a-b>0$ and that $a+(d-1)b-da^2>0$. Consider first the second factor

$$\begin{aligned} a+(d-1)b-da^2 &= \frac{1}{\binom{d+2}{2}}(a+(d-1)b) \quad \text{(by (16))} \\ &= \frac{1}{\binom{d+2}{2}}\left(a+\frac{(d+1)(d+2)a^2-(d+3)a}{d+3}\right) \quad \text{(by (18))} \\ &= \frac{1}{\binom{d+2}{2}}\frac{(d+1)(d+2)a^2}{d+3} \\ &= \frac{2a^2}{d+3}>0. \end{aligned} \tag{22}$$

Further, by direct calculation,

$$a-b=\frac{d+3}{8(d+1)(d+2)^3}\left\{3(2d^2+5d+11)+(d-7)\sqrt{4d^2+12d+17}\right\}.$$

To see that this is always positive, denote the expression inside the parentheses by $p+q\sqrt{R}$. Certainly $p=3(2d^2+5d+11)>0$ and also

$$p^2-q^2R=9(2d^2+5d+11)^2-(d-7)^2(4d^2+12d+17)=32(d+1)(d+2)^3>0$$

so that $p>|q|\sqrt{R}$ and hence $p+q\sqrt{R}>0$. ■

Proposition 2.7. For a,b given by (20) and (21), respectively,

$$K_2(\mathbf{x})=\binom{d+2}{2}-C'\sum_{j=1}^d x_j^2(1-x_j^2)$$

where $C'=C/D>0$. Consequently,

$$\max_{\mathbf{x}\in K}K_2(\mathbf{x})=\dim(\mathcal{P}_2(K))=\binom{d+2}{2}$$

and the maximum is attained at all points $\mathbf{x}\in X$ (despite the fact that a,b are determined from the values at two of the points in X, $(1,1,\cdots,1)$ and $(0,0,\cdots,0)$).

Proof. In general, from (15),

$$K_2(\mathbf{x})=\frac{Y}{D}+\left(2\frac{A}{D}+\frac{1}{a}\right)\sum_{j=1}^d x_j^2+\frac{C}{D}\sum_{j=1}^d x_j^4+\left(2\frac{B}{D}+\frac{1}{b}\right)\sum_{1\le j<k\le d}x_j^2x_k^2.$$

Now, first note that $Y/D=\binom{d+2}{d}$, as this indeed the condition (16) used to determine a. We claim that $2A/D+1/a=-C/D$ and that $2B/D+1/b=0$. To see the second formula, we note that $2B/D+1/b=0 \iff 2bB+D=0$ and calculate

$$\begin{aligned} 2bB+D &= 2b(a^2-b)+(a-b)(a+(d-1)b-da^2) \\ &= 2b(a^2-b)+(a-b)\frac{2a^2}{d+3} \quad \text{(by (22))} \end{aligned}$$

$$= \frac{(d+3)b(a^2-b)+2a^2(a-b)}{d+3}.$$

But, by (18),

$$b = \frac{(d+1)(d+2)a^2-(d+3)a}{(d-1)(d+3)}$$

and substituting this into the above, we obtain, after simplification,

$$a^2((d+3)^2-(d+3)(2d^2+3d+7)a+2(d+1)(d+2)^2a^2)$$

which equals 0, as a is a root precisely of this quadratic, (19).

For the first claim,

$$\begin{aligned} & 2A/D+1/a=-C/D \\ \iff & -\frac{2a}{a+(d-1)b-da^2}+\frac{1}{a}+\frac{a+(d-2)b-(d-1)a^2}{(a-b)(a+(d-1)b-da^2}=0 \\ \iff & -2a^2(a-b)+(a-b)(a+(d-1)b-da^2) \\ & \quad +a(a+(d-2)b-(d-1)a^2)=0. \end{aligned}$$

Then substituting the value of b given by (18), and simplifying, we obtain the equivalent condition

$$a^2((d+3)^2-((d+3)(2d^2+3d+7)a+2(d+1)(d+2)^2a^2)=0$$

which is indeed the case by (19).

Consequently,

$$K_2(\mathbf{x}) = \binom{d+2}{2} - C'\sum_{j=1}^{d} x_j^2(1-x_j^2)$$

with $C' = C/D$. We now proceed to show that $C' > 0$. Indeed, substituting the values of a and b given by (20) and (21), respectively, and simplifying, we obtain

$$\frac{C}{D} = \frac{d+2}{2(d+3)}\left\{(7+3d+2d^2)-(d-1)\sqrt{4d^2+12d+17}\right\}.$$

This is positive as clearly $7+3d+2d^2>0$ and also one may calculate

$$(7+3d+2d^2)^2-(d-1)^2(4d^2+12+17) = 8(d+1)(d+2)^2.$$

■

We now show that these two moments a, b are always realizable by a measure of the form (12).

Proposition 2.8. For $d \geq 2$, consider the weights

$$\begin{aligned} w_d &= 2^{-d}((d-1)b-(d-2)a), \\ w_{d-1} &= 2^{-(d-1)}(a-b), \\ w_0 &= 1-2a+b, \end{aligned}$$

and $w_j = 0$ otherwise. We claim that these weights are positive and that the corresponding measure (12) is a probability measure such that, for a given by (20) and b by (21),

$$\begin{aligned} \int_K x_j^2 d\mu &= a, \\ \int_K x_j^2 x_k^2 d\mu &= b, \ k \neq j. \end{aligned}$$

Consequently, this is an optimal measure of degree 2 for $K=[-1,1]^d$, supported on

$$X_d \cup X_{d-1} \cup X_0$$

with cardinality

$$2^d + d2^{d-1} + 1.$$

Proof. Using the expressions for moments of μ given by Lemma 2.4, we are asserting that

$$M\begin{bmatrix} w_d \\ w_{d-1} \\ w_0 \end{bmatrix} = \begin{bmatrix} 1 \\ a \\ b \end{bmatrix}$$

where

$$M := \begin{bmatrix} 2^d & d2^{d-1} & 1 \\ 2^d & (d-1)2^{d-1} & 0 \\ 2^d(& d-2)2^{d-1} & 0 \end{bmatrix}.$$

Now, it is easy to verify that

$$M^{-1} = 2^{-d} \begin{bmatrix} 0 & -(d-2) & (d-1) \\ 0 & 2 & -2 \\ 2^d & -2^{d+1} & 2^d \end{bmatrix}.$$

Multiplying M^{-1} times $[1\ a\ b]^t$ gives the listed formulas for the three non-zero weights. It remains to show that these are positive.

First note that, in the proof that $D > 0$, we have already shown that $a - b > 0$ and hence $w_{d-1} > 0$. To see that $w_d > 0$, using the formulas for a and b and simplifying, we obtain

$$\begin{aligned} (d-1)b - (d-2)a &= \frac{d+3}{8(d+1)(d+2)^3}\Big\{61 + 8d + 5d^2 - 2d^3 + \\ &\qquad (d^2 + 10d - 11)\sqrt{4d^2 + 12d + 17}\Big\} \\ &> \frac{d+3}{8(d+1)(d+2)^3}\Big\{61 + 8d + 5d^2 - 2d^3 + \\ &\qquad (d^2 + 10d - 11)(2d)\Big\} \\ &= \frac{d+3}{8(d+1)(d+2)^3}\Big\{61 - 14d + 25d^2\Big\} \\ &= \frac{d+3}{8(d+1)(d+2)^3}\Big\{61 + 14(d^2 - d) + 11d^2\Big\} > 0. \end{aligned}$$

Finally, to see that $w_0 > 0$, again after simplification, we obtain

$$\begin{aligned} w_0 &= 1 - 2a + b \\ &= \frac{1}{8(d+1)(d+2)^3}\{p + q\sqrt{R}\} \end{aligned}$$

with

$$\begin{aligned} p &= -119 - 24d + 43d^2 + 24d^3 + 4d^4, \\ q &= 33 + 2d - 9d^2 - 2d^3, \\ R &= 4d^2 + 12d + 17. \end{aligned}$$

It is easy to confirm that $p > 0$ for $d \geq 2$. Also

$$p^2 - q^2 R = 32(d+1)(d+2)^3(4d^2 + 5d - 17) > 0$$

for $d \geq 2$. ■

Remark. Such optimal measures, having only *three* out of $d+1$ non-zero weights are not unique for $d \geq 3$. Indeed there is a *continuum* of solutions for the undetermined system for the weights to reproduce the two required moments. However, other choices of weights may result in a support of increased cardinality. ■

Remark. The optimal measures presented above have the symmetry of the cube. In general, as is already evident from the degree one case, it will be possible to find optimal measures with support of lower cardinality, although they will not be symmetric. Indeed, by Tchakaloff's Theorem (c.f. [7]), there must exist a discrete positive measure supported on a subset of $X_d \cup X_{d-1} \cup X_0$ of cardinality at most $\binom{4+d}{4}$, a polynomial of degree 4 in d. In contrast, the cardinality of the symmetric support, $2^d + d2^{d-1} + 1$, grows exponenially in d and in fact, already for $d = 6$, $2^d + d2^{d-1} + 1 = 257$ whereas $\binom{4+d}{4} = 210$, a lesser number.

The problem of finding a measure of minimal support, as already seen in the degree one case which relates to the existence of Hadamard matrices, is very interesting, but likely dificult. ■

2.3 The degree 3 case for the square $K = [-1,1]^2$

Here we are only able to give numerical values. In this case

$$\dim(\mathcal{P}_3(K)) = 10$$

and we seek a measure so that $K_3(\mathbf{x}) \leq 10$ for $\mathbf{x} \in K$. Assuming that the four corners $(\pm 1, \pm 1)$ are in the support of the optimal measure, and from our experience with the degree 2 case, we seek a symmetric measure so that

$$K_3(\mathbf{x}) = 10 + (x_1^2 - 1)(\alpha x_1^2 + \beta x_2^2 - \gamma)^2 + (x_2^2 - 1)(\beta x_1^2 + \alpha x_2^2 - \gamma)^2 \tag{23}$$

for certain constants $\alpha, \beta, \gamma > 0$.

For such a $K_3(\mathbf{x})$, the support of the measure will be the points for which $K_3(\mathbf{x}) = 10$, i.e.,

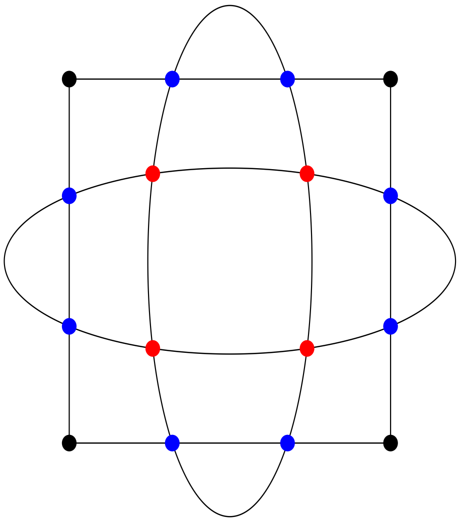

Figure 2: Sixteen Optimal Points As Interesections of Quadratic Curves

- the intersections of $x_1^2-1=0$ and x_2^2-1, i.e., the four corners, $(\pm 1, \pm 1)$
- the four intersections of $x_1^2-1=0$ with the ellipse $\beta x_1^2+\alpha x_2^2-\gamma=0$, i.e., the intersections of this ellipse with the vertical edges, $x_1=\pm 1$
- the four intersections of $x_2^2-1=0$ with the ellipse $\alpha x_1^2+\beta x_2^2-\gamma=0$, i.e., the intersections of this second ellipse with the horizontal edges $x_2=\pm 1$
- the four intersections of the two ellipses $\alpha x_1^2+\beta x_2^2-\gamma=0$ and $\beta x_1^2+\alpha x_2^2-\gamma=0$

giving a total of $4+8+4=16$ support points. These are illustrated in Figure 2.

These intersection points are easily calculated to be $(\pm 1, \pm a)$, $(\pm a, \pm 1)$ and $(\pm b, \pm b)$ for

$$\begin{aligned} a &= \sqrt{(\gamma-\beta)/\alpha}, \\ b &= \sqrt{\gamma/(\alpha+\beta)} \end{aligned}$$

(with some obvious constraints on the values of α, β and γ for these to be feasible).

We then consider measures supported on these sixteen points with weights

- w_2 for each of the four corner points,
- w_1 for each of the eight edge points,
- w_0 for each of the four interior points.

Such measures are automatically symmetric. We then have 6 variables, $\alpha, \beta, \gamma, w_0, w_1, w_2$ and 6 algebraic conditions to impose

1. $4w_2+8w_1+4w_0=1$
2. $K_3((1,1))=10$
3. $K_3((a,1))=10$
4. $K_3((b,b))=10$
5. $(a,1)$ is a double zero of $K_3(\mathbf{x})-10=0$ along the upper edge
6. (b,b) is a double zero of $K_3(\mathbf{x})-10=0$ along the diagonal $x_2=x_1$.

This non-linear system may be solved numerically to find

- $w_2=0.0918460976$
- $w_1=0.0576169752$

- $w_0 = 0.0429199521$
- $\alpha = 4.934688892$
- $\beta = 0.6529908043$
- $\gamma = 1.287921748$
- $a = 0.3587016362$
- $b = 0.4800969941$.

Notice that this configuration is not on a regular grid, as in the degree 2 case.

We also remark that it would be interesting to know if the special form of the optimal $K_n(\mathbf{x})$ made evident in the cases here considered, persists in the general case.

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