

Report on Conducted Research in Minneapolis

Damir Ferizović

Preface

During my stay in Minneapolis, the three of us: D. Bilyk, R. Matzke and D. Ferizović worked on energy optimization with functions in two and three variables and we obtained some new results in that direction. Simultaneously, I worked on a stand alone-project with the title:

On the L^2 -norm of Gegenbauer polynomials

There, results are obtained which deal with special functions called Gegenbauer polynomials, denoted by:

$$\mathcal{C}_n^{(\lambda)}(t),$$

where n is the degree and λ is the index of these polynomials. This is finished and publicly available from the pre-print server arXiv.org. The Austrian Marshall Plan Foundation is mentioned next to my other funds which are acknowledged.

Since the theory for three variable input is still in its infancy, I expect a presentable paper not before May and kindly ask the Marshall Plan Foundation not to make this work publicly available yet. The present report relies heavily on mathematical jargon and I have made efforts to give short descriptions of the main ideas and concepts involved. Notation will be explained as the text proceeds if it is necessary for the understanding of the reader.

We obtained some surprising examples that prove natural assumptions on these circle of problems wrong. In the following report, you will find an overview of what has been worked on.

In due time, there will be a publication on the subject and the support by the Marshall Plan Foundation will be acknowledged.

Damir Ferizović
Graz, February 26th 2020.

Contents

0.1	Overview for August 2019	2
0.2	Overview for September 2019	7
0.2.1	Summary of the paper [7] on Gegenbauer polynomials	8
0.2.2	A detailed commentary on the paper [7]	9
0.2.3	Investigating the three-input case	15
0.2.4	Small excerpt of calculations for the three-input case	16
0.3	Overview for October 2019	17
0.3.1	Functions uvt and $u^2v^2t^2$	18
0.3.2	The algorithm that looks for positive semi-definite matrices	19
0.3.3	Estimates of multiple integrals with respect to energies	23
0.3.4	Functions of the form $F(u, v, t) = h(u)h(v)h(t)$	26

0.1 Overview for August 2019

The first couple of days were spent on practical things and necessities. Soon thereafter I have been introduced to a couple of problems that prof. D. Bilyk and R. Matzke were working on and off in the past years. Prominent among their source of problems are questions asked or related to the Hungarian mathematician L. Fejes Tóth. We next present a couple of those difficult questions, which I am looking forward to continue work on, once we have published results on the three-input energies. Simultaneously, I started generalizing results on the L^2 -norm of Gegenbauer polynomials which I obtained during a vacation in Bosnia for λ (pronounced “lambda”) being an integer.

Ratio of wedges on the surface of a sphere

If we think of the surface of a ball, which we call sphere, and draw two distinct great circles on it, what is the maximal ratio of areas bounded by the lines of great circles on the sphere? (A great circle on a sphere is such that if we cut the sphere along the circle, we obtain two halves.) The answer is there is no maximum, as it is not bounded - just think of two great circles very close to each other, the sphere will be cut into four pieces, two of them being almost halves (hemispheres), while the other two parts are just very thin stripes (diangle): the maximal ratio is the almost

hemisphere divided by a thin stripe, which tends to infinity as the stripe gets narrower (hence the circles approach each other). Let us then ask for the constellation such that the maximal ratio is smallest among all constellations, what is the answer in this case?

The answer is rather simple, the smallest maximal ratio is one. Just draw two circles perpendicular to each other (intersecting in right angles), cutting the sphere into four equal parts. But what if we draw a third great circle? Again, the answer is one, as we can let three great circles intersect, say in the north pole, such that they cut the sphere into six equal parts.

But let us exclude the possibility that three or more great circles intersect in one point on the sphere! For three circle, the answer is still easy, as one can have two circles intersecting at the north pole cutting the sphere into four equal parts, and let the third great circle play the role of the equator, cutting the sphere in total of eight parts of equal areas - thus the maximal ratio is one, once more.

Now we are ready to formulate the problem: Place n many great circles on the sphere such that no more than two circles intersect in a common point of the sphere, what is the behavior of the maximal ratio of areas inscribed by them, i.e. does the maximal ratio has to grow without bound for any constellation, or is there a clever way to place great circles such that the ratio stays bounded?

My contribution to that problem was to consider inner products (written (x, y)) for elements x, y of the sphere: The inner product (or sometimes scalar or dot product) in our case just measures the cosine of the short angle ϕ between two elements, thus if x, y are points on the sphere which we regard as vectors in 3-dimensional space, they have two angles between them - a short (ϕ) and long one; then $\cos(\phi) = (x, y)$. To every great circle on the sphere, we can draw two antipodal points, so that if we name the points north and south pole, the circle will be the equator, i.e. every point on the sphere determines a unique great, and any great circle determines a north and south pole.

For n -great circles consider a set of associated points on the sphere $\{x_1, \dots, x_n\}$, i.e. if we draw an equator to each point x_j , we will obtain the great circles that we started with (note that the set is not unique, as instead of x_1 we could have chosen the antipodal point $-x_1$, and we would have the same property). My idea was to consider functions on the sphere build by inner products and associated points:

$$f_j(y) = (x_j, y).$$

Since the inner product measures the cosine of the angle between points, f_j will be positive for points on the same hemisphere as x_j , save the equator associated to x_j - it will be negative if the point belongs to the hemisphere of $-x_j$, and zero along the equator (where each point is perpendicular to x_j , the angle hence being $\pi/2$, where the cosine assumes the value zero). Thus each point on the sphere determines a unique code in which area inscribed by great circles it belongs to:

$$y \approx (\text{sgn}(f_1(y)), \dots, \text{sgn}(f_n(y))),$$

where $\text{sgn}(f_j(y))$ is one of three numbers: -1,0,1, depending whether $f_j(y)$ is negative, zero or positive respectively. Unfortunately, not every such code determines an area on the sphere: A counter example is given by five great circles such that three of them (with associated points x_1, x_2, x_3) inscribe a small triangle centered at the north pole (and hence they also inscribe a small triangle centered at the south pole), and the remaining two great circles are close to the equator, their associated points x_4, x_5 thus can be chosen to lie in the inscribed triangle. Thus we see that any point y from the small triangle centered at the north pole, would have the code

$$y \approx (\text{sgn}(f_1(y)), \text{sgn}(f_2(y)), \text{sgn}(f_3(y)), 1, 1),$$

by choice of x_4, x_5 ; and a code of the form

$$(\text{sgn}(f_1(y)), \text{sgn}(f_2(y)), \text{sgn}(f_3(y)), 1, -1),$$

would not make sense (note the sign change in the last coordinate). It is still a problem to find the right functions so as to make a coding refer to an area and vice versa in a meaningful way.

A further function that I introduced to investigate this question is the product of all the f_j 's:

$$b(y) := f_1(y) \cdot \dots \cdot f_n(y).$$

This function helps me to find the boundaries of the areas, as every function $f_j(y)$ is zero for y being on the great circle determined as the equator to x_j , $b(y)$ will be zero if one of the f_j 's is. It also has the nice property to be strictly positive or strictly negative in each area, and to change sign if we cross the boundary from one area to the next (unless the crossing is over a point of intersection of two great circles, in which case the sign doesn't change).

Also useful are following functions which are products of almost all the f_j 's save one:

$$\begin{aligned} p_1(y) &:= f_2(y) \cdot \dots \cdot f_n(y) \\ p_2(y) &:= f_1(y) \cdot f_3(y) \cdot \dots \cdot f_n(y) \\ &\vdots \\ p_n(y) &:= f_1(y) \cdot \dots \cdot f_{n-1}(y). \end{aligned}$$

They make it possible to define a function that detects intersections of great circles:

$$c(y) := (1 - p_1(y)) \cdot \dots \cdot (1 - p_n(y)).$$

At an intersection, there are two indices, for the sake of argument say 1, 2, such that $f_1(y) = f_2(y) = 0$. But this means all the $p_j(y)$ are zero, as either f_1 or f_2 is part of their product, thus $c(y) = 1$. Since each f_j is essentially a cosine of some value, the functions p_j have values in the

open interval $(-1, 1)$ if $n > 2$, and so $c(y) = 1$ only at intersections and has otherwise positive values less than one.

The last idea I had in this direction was to change the setting, regard the polyhedron made from the intersection points of great circles and try to use results from convex bodies. There we have a famous formula at our disposal, Euler's polyhedron formula: the amount of vertices minus the amount of edges plus the amount of faces equals 2, or $V - E + F = 2$.

As every time we draw another great circle, we have to intersect all of the previous ones at two antipodal points, this means for n -circles we have $n(n - 1)$ many intersections. Similarly, for n great circles we have $2n(n - 1)$ edges, as by going from n -th circle to the $n + 1$ -th circle, add $2n$ edges lying on the new circle by intersecting n former circles, and in addition we have cut through $2n$ former edges, thus adding $4n$ edges in the process.

All in all we hence can deduce that no matter what, we always have $n(n - 1) + 2$ many areas on the sphere. Further investigations are planned once in a while...

Mutually unbiased bases

We will state some notation before the problem. We are working in the n -dimensional complex vector space \mathbb{C}^n , i.e. a set with elements of the form (x_1, \dots, x_n) (an n -tuple) where x_1 to x_n are complex numbers and where we can add two such elements by adding component-wise and multiplication by complex numbers is again understood to be component-wise. Each of those elements can be written as a finite sum of special n -tuples and some factors from the complex numbers:

$$(x_1, \dots, x_n) = x_1 \cdot (1, 0, \dots, 0) + \dots + x_n(0, \dots, 0, 1) = \sum_{j=1}^n x_j e_j.$$

(Here e_j is the n -tuple with zeros everywhere except of the j -th entry.) A collection of those special n -tuples like above, that have the property to construct every other element by just adding appropriate multiples of them is called a spanning set. If the spanning set is such that by excluding one of them, the reconstructive property is lost, we call the spanning set minimal - or in short: A basis.

We already talked about the inner product in the previous section, but there are actually many inner products - so in the space \mathbb{C}^n . There is a standard one which again can be related to the angle between two vectors - so again, we call two vectors $x, y \in \mathbb{C}^n$ orthogonal or perpendicular if for the given inner product we have $(x, y) = 0$. The basis introduced above has the following nice property: $(e_j, e_i) = 0$ for $i \neq j$ and $(e_i, e_i) = 1$. Bases with this property are very important, so much so that they have a standard abbreviation: ONB (ortho-normal basis).

Given two such ONB, say $E = \{e_1, \dots, e_n\}$ and $B = \{b_1, \dots, b_n\}$ with the property

$$|(e_i, b_j)|^2 = \frac{1}{d},$$

for any $i, j \leq n$, then we call E and B mutually unbiased, or MUB's. These objects appear in Quantum State Topography for instance.

The problem is as follows, given the dimension n we want to work in, what is the maximal amount of MUB's we can find? In case n is a power of a prime number, the answer is known to be $n + 1$. Actually, $n + 1$ is an upper bound, that is, there are not more than that. It is also known that if n can be written as decomposition of prime powers $p_j^{m_j}$ ordered such that $p_1^{m_1} < p_j^{m_j}$ for all $j > 1$, then we know that the amount of MUB's is bigger or equal to $p_1^{m_1} + 1$.

As an example, take $n = 6$. Its prime power decomposition is 2, 3 with $m_1 = m_2 = 1$, thus there are at least 3 MUB's - and there is evidence that this is the maximum. I have left this problem aside without any idea so far.

Two-input energies

We soon started working on two-input energies, i.e. given a reasonable nice function $G(x, y)$ in two variables defined for inputs x and y from the sphere; which probability measure μ would minimize following double integral:

$$I_G[\mu] := \iint_{S_2} G(x, y) d\mu(x) d\mu(y)?$$

This kind of question has been under investigation for a long time now, by D. Bilyk, R. Matzke and many more. If $G(x, y)$ just depends on the angle between the vectors x and y and posses a Gegenbauer expansion with non-negative coefficients only, then it is known that the standard surface measure, denoted by σ (pronounced "sigma"), is a minimizer.

The discrete version is closely related to uniform point distributions. Given a set of N many points on the sphere x_1, \dots, x_N , we can regard the discrete energy

$$\sum_{i,j=1}^N \frac{1}{N^2} G(x_i, x_j).$$

As N increases, so will the discrete energy, and for certain nice functions G the limit will be the double integral; and the points will tend to be uniformly spread out. The question is still open for certain not so "nice" functions.

Consider the function $K(x, y) = \arccos |(x, y)|$, which is the inverse function to the cosine, applied to the absolute value of the inner product of x, y . The question is, what constellation of points, or which probability measure minimizes the (discrete) energy, the double integral? Also interesting is the function $H(x, y) = \arcsin |(x, y)|$, which is the inverse function to the sine, applied to the absolute value of the inner product of x, y .

Definition 0.1.1. A function $F(t)$ with $t \in [-1, 1]$ is called positive (semi-)definite if for any set of points x_1, \dots, x_N from the sphere, any integer N , and any N -tuple of real numbers (y_1, \dots, y_N) , we

have following inequality:

$$\sum_{i=1}^N \sum_{j=1}^N F((x_i, x_j)) y_i y_j \geq 0.$$

A symmetric function in two variables K , i.e. $K(x, y) = K(y, x)$ where x, y are points from the sphere, is called positive (semi-)definite if

$$\sum_{i=1}^N \sum_{j=1}^N K(x_i, x_j) y_i y_j \geq 0.$$

Tools that have been used for positive semi-definite functions are for instance Mercer's theorem, which enables us to write the function as an infinite sum of a certain orthonormal basis - but the functions above do not have this particular property, which makes it of course a lot harder to handle. The three of us worked on question when σ is a unique minimizer and which type of functions are always minimized by σ . R. Matzke contributed most to this problem.

0.2 Overview for September 2019

During this month I finished a paper on the the L^2 -Norm of Gegenbauer Polynomials, and this section contains a summary and detailed version of the aforementioned paper which can be downloaded from the pre-print server arXiv.org by searching for Ferizovic.

The reason to investigate the norm of these polynomials lies essentially at the heart of a joint work with C. Beltrán, where we needed estimates of integrals of squares of those functions for and in the paper:

Approximation to uniform distribution in $SO(3)$

There we obtained exact results for the special case of $\lambda = 2$ (pronounced "lambda"), but the question what asymptotic behavior (i.e. "speed" of growth with respect to the degree "n": one regards the quotient of the expression of interest with the right power of n , so that the quotient becomes neither 0 nor ∞ as n increases without bound [finding the right power of n is hard, finding the value the quotient approaches is hard too - both together are the first term of the asymptotic expansion]) following integral for $\lambda > 1$ (pronounced "lambda") has remained open:

$$\int_0^1 \mathcal{C}_n^{(\lambda)}(t)^2 dt.$$

This is a highly non-trivial question, as the Gegenbauer polynomials are oscillating wildly and is now answered at least asymptotically. This result is obtained by first deriving an exact recursive formula, and then applying the principle of induction. It has been submitted and is publicly available at the pre-print server arXiv.org.

Currently, I am planning to extend the results to integrals of the form

$$\int_0^1 \mathcal{C}_n^{(\lambda)}(t)^2 (1-t^2)^{\beta-\frac{1}{2}} dt.$$

0.2.1 Summary of the paper [7] on Gegenbauer polynomials

The formal introduction for Gegenbauer polynomials $\mathcal{C}_n^{(\lambda)}(x)$, where $n \in \mathbb{N}_0$ (i.e. n is a natural number including zero $[0,1,2,3,\dots]$) is the degree and $\lambda > -\frac{1}{2}$ called the index, are as the coefficients of following power series expansion in α :

$$(1 - 2t\alpha + \alpha^2)^{-\lambda} = \sum_{n=0}^{\infty} \mathcal{C}_n^{(\lambda)}(t) \alpha^n.$$

(Thus we choose arbitrary fixed numbers $t \in [-1, 1]$ and λ as above, then the Gegenbauer polynomials are those polynomials such that the above equation is true for any complex number α in a "small enough" disc around zero.) They are orthogonal with respect to the measure $(1-t^2)^{\lambda-1/2} dx$ over $[-1, 1]$, meaning

$$\int_{-1}^1 \mathcal{C}_m^{(\lambda)}(t) \mathcal{C}_n^{(\lambda)}(t) (1-t^2)^{\lambda-1/2} dt = 0 \text{ for } n \neq m.$$

As already mentioned, in [3] following results were obtained, where γ is the Euler-Mascheroni constant (a rather famous number starting with the decimal expression 0.5772...) and $\psi(x)$ is the digamma function (a well understood special function):

Lemma 0.2.1. *The Gegenbauer polynomials satisfy for $n \geq 2$*

$$\begin{aligned} \int_0^1 (1-x^2) [\mathcal{C}_{n-2}^{(2)}(x)]^2 dx &= \frac{2n^2-1}{16} \left(\psi(n+\frac{1}{2}) + \gamma + \log(4) \right) - \frac{n^2}{8}, \\ \int_0^1 [\mathcal{C}_{n-2}^{(2)}(x)]^2 dx &= \frac{n^4}{16} + \frac{4n^2-1}{64} \left(\psi(n+\frac{1}{2}) + \gamma + \log(4) \right) - \frac{5}{32}n^2. \end{aligned}$$

I was able to prove following recursive formula:

Theorem 0.2.2 (Main Result). *The L^2 -norm of Gegenbauer polynomials satisfies*

$$\begin{aligned} \int_0^1 [\mathcal{C}_{n-2}^{(\lambda+1)}(x)]^2 dx &= \frac{n^2-2\lambda n}{4^2\lambda^3} [\mathcal{C}_n^{(\lambda)}(1)]^2 + \frac{n(2n+1)}{8\lambda^2} \int_0^1 [\mathcal{C}_n^{(\lambda)}(x)]^2 dx \\ &\quad - \sum_{k=0}^n \frac{\lambda+k}{4\lambda^2} \int_0^1 [\mathcal{C}_k^{(\lambda)}(x)]^2 dx. \end{aligned}$$

With this in hand, the asymptotic expansion was derived:

Corollary 0.2.2.1. *For $\lambda \in \mathbb{N}_{>1}$ we have following asymptotic for the L^2 -norm*

$$\int_0^1 [\mathcal{C}_{n-2}^{(\lambda+1)}(x)]^2 dx = \frac{n^{4\lambda}}{4\lambda\Gamma(2\lambda+1)^2} + \frac{\lambda-1}{\Gamma(2\lambda+1)^2} n^{4\lambda-1} + O_\lambda(n^{4\lambda-2}).$$

0.2.2 A detailed commentary on the paper [7]

Gegenbauer polynomials $\mathcal{C}_n^{(\lambda)}$, where $\lambda \in I_G := (-\frac{1}{2}, 0) \cup (0, \infty)$ is called the index and $n \in \mathbb{N}_0$ is the degree, are the coefficients of following power series expansion in α :

$$(1 - 2x\alpha + \alpha^2)^{-\lambda} = \sum_{n=0}^{\infty} \mathcal{C}_n^{(\lambda)}(x)\alpha^n.$$

The case $\lambda = 0$ is not considered here. $\{\mathcal{C}_n^{(\lambda)}\}_{n \in \mathbb{N}_0}$ are orthogonal with respect to the measure $(1 - x^2)^{\lambda-1/2} dx$ over $[-1, 1]$, and by [8, Eq. 8.930]:

$$\forall \lambda \in I_G : \quad \mathcal{C}_0^{(\lambda)}(x) = 1, \quad \mathcal{C}_1^{(\lambda)}(x) = 2\lambda x. \quad (1)$$

For continuous $f : [0, 1] \rightarrow \mathbb{R}$ (continuity can be thought of as no jumps in the graph of the function "f"), the following notation will be used:

$$\|f\|_2^2 := \int_0^1 [f(x)]^2 dx.$$

We show, as a corollary to our Theorem 0.2.5, an asymptotic formula for $\|\mathcal{C}_n^{(\lambda)}\|_2^2$ for $\lambda > 1$. Indeed, one of the key ingredients in [7] was the asymptotic nature of $\|\mathcal{C}_n^{(2)}\|_2^2$ in n , and the following lemmas were proved in section 6 of [7].

Lemma 0.2.3. *Let ψ denote the digamma function and γ the Euler-Mascheroni constant. Then the Gegenbauer polynomials satisfy for $n \geq 2$:*

$$\begin{aligned} \|\sqrt{1-x^2} \mathcal{C}_{n-2}^{(2)}\|_2^2 &= \frac{1}{16}(2n^2 - 1)(\psi(n + \frac{1}{2}) + \gamma + \log(4)) - \frac{1}{8}n^2, \\ \|\mathcal{C}_{n-2}^{(2)}\|_2^2 &= \frac{1}{16}n^4 + \frac{1}{64}(4n^2 - 1)(\psi(n + \frac{1}{2}) + \gamma + \log(4)) - \frac{5}{32}n^2. \end{aligned}$$

The following result of Corollary 5.2 from [6] will prove to be indispensable.

Theorem 0.2.4 (Dette [6]). *The Gegenbauer polynomials satisfy for $\lambda \in I_G$*

$$\left(\frac{n}{2\lambda}\right)^2 [\mathcal{C}_n^{(\lambda)}(x)]^2 + (1-x^2)[\mathcal{C}_{n-1}^{(\lambda+1)}(x)]^2 = \sum_{k=0}^{n-1} \frac{\lambda+k}{\lambda} [\mathcal{C}_k^{(\lambda)}(x)]^2. \quad (2)$$

With this we show that

Theorem 0.2.5. *The Gegenbauer polynomials satisfy for $\lambda \in I_G$:*

$$\|\mathcal{C}_{n-2}^{(\lambda+1)}\|_2^2 = \frac{n^2 - 2\lambda n}{2^4 \lambda^3} [\mathcal{C}_n^{(\lambda)}(1)]^2 + \frac{n(2n+1)}{2^3 \lambda^2} \|\mathcal{C}_n^{(\lambda)}\|_2^2 - \sum_{k=0}^{n-1} \frac{\lambda+k}{2^2 \lambda^2} \|\mathcal{C}_k^{(\lambda)}\|_2^2.$$

The first term on the right-hand side above is asymptotically most important (thus as n increases, all we had to do was to give a detailed description of the behavior of the first term):

Corollary 0.2.5.1. *For $\lambda \in \mathbb{R}_{>0}$, $\lambda \neq 1$, we have following asymptotics in n :*

$$\begin{aligned} \|\mathcal{C}_{n-2}^{(\lambda+1)}\|_2^2 &= \frac{n^{4\lambda}}{4\lambda\Gamma(2\lambda+1)^2} + \frac{\lambda-1}{\Gamma(2\lambda+1)^2} n^{4\lambda-1} + O(n^{4\lambda-2}), \\ \|\sqrt{1-x^2} \mathcal{C}_{n-1}^{(\lambda+2)}\|_2^2 &= \frac{2\lambda+1}{4\lambda\Gamma(2\lambda+3)^2} n^{4\lambda+2} + O(n^{4\lambda+1}). \end{aligned}$$

Bounds for the cases $-\frac{3}{2} < \lambda < 0$ are implicit in the proof. The cases $\lambda \in \{0, 1\}$ follow by Equation (19) in [7] and Lemma 0.2.3, respectively.

Ingredients for the Proof of the Theorem

In this section we collect known results concerning Gegenbauer polynomials for later reference and the reader's convenience, and we derive some technical lemmas in Subsection 0.2.2 to prove Theorem 0.2.5. To avoid repetition, we will assume $\lambda \in I_G$ for the rest of the text if not stated otherwise. Note first that (since one can take derivatives of polynomials, it is nice to know how they look like)

$$\begin{aligned} \frac{d}{dx} \mathcal{C}_{n+1}^{(\lambda)}(x) &= 2\lambda \mathcal{C}_n^{(\lambda+1)}(x) && [8, \text{Eq. 8.935}], \\ \mathcal{C}_n^{(\lambda)}(1) &= \frac{\Gamma(n+2\lambda)}{\Gamma(2\lambda)n!} = \frac{\prod_{j=1}^n (2\lambda+n-j)}{n!} && [8, \text{Eq. 8.937}; \end{aligned} \tag{3}$$

and $\mathcal{C}_n^{(\lambda)}(1)$ is the maximum on $[-1, 1]$ for $\lambda > 0$ by [10, Eq. 7.33.1]. It will also be beneficial to know following relations, which follow by an application of (3) and the sources stated:

$$(n+2) \mathcal{C}_{n+2}^{(\lambda)}(x) = 2\lambda \left(x \mathcal{C}_{n+1}^{(\lambda+1)}(x) - \mathcal{C}_n^{(\lambda+1)}(x) \right) \quad [8, \text{Eq. 8.933.2}], \tag{4}$$

$$(n+\lambda) \mathcal{C}_n^{(\lambda)}(x) = \lambda \left(\mathcal{C}_n^{(\lambda+1)}(x) - \mathcal{C}_{n-2}^{(\lambda+1)}(x) \right) \quad [8, \text{Eq. 8.939.6}]. \tag{5}$$

Identities for Gegenbauer polynomials

Next we will derive some identities that have not been found elsewhere, but will be used in consequent calculations.

Lemma 0.2.6. *The Gegenbauer polynomials satisfy following identities:*

$$\begin{aligned} \mathcal{C}_n^{(\lambda+1)}(x) + \mathcal{C}_{n-2}^{(\lambda+1)}(x) &= 2x \mathcal{C}_{n-1}^{(\lambda+1)}(x) + \mathcal{C}_n^{(\lambda)}(x), & (\star) \\ \int_0^1 [\mathcal{C}_n^{(\lambda+1)}(x)]^2 - [\mathcal{C}_{n-2}^{(\lambda+1)}(x)]^2 dx &= \frac{n+\lambda}{2\lambda^2} \left([\mathcal{C}_n^{(\lambda)}(1)]^2 + (2\lambda-1) \|\mathcal{C}_n^{(\lambda)}\|_2^2 \right). \end{aligned}$$

Proof. Let us abbreviate $\ell := \lambda + 1$ to have nicer formulas. Next we use equation (5) and apply equation (4) to the right-hand side below to prove identity (\star) :

$$\mathcal{C}_n^{(\ell)}(x) + \mathcal{C}_{n-2}^{(\ell)}(x) = \frac{n+\lambda}{\lambda} \mathcal{C}_n^{(\lambda)}(x) + 2x \mathcal{C}_{n-1}^{(\ell)}(x) - \left(2x \mathcal{C}_{n-1}^{(\ell)}(x) - 2\mathcal{C}_{n-2}^{(\ell)}(x) \right),$$

By the binomial theorem: $a^2 - b^2 = (a-b)(a+b)$ we obtain with the readily available equations (5), (\star) and (3) following identity

$$\begin{aligned} [\mathcal{C}_n^{(\lambda+1)}(x)]^2 - [\mathcal{C}_{n-2}^{(\lambda+1)}(x)]^2 &= \frac{n+\lambda}{\lambda} \mathcal{C}_n^{(\lambda)}(x) \left(2x \mathcal{C}_{n-1}^{(\lambda+1)}(x) + \mathcal{C}_n^{(\lambda)}(x) \right) \\ &= \frac{n+\lambda}{\lambda} \left(\frac{x}{2\lambda} \frac{d}{dx} [\mathcal{C}_n^{(\lambda)}(x)]^2 + [\mathcal{C}_n^{(\lambda)}(x)]^2 \right). \end{aligned}$$

Next we can integrate both sides and use integration by parts on the first term on the right-hand side. This will give the desired expression. ■

Lemma 0.2.7. *The Gegenbauer polynomials satisfy the following identity:*

$$\begin{aligned} \int_0^1 x^2 [\mathcal{C}_{n+1}^{(\lambda+1)}(x)]^2 + [\mathcal{C}_n^{(\lambda+1)}(x)]^2 dx + \frac{1}{2\lambda} \int_0^1 (1-x^2) [\mathcal{C}_{n+1}^{(\lambda+1)}(x)]^2 dx \\ = \frac{(n+2)^2}{8\lambda^3} [\mathcal{C}_{n+2}^{(\lambda)}(1)]^2 + \frac{2\lambda-1}{2\lambda} \frac{(n+2)^2}{4\lambda^2} \|\mathcal{C}_{n+2}^{(\lambda)}\|_2^2. \end{aligned}$$

Proof. We will have to divide the parameter n by 2, so it makes sense to assume $n = 2m$ for now, i.e. n is supposed to be an even number. The case n odd works just the same. By Lemma 0.2.6 and a telescoping sum argument (we hence add up terms as follows:

$C_n - C_{n-2} + C_{n-2} - C_{n-4} + C_{n-4} - C_{n-6} \dots$ and since n is even this will terminate at C_0 , for each difference we apply the lemma as mentioned):

$$\begin{aligned} \|\mathcal{C}_n^{(\lambda+1)}\|_2^2 - \|\mathcal{C}_0^{(\lambda+1)}\|_2^2 &= \sum_{j=1}^m \frac{2j+\lambda}{2\lambda^2} \left([\mathcal{C}_{2j}^{(\lambda)}(1)]^2 + (2\lambda-1) \|\mathcal{C}_{2j}^{(\lambda)}\|_2^2 \right), \\ \|\mathcal{C}_{n+1}^{(\lambda+1)}\|_2^2 - \|\mathcal{C}_1^{(\lambda+1)}\|_2^2 &= \sum_{j=1}^m \frac{2j+1+\lambda}{2\lambda^2} \left([\mathcal{C}_{2j+1}^{(\lambda)}(1)]^2 + (2\lambda-1) \|\mathcal{C}_{2j+1}^{(\lambda)}\|_2^2 \right). \end{aligned}$$

Using (1) and summing up, and an application of Dette's result (2) yields:

$$\begin{aligned}
& \int_0^1 [\mathcal{C}_{n+1}^{(\lambda+1)}(x)]^2 + [\mathcal{C}_n^{(\lambda+1)}(x)]^2 dx \\
&= \frac{4}{3}(\lambda+1)^2 + 1 + \frac{1}{2\lambda} \sum_{j=2}^{n+1} \frac{j+\lambda}{\lambda} [\mathcal{C}_j^{(\lambda)}(1)]^2 + \frac{2\lambda-1}{2\lambda} \sum_{j=2}^{n+1} \frac{j+\lambda}{\lambda} \|\mathcal{C}_j^{(\lambda)}\|_2^2 \\
&= \frac{(n+2)^2}{8\lambda^3} [\mathcal{C}_{n+2}^{(\lambda)}(1)]^2 + \frac{2\lambda-1}{2\lambda} \sum_{j=0}^{n+1} \frac{j+\lambda}{\lambda} \|\mathcal{C}_j^{(\lambda)}\|_2^2 \\
&= \frac{(n+2)^2}{8\lambda^3} [\mathcal{C}_{n+2}^{(\lambda)}(1)]^2 + \frac{2\lambda-1}{2\lambda} \left(\frac{(n+2)^2}{4\lambda^2} \|\mathcal{C}_{n+2}^{(\lambda)}\|_2^2 + \|\sqrt{1-x^2} \mathcal{C}_{n+1}^{(\lambda+1)}\|_2^2 \right).
\end{aligned}$$

Note that the right-hand side above has an integral of the function $(1-x^2)[\mathcal{C}_{n+1}^{(\lambda+1)}]^2$, which we can subtract from the left-hand side to obtain the claim. The case $n+1=2m$ is analogous. ■

This time we obtain a complicated expression, the next lemma already will give us almost the same integral but luckily with just on sign reversed - this we will use to simply subtract both integrals and obtain an expression of the desired term only. We will skip a proof though as it is more of the same - the interested read can download the original paper from arXiv.org.

Lemma 0.2.8. *The Gegenbauer polynomials satisfy the following identity:*

$$\int_0^1 x^2 [\mathcal{C}_{n+1}^{(\lambda+1)}(x)]^2 - [\mathcal{C}_n^{(\lambda+1)}(x)]^2 dx = \frac{n+2}{4\lambda^2} \left([\mathcal{C}_{n+2}^{(\lambda)}(1)]^2 - (n+3) \|\mathcal{C}_{n+2}^{(\lambda)}\|_2^2 \right).$$

Proof of the Main Results

Proof of Theorem 0.2.5. Subtract the left hand sides of Lemma 0.2.7 and Lemma 0.2.8:

$$\begin{aligned}
2\|\mathcal{C}_n^{(\lambda+1)}\|_2^2 + \frac{1}{2\lambda} \|\sqrt{1-x^2} \mathcal{C}_{n+1}^{(\lambda+1)}\|_2^2 &= \left(\frac{(n+2)^2}{8\lambda^3} - \frac{n+2}{4\lambda^2} \right) [\mathcal{C}_{n+2}^{(\lambda)}(1)]^2 \\
&+ \left(\frac{(n+2)^2}{4\lambda^2} + \frac{(n+2)(n+3)}{4\lambda^2} \right) \|\mathcal{C}_{n+2}^{(\lambda)}\|_2^2 - \frac{1}{2\lambda} \frac{(n+2)^2}{4\lambda^2} \|\mathcal{C}_{n+2}^{(\lambda)}\|_2^2;
\end{aligned}$$

an application of Dette's formula (2) then gives the desired expression. ■

Also without proof comes the next corollary which enables us to compute its asymptotic expansion.

Corollary 0.2.8.1. *The Gegenbauer polynomials satisfy the following identity:*

$$\begin{aligned}
& \|\sqrt{1-x^2} \mathcal{C}_{n-1}^{(\lambda+1)}\|_2^2 \\
&= [\mathcal{C}_n^{(\lambda)}(1)]^2 \frac{n+2\lambda}{n+1} \frac{1-2\lambda}{2^3\lambda^2} + \frac{(n+1)(2n+3)}{2^3\lambda^2} \|\mathcal{C}_{n+1}^{(\lambda)}\|_2^2 - \|\mathcal{C}_n^{(\lambda)}\|_2^2 \frac{n+2\lambda}{2^3\lambda^2}.
\end{aligned}$$

The next remark perhaps deserves more attention, as it gives an exact and short formula.

Remark. For our asymptotic analysis we will need the following identity, which follows from the proof of Theorem 0.2.5 and Corollary 0.2.8.1:

$$\begin{aligned} \|\mathcal{C}_{n-2}^{(\lambda+1)}\|_2^2 &= \frac{n^2 - 2\lambda n}{2^4 \lambda^3} [\mathcal{C}_n^{(\lambda)}(1)]^2 + \frac{2n^2(4\lambda - 1) + n(4\lambda + 1) + 2\lambda}{2^5 \lambda^3} \|\mathcal{C}_n^{(\lambda)}\|_2^2 \\ &\quad - [\mathcal{C}_n^{(\lambda)}(1)]^2 \frac{n + 2\lambda}{n + 1} \frac{1 - 2\lambda}{2^5 \lambda^3} - \frac{(n + 1)(2n + 3)}{2^5 \lambda^3} \|\mathcal{C}_{n+1}^{(\lambda)}\|_2^2. \end{aligned} \quad (6)$$

This we use with following asymptotic form, see [11]: For $|z| \rightarrow \infty$ and $\alpha, \beta \geq 0$:

$$\frac{\Gamma(z + \alpha)}{\Gamma(z + \beta)} = z^{\alpha - \beta} \left(1 + \frac{(\alpha - \beta)(\alpha + \beta - 1)}{2z} + O(|z|^{-2}) \right). \quad (7)$$

Proof of Corollary 0.2.5.1. Let us denote the order of $\|\mathcal{C}_n^{(\lambda)}\|_2^2$ with respect to n by $\Phi(\lambda)$, i.e. $c_1 n^{\Phi(\lambda)} \leq \|\mathcal{C}_n^{(\lambda)}\|_2^2 \leq c_2 n^{\Phi(\lambda)}$ for some positive constants c_1, c_2 . When this holds, we write $\|\mathcal{C}_n^{(\lambda)}\|_2^2 = \Theta(n^{\Phi(\lambda)})$. We will first use (6) to show by induction that $[\mathcal{C}_n^{(\lambda)}(1)]^2 = \Theta(n^{\Phi(\lambda)+2})$ for $\lambda > 1, \lambda \neq 2$; as outlined below.

The case $\lambda = m \in \mathbb{N}_{>2}$: It can be easily seen with Lemma 0.2.3 and (6), that $[\mathcal{C}_n^{(3)}(1)]^2 = \Theta(n^{\Phi(3)+2})$. If it holds for m , then by abusing notation and (6):

$$\|\mathcal{C}_{n-2}^{(m+1)}\|_2^2 = n^2 \Theta(n^{\Phi(m)+2}) + n^2 \Theta(n^{\Phi(m)}) + \Theta(n^{\Phi(m)+2}) + n \Theta(n^{\Phi(m)}).$$

This proves the assertion as it shows that $\|\mathcal{C}_n^{(m+1)}\|_2^2 = \Theta(n^{\Phi(m)+4})$, but by (3):

$$\mathcal{C}_n^{(\lambda+1)}(1) = \frac{(2\lambda + n + 1)(2\lambda + n)}{2\lambda(2\lambda + 1)} \mathcal{C}_n^{(\lambda)}(1) = \Theta(n^2 \mathcal{C}_n^{(\lambda)}(1)), \quad (8)$$

which, when squared, is of order $\Phi(m) + 6$. We will use this reasoning throughout.

The case $\lambda \in (m, m + 1)$ for $m \in \mathbb{N}$: For $\lambda \in (0, 1)$ and $\theta \in [0, \pi]$:

$$\sin(\theta)^\lambda |\mathcal{C}_n^{(\lambda)}(\cos(\theta))| < \frac{2^{1-\lambda}}{\Gamma(\lambda)} n^{\lambda-1} \quad \text{see [10, Eq. 7.33.5].}$$

We square this inequality, multiply by $\sin(\varphi)^{1-2\lambda} \approx \varphi^{1-2\lambda}$ and integrate:

$$\|\mathcal{C}_n^{(\lambda)}\|_2^2 < \frac{2^{2-2\lambda}}{\Gamma(\lambda)^2} n^{2\lambda-2} \int_0^{\pi/2} \sin(t)^{1-2\lambda} dt \approx \frac{2^{2-2\lambda}}{\Gamma(\lambda)^2} \frac{n^{2\lambda-2}}{2-2\lambda} \left(\frac{\pi}{2}\right)^{2-2\lambda}.$$

Note that $\mathcal{C}_n^{(\lambda)}(1) = \Theta(n^{2\lambda-1})$ by (3) and (7) for $z = n$, thus $n\mathcal{C}_n^{(\lambda)}(1) = \Theta(n^{2\lambda})$, but

$$\|\mathcal{C}_n^{(\lambda+1)}\|_2^2 = O(n^2[\mathcal{C}_n^{(\lambda)}(1)]^2) + O(n^{2\lambda}),$$

as can be seen by (6). Thus $\Phi(\lambda + 1) = 4\lambda$, and $\mathcal{C}_n^{(\lambda+1)}(1) = \Theta(n^{2\lambda+1})$ by (7), which finishes the base case and we use induction.

Thus in order to find the two leading terms in the asymptotic form, we have to expand $\mathcal{C}_n^{(\lambda)}(1)$; which we write as ratio of Gamma functions (3), and use (7):

$$\begin{aligned} \frac{n^2 - 2\lambda n}{2^4 \lambda^3} [\mathcal{C}_n^{(\lambda)}(1)]^2 &= \frac{n^2 - 2\lambda n}{2^4 \lambda^3 \Gamma(2\lambda)^2} [n^{4\lambda-2} + n^{4\lambda-3} 2\lambda(2\lambda - 1) + O(n^{4\lambda-4})] \\ &= \frac{n^{4\lambda}}{4\lambda\Gamma(2\lambda + 1)^2} + \frac{2\lambda(2\lambda - 2)}{4\lambda\Gamma(2\lambda + 1)^2} n^{4\lambda-1} + O(n^{4\lambda-2}). \end{aligned}$$

This proves the result of the asymptotic formula of $\|\mathcal{C}_n^{(\lambda)}\|_2^2$; and this in combination with Corollary 0.2.8.1 and (7), will finish the argument using $x\Gamma(x) = \Gamma(x + 1)$:

$$\begin{aligned} \|\sqrt{1-x^2} \mathcal{C}_{n-1}^{(\lambda+2)}\|_2^2 &= -\frac{1+2\lambda}{2^3(\lambda+1)^2} [\mathcal{C}_n^{(\lambda+1)}(1)]^2 + \frac{\|\mathcal{C}_{n+1}^{(\lambda+1)}\|_2^2}{2^3(\lambda+1)^2} 2n^2 + O(n^{4\lambda+1}) \\ &= -\frac{1+2\lambda}{2^3(\lambda+1)^2} \frac{n^{4\lambda+2}}{\Gamma(2\lambda+2)^2} + \frac{2n^2}{2^3(\lambda+1)^2} \frac{n^{4\lambda}}{4\lambda\Gamma(2\lambda+1)^2} + O(n^{4\lambda+1}) \\ &= \frac{n^{4\lambda+2}}{2^3(\lambda+1)^2 \Gamma(2\lambda+1)^2} \left(\frac{1}{2\lambda} - \frac{1+2\lambda}{(2\lambda+1)^2} \right) + O(n^{4\lambda+1}) \\ &= \frac{n^{4\lambda+2}}{2^3(\lambda+1)^2 \Gamma(2\lambda+1)^2} \frac{2\lambda+1}{2\lambda(2\lambda+1)^2} + O(n^{4\lambda+1}). \quad \blacksquare \end{aligned}$$

Tackling the more complicated version

If we regard following integral

$$\int_{-1}^1 (1-x^2)^\alpha [\mathcal{C}_n^{(\lambda)}(x)]^2 dx$$

and want to know it's asymptotic, we can make use of connection coefficients as in George Andrew's Book "Special Functions", page 360 Theorem 7.1.4' for:

$$\mathcal{C}_n^{(\lambda)}(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(\lambda)_{n-k} (\lambda - \mu)_k (n + \mu - 2k)}{(\mu + 1)_{n-k} k! \mu} \mathcal{C}_{n-2k}^{(\mu)}(x).$$

Letting $\mu = \alpha + \frac{1}{2}$, we can make use of the orthogonality relation and obtain

$$\begin{aligned} & \int_{-1}^1 (1-x^2)^\alpha [\mathcal{C}_n^{(\lambda)}(x)]^2 dx \\ &= \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(\lambda)_{n-k}^2 (\lambda - \mu)_k^2 (n + \mu - 2k)^2}{(\mu + 1)_{n-k}^2 k!^2 \mu^2} \int_{-1}^1 (1-x^2)^\alpha [\mathcal{C}_{n-2k}^{(\alpha+1/2)}(x)]^2 dx \end{aligned}$$

where the last integral is known:

$$\int_{-1}^1 (1-x^2)^{\lambda-1/2} [\mathcal{C}_n^{(\lambda)}(x)]^2 dx = \frac{\pi 2^{1-2\lambda} \Gamma(2\lambda + n)}{n!(n+\lambda)\Gamma(\lambda)^2} \quad \text{see [8, Eq. 7.313];}$$

These are the first steps in extending the obtained results - but my ideas do not seem applicable here. It is a side project that I am working on, trying to get this done in the next months or so.

0.2.3 Investigating the three-input case

We started to investigate the behavior of the three-input case, i.e. we were looking at triple integrals of the form:

$$I_F^3[\mu] := \iiint_{S_2} F(x, y, z) d\mu(x) d\mu(y) d\mu(z).$$

We want to pursue the same kind of questions as for the familiar two-input case: What is the minimizer of this energy, when is the standard surface measure σ a minimizer, when is σ a unique minimizer, for what kind of functions $F(x, y, z)$ is σ always a minimizer?

Natural questions ask for the structure of functions whose energy is minimized by σ :

Suppose $F_1(x, y, z)$ and $F_2(x, y, z)$ are minimized by σ , is the same true for the product function $F(x, y, z) = F_1(x, y, z)F_2(x, y, z)$?

Suppose $F(x, y, z)$ just depends only on the angles between the vectors x, y and z , denote them by u, v, t and $F(x, y, z) = h(u)h(v)h(t)$ where h is a known simple function. If $\int F(x, y, z)d\sigma(z)$ is positive semi-definite, can the same be said about h ?

In order to answer these questions, we follow the paper of C. Bachoc and F. Vallentin [2], where one can regard spheres of arbitrary dimension: $S_{n-1} \subset \mathbb{R}^n$ and set $\lambda = \frac{n-2}{2}$. We will focus our attention on the case $n = 3$ though. We further define the normalized Gegenbauer polynomials as $P_k^n(x)C_k^\lambda(1) := C_k^\lambda(x)$ and note that $P_1^m(x) = x$ and $P_0^m = 1$ for all $m \in \mathbb{N}$. Thus, as a sample list

we have for $\lambda > -\frac{1}{2}$:

$$\begin{aligned}
C_0^\lambda(x) &= 1, \\
C_1^\lambda(x) &= 2\lambda x, \\
C_2^\lambda(x) &= x^2(\lambda + 1)2\lambda - \lambda, \\
C_3^\lambda(x) &= x^3\frac{4}{3}(\lambda + 2)(\lambda + 1)\lambda - x(\lambda + 1)2\lambda, \\
C_4^\lambda(x) &= x^4\frac{2}{3}(\lambda + 3)(\lambda + 2)(\lambda + 1)\lambda - x^2\lambda(2\lambda^3 + 6\lambda + 4) + \frac{1}{2}(\lambda + 1)\lambda.
\end{aligned}$$

0.2.4 Small excerpt of calculations for the three-input case

For the decomposition as in [5], we will need matrices S_k^n symmetric in the entries u, v, t , and while the derivation is rather technically involved, I want to present just a specific one to convey the feeling how complicated things get. We first define the elementary functions

$$D_i^j(u, v, t) = D_j^i(u, v, t) = \frac{1}{2} \left(u^i(v^j + t^j) + v^i(t^j + u^j) + t^i(v^j + u^j) \right),$$

where we clearly have $(D_0^i(u, v, t))^2 = D_0^{2i}(u, v, t) + 4D_i^i(u, v, t)$. Then

$$\begin{aligned}
(S_0^3)_{0,0} &= 1, \\
(S_0^3)_{1,1} &= uv + vt + tu = D_1^1(u, v, t), \\
(S_0^3)_{2,2} &= \frac{5}{12} \left(9(u^2v^2 + v^2t^2 + t^2u^2) - 6(u^2 + v^2 + t^2) + 3 \right) \\
&= \frac{5}{12} \left(9D_2^2(u, v, t) - 6D_0^2(u, v, t) + D_0^0(u, v, t) \right) \\
(S_0^3)_{3,3} &= \frac{7}{12} \left(25(u^3v^3 + v^3t^3 + t^3u^3) - 15(\dots) + 9(uv + vt + tu) \right) \\
&= \frac{7}{12} \left(25D_3^3(u, v, t) - 30D_1^3(u, v, t) + 9D_1^1(u, v, t) \right).
\end{aligned}$$

It appears one can write $(S_0^3)_{s,s}$ in terms of $D_j^i(u, v, t)$ by taking the coefficients of $C_s^{\frac{1}{2}}(x)^2$ and replacing the highest to smallest monomials by $D_{s-2j-2i}^{s-2j}(u, v, t)$ where $0 \leq j \leq i \leq \lfloor s/2 \rfloor$.

Mean Zero Property of S_k^n

It is a nice side remark, that the triple integral of any entry of $S_k^n(u, v, t)$ w.r.t. the surface measure equals zero. To see this, note that

$$(Y_k^n)_{i,j} := P_i^{n+2k}(u)P_j^{n+2k}(v) \left((1-u^2)(1-v^2) \right)^{k/2} P_k^{n-1} \left(\frac{t-uv}{\sqrt{(1-u^2)(1-v^2)}} \right)$$

integrates to zero - we will further omit the normalization and deal with

$$(V_k^n)_{i,j} := C_i^{\lambda(k)}(u)C_j^{\lambda(k)}(v)\left((1-u^2)(1-v^2)\right)^{\frac{k}{2}}C_k^{\lambda(-\frac{1}{2})}\left(\frac{t-uv}{\sqrt{(1-u^2)(1-v^2)}}\right),$$

where $\lambda(k) = \frac{n+2k-2}{2}$. Recall:

$$\begin{aligned} u &= \langle x, y \rangle \\ v &= \langle y, z \rangle \\ t &= \langle x, z \rangle \end{aligned}$$

Also we note following relation for $\lambda, \mu > -\frac{1}{2}$ found in [1]:

$$C_n^\lambda(x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{(\lambda)_{n-k}(\lambda-\mu)_k}{(\mu+1)_{n-k}k!} \frac{n+\mu-2k}{\mu} C_{n-2k}^\mu(x),$$

where $(\lambda)_n = \prod_{j=0}^{n-1}(\lambda+j)$; thus for $\lambda = \lambda(k)$ and $\mu = \frac{1}{2}$ we have:

$$C_n^{\lambda(k)}(x) = \sum_{s=0}^{\lfloor \frac{n}{2} \rfloor} \frac{\binom{n+2k-2}{2}_{n-s} \binom{n+2k-3}{2}_s}{\left(\frac{3}{2}\right)_{n-s} s!} (2n+1-4s) C_{n-2s}^{\frac{1}{2}}(x). \quad (9)$$

We recall that the homogeneous harmonic polynomials of degree d restricted to S^{n-1} , denoted by H_d^n - also called spherical harmonics, have dimension h_d^n and any orthonormal basis $\{Y_{d,j}^n(x)\}$ of H_d^n satisfies, again with $\lambda(k) = \frac{n+2k-2}{2}$:

$$\sum_{j=1}^{h_d^n} Y_{d,j}^n(x)Y_{d,j}^n(y) = \frac{d+\lambda(0)}{\lambda(0)} C_d^{\lambda(0)}(\langle x, y \rangle).$$

Lemma 0.2.9. *With notation as above and for all $k, i, j \in \mathbb{N}_0$ with $k+i+j > 0$ and $n > 2$:*

$$\iiint_{S^{n-1}} (V_k^n)_{i,j}(u, v, t) d\sigma(x, y, z) = 0.$$

0.3 Overview for October 2019

This month was rather interesting as we obtained many results, proving some of the open questions to be wrong, which was rather surprising.

0.3.1 Functions $uv t$ and $u^2 v^2 t^2$

The simplest functions which depend only on the angle of their inputs are powers of $uv t$, so it is just natural to explore these basic functions first.

In the previous section we calculated some of the matrices $(S_k^d)_{i,j}$, which are important to obtain a decomposition of our functions of interest into sums that behave in a certain nice way, a result found in [2]. The functions in the title have an expansion in terms of positive semi-definite matrices F_j as written out in [5] and using most of the notation found there:

$$uv t = \sum_{k=0} \text{Trace}(F_k^1 S_k(u, v, t)),$$

$$u^2 v^2 t^2 = \sum_{k=0} \text{Trace}(F_k^2 S_k(u, v, t));$$

where

$$F_0^1 = \begin{pmatrix} \frac{1}{9} & 0 & \frac{2}{9\sqrt{5}} \\ 0 & 0 & 0 \\ \frac{2}{9\sqrt{5}} & 0 & \frac{4}{45} \end{pmatrix} \quad F_1^1 = \begin{pmatrix} 0 & 0 \\ 0 & \frac{2}{15} \end{pmatrix}$$

and

$$F_0^2 = \begin{pmatrix} \frac{11}{225} & 0 & \frac{293}{2205\sqrt{5}} & 0 & \frac{16}{1575} \\ 0 & 0 & 0 & 0 & 0 \\ \frac{293}{2205\sqrt{5}} & 0 & \frac{164}{2205} & 0 & \frac{64}{2205\sqrt{5}} \\ 0 & 0 & 0 & 0 & 0 \\ \frac{16}{1575} & 0 & \frac{64}{2205\sqrt{5}} & 0 & \frac{32}{3675} \end{pmatrix} \quad F_1^2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{16}{735} & 0 & \frac{16\sqrt{2/3}}{735} \\ 0 & 0 & 0 & 0 \\ 0 & \frac{16\sqrt{2/3}}{735} & 0 & \frac{32}{2205} \end{pmatrix} \quad F_2^2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{16}{2205} \end{pmatrix}.$$

Since the elements of the matrices S_k are positive definite functions, every measure will contribute a non-negative number - but σ integrates all, save the constant term $(S_0)_{0,0}$ to zero proving that the standard surface measure is a minimizer.

A second way to write them in terms of diagonal matrices only is:

$$F_0^1 = \begin{pmatrix} \frac{1}{9} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{8}{45} \end{pmatrix} \quad F_1^1 = \begin{pmatrix} 0 & 0 \\ 0 & \frac{14}{45} \end{pmatrix} \quad F_2^1 = \frac{8}{45}$$

and

$$F_0^2 = \begin{pmatrix} \frac{11}{225} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{2314}{15435} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{192}{8575} \end{pmatrix} \quad F_1^2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1516}{15435} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1024}{25725} \end{pmatrix}$$

$$F_2^2 = \begin{pmatrix} \frac{1756}{15435} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{2032}{77175} \end{pmatrix} \quad F_3^2 = \begin{pmatrix} 0 & 0 \\ 0 & \frac{32}{3675} \end{pmatrix} \quad F_4^2 = -\frac{64}{11025}.$$

This already shows that the representation is neither unique, nor always positive semi-definite. Once the matrices are found, it is rather easy to check that they work - but how to get them and why stop at degree two? Well, both questions are answered by the same fact really, they have been found by a computer algorithm which I wrote. This algorithm just needs you to enter the function you are interested in, in this case uv or $(uv)^2$, and it will compute the matrices and check if they are positive semi-definite as required by the theoretical result obtained by Bachoc and Vallentin. In case the degree was three or four, the computer wasn't able to find positive semi-definite matrices, in degree five my algorithm came to its boundaries. The intention is to improve the algorithm to search a wider spectrum of possibilities. Next we describe it.

0.3.2 The algorithm that looks for positive semi-definite matrices

Here we present the algorithm that found the representation by positive semi-definite matrices in the previous sections, written for Mathematica 11 (this is a well known computer program among scientists that need to do computations - and nowadays people outside any scientific field might have heard about its parent company: Wolfram, with their famous "ask anything"-website WolframAlpha). First we give the definition of functions that we need to manipulate and follow the paper of Bachoc and Vallentin.

$$\begin{aligned} f[i, n, x] &:= \text{GegenbauerC}[i, n/2 - 1, x] / \text{GegenbauerC}[i, n/2 - 1, 1]; \\ h[i, k] &:= \text{Binomial}[3 + 2k + i - 1, 2 + 2k] - \text{Binomial}[2k + i, 2 + 2k]; \\ w[n] &:= 2 * \text{Pi}^{(n/2)} / \text{Gamma}[n/2]; \\ l[i, j, k, n] &:= w[n] / w[n - 1] * w[n + 2k - 1] / w[n + 2k] * \text{Sqrt}[h[i, k] * h[j, k]]; \\ q[k, u, v, t] &:= ((1 - u^2) * (1 - v^2))^{(k/2)} * \text{ChebyshevT}[k, (t - u * v) / \text{Sqrt}[(1 - u^2) * (1 - v^2)]]; \\ y[n, k, i, j, u, v, t] &:= l[i, j, k, n] * f[i, n + 2k, u] * f[j, n + 2k, v] * q[k, u, v, t]; \\ s[n, k, i, j, u, v, t] &:= (y[n, k, i, j, t, u, v] + y[n, k, i, j, u, v, t] + y[n, k, i, j, u, t, v] + y[n, k, i, j, v, u, t] + \\ &\quad y[n, k, i, j, v, t, u] + y[n, k, i, j, t, v, u]) / 6; \end{aligned}$$

The next step is to program the actual algorithm that does the work for us automatically.

```

maxterm = 1000;
ident = IdentityMatrix[1000];
replacement = Reverse[Flatten[Table[ui * vj * ts * z - >
                                ident[[FromDigits[i, j, s] + 1]], i, 0, 9, j, 0, 9, s, 0, 9]]];
mat = ConstantArray[0, 750, maxterm];
Table[mat[[FromDigits[i, j] + 1]] =
      (Expand[Simplify[s[3, 0, i, j, u, v, t] * z]]/.replacement), i, 0, 9, j, 0, 9];
Table[mat[[FromDigits[i, j] + 101]] =
      (Expand[Simplify[s[3, 1, i, j, u, v, t] * z]]/.replacement), i, 0, 8, j, 0, 8];
:

```

The heart of the whole script is to use the most basic of non trivial mathematics: Linear Algebra. Thus we need to find a way of replacing in a one to one fashion our polynomials in the variables u, v, t by vectors.

The idea I had was to use the row of a matrix with a million entries. The expression “replacement” defines hundreds of rules how to make this association, i.e. $u^3v^7t^0z$ is associated to the basic vector e_{371} (a 1000-tuple with zero’s everywhere except for the entry 371, where we find a one) - note there is a shift by one, this is to avoid the problem of $u^0v^0t^0z$ not being associated to any basic vector. Next we define a dummy object where we will store data: mat . For each $0 \leq i, j \leq 9$, we take the polynomials $s[3, 0, i, j, u, v, t] * z$, apply our replacement rules to it and store the resulting vector as the $(ij + 1)$ -th row of the matrix mat (note ij here denotes the number $i * 10 + j$).

To see how this works, take for instance $s[3, 0, 1, 1, u, v, t] = uv + vt + tu$ (as can be seen from the subsection “small excerpt of calculations for the three-input case”), thus

$s[3, 0, 1, 1, u, v, t] * z = uvz + vtz + tuz$ gets replaced by $e_{111} + e_{12} + e_{101}$, which is the vector (or 1000-tuple) with zero’s everywhere except for the entries 111, 101, and 12 where we the integer one. Proceeding this way, we fill the first hundred rows by replacements for $s[3, 0, i, j, u, v, t] * z$, the next hundred rows with replacements for $s[3, 1, i, j, u, v, t] * z$ (note the entry 1 as the second coefficient) and so forth. We stop at row 750 to save some computation time, as the whole script is rather time consuming.

All is set right now, we translated our problem into Linear Algebra, something the computer

program Mathematica 11 has plenty of tools to work with. Let us see how this works actually.

```

b = Expand[Simplify[(u3v3t3) * z]]/.replacement;
aunflat = LinearSolve[Transpose[mat], b];
a = Flatten[aunflat];
pol[x] := Sum[a[[j + 1]] * xj, j, 0, 749];
replacex = Reverse[Flatten[Table[xs - > kFloor[s/100]iMod[Floor[s/10],10]jMod[s,10], s, 0, 749]]];

```

First and foremost we have to enter the term we want to investigate, in this case $(uvt)^3$ - where we use our replacement rules to associate a vector b to it. What are possible combinations of the functions $s[n, k, i, j, u, v, t]$, scaled by some factors, to reconstruct our term above? This same question posed in the language of Linear Algebra becomes: Is the vector b in the span of vectors given by the rows of the matrix mat ?

This is what “LinearSolve” does, and promptly finds *a* solution - there might be many actually. The obtained vector a has now the solution as its coefficients, i.e. our vector b can now be written as: the first row of mat multiplied by the first entry of the vector a plus the second row of mat multiplied by the second entry of a plus, etc.

But we want to know which polynomials in u, v, t constitute $(uvt)^3$, so we write the solution vector a as a polynomial of degree 750 and write another set of rules to replace a power of x with the right function $s[n, k, i, j, u, v, t]$ (here we use the fact that we know how the rows were constructed). If everything works as expected, we should obtain the term we entered. Thus the computational part is now done, all we have to do is print out the results in a way readable by humans:

```

Print[" The suggested linear combination looks like this:"]
pol[x]/.replacex
Print[" Just to make sure, when we substitute the corresponding functions, we obtain:"]
Simplify[Sum[a[[j + 1]] * s[3, Floor[j/100], Mod[Floor[j/10], 10], Mod[j, 10], u, v, t], j, 0, 749]]
mat0 = ConstantArray[0, 10, 10];
mat1 = mat0;
mat2 = mat0;
:

```

We let the computer first print its findings, and then let it use the found linear combination and apply it to the base functions to see if we really obtain the polynomial we entered. But we are not finished just yet. We need to know if the associated matrices are positive semi-definite. So first we

define dummy matrices that will contain the found solution factors.

```

Table[mat0[[Mod[Floor[j/10], 10] + 1, Mod[j, 10] + 1]] = a[[j + 1]], j, 0, 99];
Table[mat1[[Mod[Floor[j/10], 10] + 1, Mod[j, 10] + 1]] = a[[j + 101]], j, 0, 99];
:
F0 = (mat0 + Transpose[mat0])/2;
F1 = (mat1 + Transpose[mat1])/2;
F2 = (mat2 + Transpose[mat2])/2;
:
Print["Are the matrices F0, F1, ..., F7 respectively positive semidefinite?"]
PositiveSemidefiniteMatrixQ[F0]
PositiveSemidefiniteMatrixQ[F1]
:

```

We enter all the coefficients and let Mathematica 11 check if they are positive definite or not. What we obtain as output is written here:

The suggested linear combination looks like this:

Out[62] =

$31/1225 + (43334j^2)/(266805\text{Sqrt}[5]) + (4684i^2j^2)/88935\dots$

Just to make sure, when we substitute the corresponding functions, we obtain:

Out[64] = $t^3u^3v^3$

Are the matrices F_0, F_1, \dots, F_7 respectively positive semidefinite?

Out[69] = False

Out[70] = True

Out[71] = True

Out[72] = True

Out[73] = True

Out[74] = True

Out[75] = True

Out[76] = True

First the suggested linear combination, parts of it as it has no real value at this point; note again that it is neither unique nor exhaustive. Next the algorithm automatically checks if the suggestion

is correct, just to be sure, we want the inserted polynomial to be reconstructed at this place. Everything looks good so far, but the last check (if the matrices are positive semidefinite), shows that the first one is not. This is a big problem as we cannot simply copy and paste the result to our paper, nor does it mean that there is no such combination as we already saw in the previous section, it is possible to have multiple possibilities for reconstruction. Something similar happens for $(uv)^4$.

0.3.3 Estimates of multiple integrals with respect to energies

When working with multiple integrals with respect to various probability measures, it is useful to have estimates on these terms using multiple integrals of the same measure. In order to do so, we found at the beginning of chapter 4 of [4] following lemma.

Lemma 0.3.1. *Suppose K is symmetric, lower semi-continuous, and conditionally strictly positive definite kernel on $A \times A$. Then for every pair of Borel probability measures μ_1 and μ_2 supported on A and having finite K -energies, the mutual energy $(\mu_1, \mu_2)_K$ is finite and satisfies*

$$2(\mu_1, \mu_2)_K \leq I[\mu_1] + I[\mu_2],$$

where the equality holds if and only if $\mu_1 = \mu_2$ on Borel subsets of A .

To be symmetric simply means that $K(x, y) = K(y, x)$ holds for any pair of points from the sphere; lower semi-continuity makes sure the function K behaves in a certain controlled way for nearby points, and it also makes sure the function has a minimum on the sphere. The property of being conditionally strictly positive definite is a technicality that is used to show uniqueness - but since we do not pursue this goal, we will leave it undefined and refer to the source material for the interested reader. Further, we abbreviated

$$(\mu_1, \mu_2)_K = \iint_A K(x, y) d\mu_1(x) d\mu_2(y).$$

Although we are mainly interested in triple integrals, we will try to transfer this result to multiple input energies.

Definition 0.3.1. We call a function K of s -inputs, $s > 1$, positive semidefinite if this is true for all the functions K_{x_3, \dots, x_s} , where $K_{x_3, \dots, x_s}(x, y) := K(x, y, x_3, \dots, x_s)$ and x_3, \dots, x_s are chosen from the domain of K .

Definition 0.3.2. For fixed $s > 1$ and an s -input function K , we set for $1 \leq s' \leq s$, and some Borel probability measures μ_1, \dots, μ_s , natural numbers $n_1, \dots, n_{s'}$ with $\Sigma = n_1 + \dots + n_{s'} \leq s$:

$$I_K[\mu_1^{n_1}, \dots, \mu_{s'}^{n_{s'}}](x_{\Sigma+1}, \dots, x_s) := \underbrace{\int \dots \int}_{\Sigma} K(x_1, \dots, x_s) d\mu_1(x_1, \dots, x_{n_1}) \dots d\mu_{s'}(x_{n_{s'}-1+1}, \dots, x_{n_{s'}}),$$

where $d\mu(x_1, \dots, x_n)$ is an abbreviation for $d\mu(x_1) \dots d\mu(x_n)$.

Given the necessary definitions and notation, we are ready to extend the result in the next lemma.

Lemma 0.3.2. *Suppose K is a symmetric, continuous, and positive semi-definite kernel on A^s for $s > 1$. Then for every s -tuple of Borel probability measures μ_1, \dots, μ_s supported on A , the mutual energy $I_K[\mu_1, \dots, \mu_s]$ satisfies*

$$I_K[\mu_1, \dots, \mu_s] \leq \frac{1}{s} \sum_{j=1}^s I_K[\mu_j^s].$$

Proof. By the previous lemma, this is true for $s = 2$. We proceed by induction and assume it is correct for s , and prove it for the case $s + 1$. We regard the s -input functions $K_{x_{s+1}}$, for which we know by the induction hypothesis that

$$I_K[\mu_1, \dots, \mu_s](x_{s+1}) \leq \frac{1}{s} \sum_{j=1}^s I_K[\mu_j^s](x_{s+1});$$

which we integrate with respect to the probability measure μ_{s+1} to obtain

$$I_K[\mu_1, \dots, \mu_s, \mu_{s+1}] \leq \frac{1}{s} \sum_{j=1}^s I_K[\mu_j^s, \mu_{s+1}]. \quad (10)$$

Further, we use Fubini's theorem on swapping the order of integration (which we can apply without problem as K is supposed to be continuous on a compact space) and the induction hypothesis to show

$$I[\mu^s, \rho] = I[\mu^{s-1}, \rho, \mu] \leq \frac{s-1}{s} I_K[\mu^s, \mu] + \frac{1}{s} I_K[\rho^s, \mu].$$

On the right-hand side we see a term of the same form appearing as on the left-hand side, thus we use the same inequality and obtain

$$I[\mu^s, \rho] \leq \frac{s-1}{s} I_K[\mu^s, \mu] + \frac{1}{s} \left(\frac{s-1}{s} I_K[\rho^s, \rho] + \frac{1}{s} I_K[\mu^s, \rho] \right),$$

which after elementary manipulations has the form

$$I[\mu^s, \rho] \leq \frac{s}{s+1} I_K[\mu^s, \mu] + \frac{1}{s+1} I_K[\rho^s, \rho].$$

Using this inequality and applying it to (10), finishes the proof. ■

Positive semi-definiteness of three input kernels

At this point we still do not know which property of a 3-input kernel to call positive semi-definite, let alone of an s -input kernel - the previous section introduced such a notion, but it is not clear at all

if this is the right one to use, or if there is not a better one waiting to be created. We introduced a notion of positive semi-definiteness in the previous section, next we introduce another one and show that in special cases, the old one follows from the new one (Lemma 0.3.3). We are mainly focusing on the case $K_r(x, y, z) = (x, y)^r (y, z)^r (z, x)^r$ for some $r \in \mathbb{N}$. Note that we have following equality

$$K_r(x, y, y) = K_r(y, x, x) = (x, y)^{2r},$$

and thus

$$K_r(x, y, z)^2 = K_r(x, y, y)K_r(y, z, z)K_r(z, x, x).$$

Since $(x, y)^{2r}$ is an even degree polynomial of the inner product, the kernel

$$G_r(x, y) = K_r(x, y, y)$$

is symmetric, and positive semi-definite. We are thus led to following

Definition 0.3.3. A continuous kernel $K(x_1, \dots, x_s)$ is (new) positive semi-definite iff

$$K(x, \underbrace{y, \dots, y}_{s-1}) = K(y, \underbrace{x, \dots, x}_{s-1})$$

and

$$G_K(x, y) = K(x, y, \dots, y)$$

is positive semi-definite.

By Mercer's theorem, we find for arbitrary (new) positive semi-definite kernels $K(x, y, z)$, that

$$P^z(x, y) = K(y, z, z)K(z, x, x)$$

is positive semi-definite: Write

$$K(y, z, z) = \sum_{j \geq 1} \lambda_j \psi_j(y) \psi_j(z),$$

for an ONB of $L^2(S_d, \mu)$ with given measure μ and regard

$$\iint P^z(x, y) \psi_k(x) \psi_m(y) \, d\mu(x) \, d\mu(y) = \lambda_k \psi_k(z) \lambda_m \psi_m(z);$$

thus for $\phi(z) = \sum_{j \geq 0} \alpha_j \psi_j(z)$ we have

$$\iint P^z(x, y) \phi(x) \phi(y) \, d\mu(x) \, d\mu(y) = \left(\sum_{j \geq 0} \alpha_j \lambda_j \psi_j(z) \right)^2.$$

Also note that the λ_j are a null-sequence, hence convergence cannot be a problem. Since the product of positive semi-definite kernels is positive semi-definite, all in all we have proved

Lemma 0.3.3. For (new) positive semi-definite kernels $K(x, y, z)$, the kernel

$$G^z(x, y) = K(x, y, y)K(y, z, z)K(z, x, x)$$

is (old) positive semi-definite, i.e. positive semi-definite for every fixed z .

Thus in particular, $K_r(x, y, z)^2$ is (old) positive semi-definite - also note that

$$\iint K(x, y, y)K(y, z, z)K(z, x, x) d\mu(x) d\mu(y) = \sum_{j \geq 1} \lambda_j^3 \psi_j(z) \geq 0.$$

(It follows from the definition of psd with a constant function.)

0.3.4 Functions of the form $F(u, v, t) = h(u)h(v)h(t)$

If we define

$$H(u) = \int h(v)h(t)d\sigma(z)$$

and obtain that

$$h(u)H(u) = \int F(u, v, t)\sigma(z) \text{ is positive definite;}$$

we can not conclude that $h(u)$ is positive definite:

Lemma 0.3.4. With the notation as above and any $\lambda \geq \frac{1}{2}$, $n > 1$, if we define $h(u)$ as

$$h(u) = \frac{1}{3} - C_1^\lambda(u) + \sum_{j=2}^{n+1} a_j C_j^\lambda(u), \quad (11)$$

where $a_2 = a_3 = 1$ and $\frac{\lambda+j}{\lambda+1} \geq a_j \geq 0$ for $j > 3$. Then $h(u)H(u)$ will have a Gegenbauer expansion with non-negative coefficients, save the constant term.

These were some of the results we obtained and there are many more questions to look into.

Bibliography

- [1] G. E. Andrews: *Special Functions*.
- [2] C. Bachoc and F. Vallentin: *New upper bounds for kissing numbers from semidefinite programming*. Journal of the AMS, Vol. 21 Nr. 3 Pages 909-924 (2008)
- [3] C. Beltrán and D. Ferizović: *Approximation to uniform distribution in $SO(3)$* . arXiv.org (2019)

- [4] S. V. Borodachov, D. P. Hardin and E. B. Saff: *Discrete Energy on Rectifiable Sets*, Springer (2019)
- [5] H. Cohn and J. Woo: *Three-Point Bounds for Energy Minimization*
Journal of the AMS Vol. 25 Nr. 4 Pages 929-958 (2012)
- [6] H. Dette: *New identities for orthogonal polynomials on a compact interval*; J. Math. Anal. Appl. 179, pp. 547-573 (1993).
- [7] D. Ferizović: *On the L^2 -norm of Gegenbauer polynomials*. arXiv.org (2019)
- [8] I. S. Gradshteyn, I. M. Ryzhik, A. Jeffrey, D. Zwillinger: *Table of Integrals, Series, and Products*; Academic Press; 6th edition (2000).
- [9] J. Sánchez-Ruiz and J. S. Dehesa: *Some connection and linearization problems for polynomials in and beyond Askey scheme*
Journal of Computational and Applied Mathematics 133 Pages 579-591 (2001)
- [10] G. Szegő: *Orthogonal Polynomials*; 4th Edition; Amer. Math. Soc. (1975).
- [11] F. Tricomi and A. Erdélyi: *The Asymptotic Expansion of a Ration of Gamma Functions*; Pacific Journal of Mathematics Vol. 1 Nr. 1, pp. 133-142 (1951).