

## Notes on multidimensional scaling of distances in a symmetric space

Work in progress, J. Victor jdvicto@med.cornell.edu

### Main Results

SO(2) (or, equivalently, the circle  $S_1$ ) can be isometrically embedded in a Euclidean space with an “embedding exponent”  $\frac{s}{2} \leq \frac{1}{2}$  (eq. (18))

SO( $n$ ) ( $n \geq 3$ ) cannot be isometrically embedded in a Euclidean space with any embedding exponent (eq. (19) and preceding material)

The sphere ( $S_2$ ) can be isometrically embedded in a Euclidean space with an “embedding exponent”  $\frac{s}{2} \leq \frac{1}{2}$  (eq. (34))

The hypersphere ( $S_3$ ) can be isometrically embedded in a Euclidean space with an “embedding exponent”  $\frac{s}{2} \leq \frac{1}{2}$  (eq. (42)).  $S_5$  can be similarly embedded (eq. (60)).

An interesting series for  $\mathbf{p}$  (eq. (38))

Expression of the ultraspherical (Gegenbauer) polynomials as trigonometric polynomials, involving the Catalan numbers or the binomial coefficients, depending on the parity of the dimension (eqs. (51) and (52))

### For further work

Proof of conjectured form for the hypersphere (62) for  $a = 4$  and  $a \geq 6$ , and consequent additional series for  $\mathbf{p}$

Other symmetric spaces (the  $k$ -planes in  $n$ -space) acted on by SO( $n$ )

Non-Euclidean spaces, e.g.,  $SL(n, \mathbb{R})$  and  $SL(n, \mathbb{C})$  and objects that they act on  
Minkowski space, exploiting just the translation group

### General setup

$G$ : a continuous compact group that acts on a symmetric space  $S$

$\mathbf{a}, \mathbf{b}, \mathbf{g}$ : elements of  $G$

### $G$ and $S$ are identical

The action of  $G$  on  $S$  is the regular action. Let  $d(\mathbf{a}, \mathbf{b})$  be the geodesic distance in  $G$ . It has the usual properties of a metric:  $d(\mathbf{a}, \mathbf{b}) = d(\mathbf{b}, \mathbf{a})$ ,  $d(\mathbf{a}, \mathbf{a}) = 0$ ,  $d(\mathbf{a}, \mathbf{b}) > 0$  for  $\mathbf{a} \neq \mathbf{b}$ , and the triangle inequality  $d(\mathbf{a}, \mathbf{b}) \leq d(\mathbf{a}, \mathbf{g}) + d(\mathbf{g}, \mathbf{b})$ . In addition, it is preserved by the group action:

$$d(\mathbf{ag}, \mathbf{bg}) = d(\mathbf{gb}, \mathbf{ga}) = d(\mathbf{a}, \mathbf{b}). \quad (1)$$

We want to relate the distance to a Euclidean distance, by mapping each group element  $\mathbf{a}$  to a vector  $(x_1(\mathbf{a}), x_2(\mathbf{a}), \dots, x_k(\mathbf{a}), \dots)$ , so that

$$f(d(\mathbf{a}, \mathbf{b})) = \sum_k (x_k(\mathbf{a}) - x_k(\mathbf{b}))^2, \quad (2)$$

some monotonic function  $f$ . For reasons discussed in Aronov and Victor (2004), we will only consider  $f(d) = d^s$ , where  $s/2$  is the “embedding exponent.” That is

$$(d(\mathbf{a}, \mathbf{b}))^{s/2} = \left( \sum_k (x_k(\mathbf{a}) - x_k(\mathbf{b}))^2 \right)^{1/2}. \quad (3)$$

The dimension of the embedding, and hence the number of terms in the sum, is typically infinite. That is, our goal is to recapitulate  $d$  exactly for all elements  $\mathbf{a}, \mathbf{b}$  of  $G$  via this Euclidean distance. This is in contrast to a more common viewpoint, in which the goal is to approximate  $d$  with a small number of dimensions. [Indyk, P., and Matousek, J. Low Distortion Embeddings of Finite Metric Spaces, in Handbook of Discrete and Computational Geometry, 2nd. Ed., editors: Goodman, J.E., and O'Rourke, J., in press (2004). CRC Press LLC, Boca Raton, FL]

$$\text{Let } \mathbf{m} = \langle f(d(0, \mathbf{b})) \rangle_{\mathbf{b} \in G} = \langle f(d(\mathbf{a}, \mathbf{b})) \rangle_{\mathbf{a}, \mathbf{b} \in G} = \frac{1}{|G|} \int_G f(d(0, \mathbf{b})) d\mathbf{b}, \quad (4)$$

where  $\langle \rangle$  denotes an average with respect to the invariant measure, the integral is also taken with respect to the invariant measure on  $G$ , and  $|G| = \int_G d\mathbf{b}$ .

Following Kruskal's approach for multidimensional scaling, we write

$$F(\mathbf{a}, \mathbf{b}) = -\frac{1}{2} f(d(\mathbf{a}, \mathbf{b})) + \frac{1}{2} \langle f(d(\mathbf{a}, \mathbf{g})) \rangle_{\mathbf{g} \in G} + \frac{1}{2} \langle f(d(\mathbf{g}, \mathbf{b})) \rangle_{\mathbf{g} \in G} - \frac{1}{2} \langle f(d(\mathbf{g}, \mathbf{g}')) \rangle_{\mathbf{g}, \mathbf{g}' \in G},$$

which, because of the symmetries, becomes

$$F(\mathbf{a}, \mathbf{b}) = -\frac{1}{2} f(d(\mathbf{a}, \mathbf{b})) + \mathbf{m}. \quad (5)$$

Equation (2) is now equivalent to

$$F(\mathbf{a}, \mathbf{b}) = \sum_k x_k(\mathbf{a}) x_k(\mathbf{b}). \quad (6)$$

We can assume that  $\langle x_k(\mathbf{a}) \rangle_{\mathbf{a} \in G} = 0$ , and replace  $x_k(\mathbf{a})$  by  $y_k(\mathbf{a}) = \frac{x_k(\mathbf{a})}{\sqrt{\langle |x_k(\mathbf{g})|^2 \rangle_{\mathbf{g} \in G}}}$ , so that

our goal is to write

$$F(\mathbf{a}, \mathbf{b}) = \sum_k \mathbf{I}_k y_k(\mathbf{a}) y_k(\mathbf{b}) \quad (7)$$

for orthonormal functions  $y_k$  on  $G$ . This is equivalent to finding the eigenvalues  $\mathbf{I}_k$  and eigenfunctions  $y_k$  of an integral operator:

$$\frac{1}{|G|} \int_G F(\mathbf{a}, \mathbf{b}) y_k(\mathbf{b}) d\mathbf{b} = \mathbf{I}_k y_k(\mathbf{a}).$$

### Diagonalization

$F(\mathbf{a}, \mathbf{b})$  is a function on  $G \times G$ . An orthogonal basis for such functions are the matrix elements of all the irreducible representations of  $G \times G$ . These are parameterized by a pair  $(\mathbf{r}, \mathbf{s})$ , where both  $\mathbf{r}$  and  $\mathbf{s}$  are irreducible representations of  $G$ . Say  $\mathbf{r}_{m_1 m_2}(\mathbf{a})$  is a typical matrix element of  $\mathbf{r}$  (for  $m_1$  and  $m_2$  in  $[1, \dots, \dim \mathbf{r}]$ ) and similarly for  $\mathbf{s}_{n_1 n_2}(\mathbf{b})$ . Thus,

$$F(\mathbf{a}, \mathbf{b}) = \sum_{\mathbf{r}, \mathbf{s}} \mathbf{r}_{m_1 m_2}(\mathbf{a}) \mathbf{s}_{n_1 n_2}(\mathbf{b}) \tilde{F}_{\mathbf{r}, \mathbf{s}}(m_1, m_2, n_1, n_2). \quad (8)$$

Since

$$\left\langle \mathbf{r}_{m_1 m_2}(\mathbf{a}) \overline{\mathbf{s}_{n_1 n_2}(\mathbf{a})} \right\rangle_{\mathbf{a} \in G} = \frac{1}{\dim \mathbf{r}} \mathbf{d}_{\mathbf{r}} \mathbf{d}_{m_1 n_1} \mathbf{d}_{m_2 n_2}, \quad (9)$$

it follows that

$$\tilde{F}_{\mathbf{r}, \mathbf{s}}(m_1, m_2, n_1, n_2) = \dim \mathbf{r} \dim \mathbf{s} \left\langle F(\mathbf{a}, \mathbf{b}) \overline{\mathbf{r}_{m_1 m_2}(\mathbf{a}) \mathbf{s}_{n_1 n_2}(\mathbf{b})} \right\rangle_{\mathbf{a}, \mathbf{b} \in G}. \quad (10)$$

Via a change of variables  $\mathbf{a} = \mathbf{g}\mathbf{b}$ , it follows that

$$\tilde{F}_{\mathbf{r}, \mathbf{s}}(m_1, m_2, n_1, n_2) = \dim \mathbf{r} \dim \mathbf{s} \left\langle F(\mathbf{g}\mathbf{b}, \mathbf{b}) \overline{\mathbf{r}_{m_1 m_2}(\mathbf{g}\mathbf{b}) \mathbf{s}_{n_1 n_2}(\mathbf{b})} \right\rangle_{\mathbf{b}, \mathbf{g} \in G},$$

from which the fact that  $\mathbf{r}$  is a group representation, and eq. (1), imply

$$\tilde{F}_{\mathbf{r}, \mathbf{s}}(m_1, m_2, n_1, n_2) = \dim \mathbf{r} \dim \mathbf{s} \left\langle F(0, \mathbf{g}) \overline{\sum_{r=1}^{\dim \mathbf{r}} \mathbf{r}_{m_1 r}(\mathbf{g}) \mathbf{r}_{r m_2}(\mathbf{b}) \mathbf{s}_{n_1 n_2}(\mathbf{b})} \right\rangle_{\mathbf{b}, \mathbf{g} \in G}.$$

The average over  $\mathbf{b}$  can now be computed separately, via eq. (9):

$$\left\langle \overline{\mathbf{r}_{m_2}(\mathbf{b}) \mathbf{s}_{n_1 n_2}(\mathbf{b})} \right\rangle_{\mathbf{b} \in G} = \frac{1}{\dim \mathbf{r}} \mathbf{d}_{\mathbf{r}} \mathbf{d}_{m_1 n_1} \mathbf{d}_{m_2 n_2}. \quad (11)$$

Thus,

$$\tilde{F}_{\mathbf{r}, \mathbf{r}}(m_1, m_2, n_1, m_2) = \dim \mathbf{r} \left\langle F(0, \mathbf{g}) \overline{\mathbf{r}_{m_1 n_1}(\mathbf{g})} \right\rangle_{\mathbf{g} \in G}, \quad (12)$$

and  $\tilde{F}_{\mathbf{r},\mathbf{s}}(m_1, m_2, n_1, n_2) = 0$  unless  $\mathbf{s} = \overline{\mathbf{r}}$  and  $n_2 = m_2$ .

To calculate the quantity in eq. (12), we break down the average over the group into an average over conjugate classes, parameterized by  $\mathbf{q}$ , weighted by the volume  $h(\mathbf{q})$  of each conjugate class  $c(\mathbf{q})$ :

$$\left\langle F(0, \mathbf{g}) \overline{\mathbf{r}_{m_1 n_1}(\mathbf{g})} \right\rangle_{\mathbf{g} \in G} = \int \left\langle F(0, \mathbf{g}) \overline{\mathbf{r}_{m_1 n_1}(\mathbf{g})} \right\rangle_{\mathbf{g} \in c(\mathbf{q})} h(\mathbf{q}) d\mathbf{q} .$$

The property (1) implies that  $F(0, \mathbf{q}) = F(0, \mathbf{nqn}^{-1})$ , so  $F(0, \mathbf{g}) = F(0, \mathbf{q})$  for any  $\mathbf{g} \in c(\mathbf{q})$ . Moreover, the average of  $\overline{\mathbf{r}}$  over a conjugate class  $c(\mathbf{q})$  commutes with any  $\overline{\mathbf{r}}(\mathbf{a})$  and has trace  $\mathbf{c}_{\overline{\mathbf{r}}}(\mathbf{q})$ , from which it follows that

$$\left\langle \overline{\mathbf{r}_{m_1 n_1}(\mathbf{g})} \right\rangle_{\mathbf{g} \in c(\mathbf{q})} = \frac{1}{\dim \mathbf{r}} \mathbf{d}_{m_1 n_1} \mathbf{c}_{\overline{\mathbf{r}}}(\mathbf{q}) .$$

Therefore,

$$\left\langle F(0, \mathbf{g}) \overline{\mathbf{r}_{m_1 n_1}(\mathbf{g})} \right\rangle_{\mathbf{g} \in G} = \frac{1}{\dim \mathbf{r}} \mathbf{d}_{m_1 n_1} \int F(0, \mathbf{q}) \overline{\mathbf{c}_{\overline{\mathbf{r}}}(\mathbf{q})} h(\mathbf{q}) d\mathbf{q} . \quad (13)$$

Note that since  $\left\langle F(0, \mathbf{g}) \right\rangle_{\mathbf{g} \in G} = 0$  (as a consequence of eq. (5)), eq. (13) is zero for the trivial representation. Combining eqs. (5), (12), and (13) yields

$$\tilde{F}_{\overline{\mathbf{r}}, \overline{\mathbf{r}}}(m_1, m_2, m_1, m_2) = -\frac{1}{2} \int f(d(\mathbf{q}, 0)) \overline{\mathbf{c}_{\overline{\mathbf{r}}}(\mathbf{q})} h(\mathbf{q}) d\mathbf{q} , \quad (14)$$

and  $\tilde{F}_{\mathbf{r}, \mathbf{s}}(m_1, m_2, n_1, n_2) = 0$  unless  $\mathbf{s} = \overline{\mathbf{r}}$ ,  $n_1 = m_1$ , and  $n_2 = m_2$ .

Therefore, the irreducible representation  $\mathbf{r}$  contributes  $(\dim \mathbf{r})^2$  orthogonal functions  $y_k$ , one for each matrix element  $\mathbf{r}_{m_1 m_2}$ . In view of eq. (11),  $(\sqrt{\dim \mathbf{r}}) \mathbf{r}_{m_1 m_2}(\mathbf{a})$  are orthonormal. Thus, comparing eq. (7) and (8), all of these  $(\dim \mathbf{r})^2$  eigenvalues are equal to

$$\Lambda_{\mathbf{r}} = \frac{1}{\dim \mathbf{r}} \tilde{F}_{\overline{\mathbf{r}}, \overline{\mathbf{r}}}(m_1, m_2, m_1, m_2) = -\frac{1}{2 \dim \mathbf{r}} \int f(d(\mathbf{q}, 0)) \overline{\mathbf{c}_{\overline{\mathbf{r}}}(\mathbf{q})} h(\mathbf{q}) d\mathbf{q} . \quad (15)$$

### **Parseval relation**

From the orthonormality of the  $y_k$ , it follows from eq. (6) that

$$\left\langle |F(\mathbf{a}, \mathbf{b})|^2 \right\rangle_{\mathbf{a}, \mathbf{b} \in G} = \left\langle |F(\mathbf{a}, 0)|^2 \right\rangle_{\mathbf{a} \in G} = \sum_k \mathbf{I}_k^2 . \quad (16)$$

Note that

$$4 \left\langle |F(\mathbf{a}, 0)|^2 \right\rangle_{\mathbf{a} \in G} = \left\langle |f(d(\mathbf{a}, 0) - \mathbf{m})|^2 \right\rangle_{\mathbf{a} \in G} = \left\langle |f(d(\mathbf{a}, 0)|^2 \right\rangle_{\mathbf{a} \in G} - \mathbf{m}^2 . \quad (17)$$

## Applications

We carry out this program for  $SO(n)$ .

### SO(2)

Elements of the group, and conjugate classes, are parameterized by an angle  $\mathbf{q} \in [-\mathbf{p}, \mathbf{p}]$ . Irreducible representations are parameterized by an integer  $n \in \mathbb{Z}$  (both positive and negative), with  $\mathbf{c}_n(\mathbf{q}) = e^{in\mathbf{q}}$ . Representations are one-dimensional. The weight of a conjugate class  $\mathbf{q}$  is  $h(\mathbf{q}) = \frac{1}{2\mathbf{p}}$ . The distance is given by  $d(\mathbf{q}, 0) = |\mathbf{q}|$ .

With  $f(d) = d^s$ , eq. (15) yields

$$\Lambda_n(s) = -\frac{1}{2} \int_{-\mathbf{p}}^{\mathbf{p}} |\mathbf{q}|^s e^{in\mathbf{q}} \frac{d\mathbf{q}}{2\mathbf{p}} = -\frac{1}{2\mathbf{p}} \int_0^{\mathbf{p}} |\mathbf{q}|^s \cos(n\mathbf{q}) d\mathbf{q}.$$

For  $s > 1$ , this expression becomes negative for sufficiently large even values of  $n$ , thus indicating that a Euclidean embedding is not possible.

Specializing to  $s=1$  yields

$$\Lambda_n(1) = \frac{1}{\mathbf{p}n^2} \quad (n \text{ odd}) \quad \text{and} \quad \Lambda_n(1) = 0 \quad (n \text{ even}). \quad (18)$$

For the Parseval relation (with  $s=1$ ),  $\mathbf{m} = \frac{\mathbf{p}}{2}$ ,  $\left\langle |f(d(\mathbf{a}, 0))|^2 \right\rangle_{\mathbf{a} \in G} = \frac{1}{2\mathbf{p}} \int_{-\mathbf{p}}^{\mathbf{p}} \mathbf{q}^2 d\mathbf{q} = \frac{\mathbf{p}^2}{3}$ ,

$$\left\langle |f(d(\mathbf{a}, 0))|^2 \right\rangle_{\mathbf{a} \in G} - \mathbf{m}^2 = \frac{\mathbf{p}^2}{12},$$

and (recalling that terms from  $n$  and  $-n$  contribute) the familiar series

$$\frac{\mathbf{p}^4}{96} = \frac{1}{1^4} + \frac{1}{3^4} + \frac{1}{5^4} + \dots \text{ is recovered from (16).}$$

### SO(3)

Conjugate classes, are parameterized by an angle  $\mathbf{q} \in [0, \mathbf{p}]$ , the angle of rotation.

Irreducible representations are parameterized by an integer  $n > 0$ . The  $n$ th irreducible representation is the action of  $G$  on homogeneous polynomials  $p(x, y, z)$  of degree  $n$  for

which  $\nabla^2 p = 0$ . It is of dimension  $2n+1$ , and has character  $\mathbf{c}_n(\mathbf{q}) = \sum_{m=-n}^n e^{im\mathbf{q}}$ . The weight

of a conjugate class  $\mathbf{q}$  is  $h(\mathbf{q}) = \frac{1 - \cos \mathbf{q}}{\mathbf{p}}$ . The distance is given by  $d(\mathbf{q}, 0) = |\mathbf{q}|$ .

With  $f(d) = d^s$ , eq. (15) yields

$$\Lambda_n(s) = -\frac{1}{2(2n+1)} \int_0^{\mathbf{p}} |\mathbf{q}|^s \left( \sum_{m=-n}^n e^{im\mathbf{q}} \right) \frac{1 - \cos \mathbf{q}}{\mathbf{p}} d\mathbf{q} = -\frac{1}{2\mathbf{p}(2n+1)} \int_0^{\mathbf{p}} |\mathbf{q}|^s (\cos(n\mathbf{q}) - \cos((n+1)\mathbf{q})) d\mathbf{q}$$

For  $s > 0$ , this expression becomes negative for even values of  $n$ , thus indicating that a Euclidean embedding is not possible.

Specializing to  $s=1$  yields

$$\Lambda_n(1) = \frac{1}{2n+1} \frac{1}{\mathbf{p}n^2} \quad (n \text{ odd}) \quad \text{and} \quad \Lambda_n(1) = -\frac{1}{2n+1} \frac{1}{\mathbf{p}(n+1)^2} \quad (n \text{ even}). \quad (19)$$

For the Parseval relation (with  $s=1$ ),  $\mathbf{m} = \frac{\mathbf{p}}{2} + \frac{2}{\mathbf{p}}$ ,

$$\left\langle |f(d(\mathbf{a}, 0))|^2 \right\rangle_{\mathbf{a} \in G} = \frac{1}{\mathbf{p}} \int_0^{\mathbf{p}} \mathbf{q}^2 (1 - \cos \mathbf{q}) d\mathbf{q} = \frac{\mathbf{p}^2}{3} + 2,$$

$\left\langle |f(d(\mathbf{a}, 0))|^2 \right\rangle_{\mathbf{a} \in G} - \mathbf{m}^2 = \frac{\mathbf{p}^2}{12} - \frac{4}{\mathbf{p}^2}$ , and again the familiar series  $\frac{\mathbf{p}^4}{96} = \frac{1}{1^4} + \frac{1}{3^4} + \frac{1}{5^4} + \dots$  is recovered from (16).

### Setup for $G$ and $S$ distinct

We posit a map  $\mathbf{f}$  from  $G$  to  $S$ , and  $d$  is a distance in  $S$ . The property (1) is replaced by  $d(\mathbf{f}(\mathbf{g}\mathbf{b}), \mathbf{f}(\mathbf{g}\mathbf{a})) = d(\mathbf{f}(\mathbf{a}), \mathbf{f}(\mathbf{b}))$ . (20)

The circle  $S_1$

This is identical to  $S=G=SO(2)$ ;  $G$  and  $S$  are not distinct.

The sphere  $S_2$

We use the setup with an explicit map  $\mathbf{f}$  from  $G$  to  $S$ , not the ‘‘coset’’ setup. The right-hand version of property (1) is not used until after eq. (12). Using eq. (20) rather than eq. (1), we evaluate eq. (12) as follows:

$G=SO(3)$ . The map  $\mathbf{f}$  from  $G$  to  $S_2$  takes  $\mathbf{a} \in G$  to the point  $\mathbf{a}(\hat{z})$  on  $S_2$  to which  $\mathbf{a}$  moves the north pole  $\hat{z}$ . The distance is given by  $d(\mathbf{f}(\mathbf{a}), \mathbf{f}(\mathbf{b})) = \cos^{-1}(\mathbf{a}(\hat{z}) \bullet \mathbf{b}(\hat{z}))$ . We will parameterize the distances by  $\mathbf{q}$ . Eq. (20) is satisfied, since

$$d(\mathbf{f}(\mathbf{g}\mathbf{a}), \mathbf{f}(\mathbf{g}\mathbf{b})) = \cos^{-1}((\mathbf{g}\mathbf{a})(\hat{z}) \bullet (\mathbf{g}\mathbf{b})(\hat{z})) = \cos^{-1}(\mathbf{g}(\mathbf{a}(\hat{z})) \bullet \mathbf{g}(\mathbf{b}(\hat{z}))) = \cos^{-1}(\mathbf{a}(\hat{z}) \bullet \mathbf{b}(\hat{z})).$$

The  $n$ th irreducible representation is the action of  $G$  on homogeneous polynomials  $p(x, y, z)$  of degree  $n$  for which  $\nabla^2 p = 0$ . A basis for these polynomials consists of the spherical harmonics  $Y_n^m(\mathbf{q} \cdot \mathbf{j})$  where  $m \in \{-n, \dots, n\}$ , and

$$Y_n^m(\mathbf{q}, \mathbf{j}) = \sqrt{\frac{2n+1}{4p} \frac{(n-m)!}{(n+m)!}} P_n^m(\cos \mathbf{q}) e^{imj}, \quad (21)$$

where  $P_n^m(u)$  is an associated Legendre polynomial [Eric W. Weisstein. "Spherical Harmonic." From MathWorld--A Wolfram Web Resource.

<http://mathworld.wolfram.com/SphericalHarmonic.html>].  $P_n^0(x) = P_n(x)$  is the  $n$ th Legendre polynomial, orthogonal on  $[-1,1]$ , satisfying

$$\int_{-1}^1 P_n(x) dx = \frac{2}{2n+1}. \quad (22)$$

From eqs. (5) and (12), for nontrivial representations  $\mathbf{r}$  we have

$$\tilde{F}_{\mathbf{r}, \bar{\mathbf{r}}}(m_1, m_2, n_1, m_2) = -\frac{\dim \mathbf{r}}{2} \left\langle f(d(0, \mathbf{g})) \overline{\mathbf{r}_{m_1 n_1}(\mathbf{g})} \right\rangle_{\mathbf{g} \in G}. \quad (23)$$

and (from eq. (15))

$$\Lambda_{\mathbf{r}, \bar{\mathbf{r}}}(m_1, m_2, n_1, m_2) = -\frac{1}{2} \left\langle f(d(0, \mathbf{g})) \overline{\mathbf{r}_{m_1 n_1}(\mathbf{g})} \right\rangle_{\mathbf{g} \in G}. \quad (24)$$

All matrix elements of  $\mathbf{r}(\mathbf{g})$  contain a nontrivial dependence on  $e^{if}$  except the one in the

row and column corresponding to  $Y_n^0(\mathbf{q}, \mathbf{j}) = \sqrt{\frac{2n+1}{4p}} P_n(\cos \mathbf{q})$ . We arbitrarily choose this to be the first row and column of  $\mathbf{r}(\mathbf{g})$ . Moreover, the average in eq. (23) can be replaced by an average over all products  $\mathbf{x}\mathbf{g}$ , where  $\mathbf{x}$  is a rotation by an angle  $f$  about the north pole  $\hat{z}$ . Thus, the average in eq. (23) must be zero except at  $m_1 = n_1 = 1$ .

Another consequence of the above argument is that the average in eq. (23) can be replaced by an average over the angle  $\mathbf{q}$  by which  $\mathbf{g}$  moves the north pole  $\hat{z}$ , i.e.,  $\mathbf{q}(\mathbf{g}) = \cos(\mathbf{g}(\hat{z}) \cdot \hat{z}) = d(0, \mathbf{g})$ . The weight associated with this angle  $\mathbf{q}$  is

$$w(\mathbf{q}) = \frac{1}{2} \sin \mathbf{q} \quad \left( \int_0^p w(\mathbf{q}) d\mathbf{q} = 1 \right), \quad (25)$$

since any final position of  $\mathbf{g}(\hat{z})$  on  $S_2$  is equally likely.

For a rotation  $\mathbf{g}$  that moves the north pole  $\hat{z}$  by an angle  $\mathbf{q}$ , the (1,1) matrix element of  $\mathbf{r}(\mathbf{g})$  is

$$\mathbf{r}_{1,1}(\mathbf{g}) = P_n(\cos \mathbf{q}(\mathbf{g})). \quad (26)$$

This conforms to the normalization (eq. (9)) of matrix elements of group representations:

$$\left\langle \left| \overline{\mathbf{r}_{1,1}(\mathbf{g})} \right|^2 \right\rangle_{\mathbf{g} \in G} = \left\langle |P_n(\cos \mathbf{q})|^2 \right\rangle = \int_0^p |P_n(\cos \mathbf{q})|^2 w(\mathbf{q}) d\mathbf{q} = \frac{1}{2n+1}, \quad (27)$$

where the last equality follows from eqs. (22) and (25). Combining eqs. (23),(25), and (26), and taking  $f(d) = d^s$  yields

$$\tilde{F}_{r,r}(1,m,1,m) = -\frac{2n+1}{4} \int_0^p \mathbf{q}^s P_n(\cos \mathbf{q}) \sin \mathbf{q} d\mathbf{q}, \quad (28)$$

where the average over  $\mathbf{g} \in G$  has been replaced by an average over  $\mathbf{q}(\mathbf{g})$ .

Thus, the  $n$ th irreducible representation of  $SO(3)$  contributes  $2n+1$  terms to eq. (8) (for  $m \in \{1, \dots, 2n+1\}$  in eq. (28)), and an eigenvalue  $\Lambda_n(s)$  of multiplicity  $2n+1$  to eq. (16). In view of (15),

$$\Lambda_n(s) = -\frac{1}{4} \int_0^p \mathbf{q}^s P_n(\cos \mathbf{q}) \sin \mathbf{q} d\mathbf{q}. \quad (29)$$

Evaluation of this integral is facilitated by writing the Fourier series

$$P_n(\cos \mathbf{q}) = \frac{1}{2^n n!} \sum_{q=-n}^n b_{n,q} \cos(q\mathbf{q}) = \frac{1}{4^n} \sum_{q=-n}^n B_{n,q} \cos(q\mathbf{q}), \quad (30)$$

where  $b_{n,q}$  and  $B_{n,q}$  are nonzero only for  $q = n - 2r$ . Note that both negative and positive frequencies are included. One can show (see Appendix I) that

$$b_{n,n-2r} = \frac{n! (2n-2r)! (2r)!}{2^n ((n-r)!)^2 (r!)^2} = \frac{(2n)!}{n! 2^n} \frac{\binom{n}{r}^2}{\binom{2n}{2r}}, \quad (31)$$

or equivalently, that

$$B_{n,q} = \frac{(n+q)! (n-q)!}{\left(\frac{n+q}{2}!\right)^2 \left(\frac{n-q}{2}!\right)^2}. \quad (32)$$

For  $s = 1$ , the above integral (29) can then be evaluated from the Fourier series, since

$$\int_0^p \mathbf{q} \cos q\mathbf{q} \sin \mathbf{q} d\mathbf{q} = \begin{cases} \frac{\mathbf{p}}{q^2 - 1}, & q > 1 \\ -\frac{\mathbf{p}}{4}, & q = 1 \end{cases}, \quad (33)$$

for odd  $q \geq 1$ . (For  $n$  even, the integral (29) is zero, since  $\left(\mathbf{q} - \frac{\mathbf{p}}{2}\right) P_n(\cos \mathbf{q}) \sin \mathbf{q}$  is odd-symmetric around  $\mathbf{q} = \frac{\mathbf{p}}{2}$ , and  $\int_0^p \cos q\mathbf{q} \sin \mathbf{q} d\mathbf{q} = 0$ .)

Appendix II shows that



$$\Lambda_n(1) = -\frac{1}{4} \int_0^{\mathbf{p}} \mathbf{q} P_n(\cos \mathbf{q}) \sin \mathbf{q} d\mathbf{q} = \frac{\mathbf{p}}{2^{2n+2}} \left( \frac{(n-1)!}{\left(\frac{n-1}{2}\right)! \left(\frac{n+1}{2}\right)!} \right)^2 = \frac{\mathbf{p}}{2^{2n+2}} C_m^2, \quad (34)$$

where  $n = 2m + 1$  and  $C_m$  is the  $m$ th Catalan number

$$C_m = \frac{(2m)!}{m!(m+1)!} = \frac{1}{m+1} \binom{2m}{m}. \quad (35)$$

[Sloane citation A000108, <http://www.research.att.com/projects/OEIS?Anum=A000108>].

To apply the Parseval relation (16) (for  $s = 1$ ), note that  $\mathbf{m} = \frac{\mathbf{p}}{2}$ , and, with  $f(d(\mathbf{q}, 0)) = |\mathbf{q}|$ , that

$$\langle (\mathbf{q} - \mathbf{m})^2 \rangle = \frac{1}{2} \int_0^{\mathbf{p}} \left( \mathbf{q} - \frac{\mathbf{p}}{2} \right)^2 \sin \mathbf{q} d\mathbf{q} = \frac{\mathbf{p}^2}{4} - 2, \quad (36)$$

where  $\frac{1}{2} \sin \mathbf{q}$  is the weight associated with a point on  $S_2$  at polar angle  $\mathbf{q}$ .

With these, eqs. (16) and (17) give

$$\frac{\mathbf{p}^2}{16} - \frac{1}{2} = \sum_{n=2m+1} (2n+1) \frac{\mathbf{p}^2}{2^{4n+4}} C_m^4. \quad (37)$$

This can be re-arranged to

$$1 - \frac{8}{\mathbf{p}^2} = \sum_{n=2m+1} \frac{2n+1}{2^{4n}} C_m^4. \quad (38)$$

Left and right-hand sides are both approximately 0.18943.

### The hypersphere $S_3$

Here,  $G = \text{SO}(4)$ . Analogous to the case of  $S_2$ , The map  $\mathbf{f}$  from  $G$  to  $S_3$  takes  $\mathbf{a} \in G$  to the point  $\mathbf{a}(\hat{z})$  on  $S_3$  to which  $\mathbf{a}$  moves  $\hat{z}$ , and the distance is given by

$$d(\mathbf{f}(\mathbf{a}), \mathbf{f}(\mathbf{b})) = \cos^{-1}(\mathbf{a}(\hat{z}) \cdot \mathbf{b}(\hat{z})).$$

The irreducible representations of  $G$  are parameterized by a pair of integer indices,  $g_+$  and  $g_-$ , corresponding to the largest Fourier coefficients with respect to  $\mathbf{w}_1 + \mathbf{w}_2$  and  $\mathbf{w}_1 - \mathbf{w}_2$  present in the characters, where  $\mathbf{w}_1$  and  $\mathbf{w}_2$  are the principal angles of the rotation of a typical group element  $\mathbf{a} \in G$ . All matrix elements of  $\mathbf{r}_{g_+, g_-}(\mathbf{g})$  contain a nontrivial dependence on a rotation about  $\hat{z}$ , of the form  $e^{if}$  except for one. That one is the matrix element in  $\mathbf{r}_{n, n}(\mathbf{g})$  that corresponds to transformations of the homogeneous polynomial of degree  $n$  that depends only on  $z = \cos \mathbf{q}$ . The dimension of  $\mathbf{r}_{n, n}(\mathbf{g})$ , which describes the

transformation of all homogenous polynomials of degree  $n$  (including those that do not depend only on  $z$ ), is

$$\binom{n+3}{3} - \binom{n+1}{3} = (n+1)^2.$$

Denote the polynomial that depends only on  $z$  by  $Q_n(\cos \mathbf{q})$ . These polynomials must be orthogonal with respect to the weight

$$w(\mathbf{q}) = \frac{2}{\mathbf{p}} \sin^2 \mathbf{q} \quad \left( \int_0^{\mathbf{p}} w(\mathbf{q}) d\mathbf{q} = 1 \right). \quad (39)$$

Since  $w(\mathbf{q}) = \frac{1}{2}(1 - \cos(2\mathbf{q}))$ , it follows that

$$Q_n(\cos \mathbf{q}) = K_n \sum_{a \equiv n}^n \cos(a\mathbf{q}), \quad (40)$$

where only terms for which  $a \equiv n \pmod{2}$  are included.  $K_n$  can be determined from eq. (11), as follows:

$$\frac{1}{(n+1)^2} = \int_0^{\mathbf{p}} (Q_n(\cos \mathbf{q}))^2 w(\mathbf{q}) d\mathbf{q} = \frac{1}{\mathbf{p}} \int_0^{\mathbf{p}} (Q_n(\cos \mathbf{q}))^2 (1 - \cos(2\mathbf{q})) d\mathbf{q} = K_n^2,$$

$$\text{so } K_n = \frac{1}{n+1}.$$

Again, the average corresponding to eq. (24) can be replaced by an average over the angle  $\mathbf{q}$  by which  $\mathbf{g}$  moves  $\hat{z}$ , weighted by  $w(\mathbf{q})$ . This is because any final position of  $\mathbf{g}(\hat{z})$  on  $S_3$  is equally likely, and the points at angle  $\mathbf{q}$  correspond to the surface of an  $S_2$ -sphere of radius  $\sin \mathbf{q}$ .

Thus, the irreducible representation of  $\text{SO}(4)$  corresponding to  $(g_+, g_-) = (n, n)$  contributes  $(n+1)^2$  terms to eq. (8), and an eigenvalue  $\Lambda_n(s)$  of multiplicity  $(n+1)^2$  to eq. (16). In view of (15),

$$\Lambda_n(s) = -\frac{1}{2} \int_0^{\mathbf{p}} |\mathbf{q}|^s Q_n(\cos \mathbf{q}) w(\mathbf{q}) d\mathbf{q} = -\frac{1}{\mathbf{p}} \int_0^{\mathbf{p}} \mathbf{q}^s Q_n(\cos \mathbf{q}) \sin^2 \mathbf{q} d\mathbf{q}. \quad (41)$$

For  $s=1$ ,

$$\Lambda_n(1) = \frac{4}{\mathbf{p} n^2 (n+2)^2}. \quad (42)$$

To apply the Parseval relation (16) (for  $s=1$ ), note that  $\mathbf{m} = \frac{\mathbf{p}}{2}$ , and, with  $f(d(\mathbf{q}, 0)) = |\mathbf{q}|$ , that

$$\langle (\mathbf{q} - \mathbf{m})^2 \rangle = \frac{2}{\mathbf{p}} \int_0^{\mathbf{p}} \left( \mathbf{q} - \frac{\mathbf{p}}{2} \right)^2 \sin^2 \mathbf{q} d\mathbf{q} = \frac{\mathbf{p}^2}{12} - \frac{1}{2}, \quad (43)$$

where  $\frac{2}{\mathbf{p}} \sin^2 \mathbf{q}$  is the weight associated with a point on  $S_3$  at polar angle  $\mathbf{q}$ . Eq. (16), eq. (42), eq. (43), and the fact that the multiplicity of  $\Lambda_n(1)$  is  $(n+1)^2$  lead to

$$\frac{\mathbf{p}^2}{128} \left( \frac{\mathbf{p}^2}{6} - 1 \right) = \sum_{n=2m+1} \frac{(n+1)^2}{n^4 (n+2)^4}. \quad (44)$$

This is equivalent to the sum of the following two series for  $\mathbf{p}$  attributed to Euler (Xavier Gourdon and Pascal Sebah, <http://numbers.computation.free.fr/Constants/Pi/piSeries.html>):

$$-\frac{3\mathbf{p}^2}{64} + \frac{1}{2} = \sum_{k=1}^{\infty} \frac{1}{(4k^2 - 1)^3} \quad (45)$$

and

$$\frac{\mathbf{p}^4 + 30\mathbf{p}^2}{768} - \frac{1}{2} = \sum_{k=1}^{\infty} \frac{1}{(4k^2 - 1)^4}. \quad (46)$$

(Prior to February 2004, that there had is a typographical error in eq. (45) on the above website).

## The hypersphere $S_a$

Here,  $G=SO(a+1)$ .  $a=1$  corresponds to the circle,  $a=2$  corresponds to the sphere, and  $a=3$  corresponds to the hypersphere. The map  $\mathbf{f}$  from  $G$  to  $S_a$  takes  $\mathbf{a} \in G$  to the point  $\mathbf{a}(\hat{z})$  on  $S_a$  to which  $\mathbf{a}$  moves  $\hat{z}$ , and the distance is given by  $d(\mathbf{f}(\mathbf{a}), \mathbf{f}(\mathbf{b})) = \cos^{-1}(\mathbf{a}(\hat{z}) \cdot \mathbf{b}(\hat{z}))$ .

The irreducible representations of  $G$  are parameterized by an  $\left\lfloor \frac{a+1}{2} \right\rfloor$ -tuple of integer

indices. The dimension of the representation which describes the transformation of all homogenous polynomials of degree  $n$  (including those that do not depend only on  $z$ ), is

$$\binom{n+a}{a} - \binom{n+a-2}{a}. \quad (47)$$

Denote the polynomial that depends only on  $z$  by  $R_{n,a}(\cos \mathbf{q})$ . These polynomials must be orthogonal with respect to the weight

$$w_a(\mathbf{q}) = A_a \sin^{a-1} \mathbf{q} = \frac{\Gamma(\frac{a+1}{2})}{\Gamma(\frac{a}{2}) \sqrt{\mathbf{p}}} \sin^{a-1} \mathbf{q}, \quad (48)$$

where  $A_a = \frac{1}{M_0^{(a-1)}}$  (eq. (54)) o ensure that  $\int_0^p w(\mathbf{q}) d\mathbf{q} = 1$ . (49)

### Polynomials for $\mathbf{S}_a$

The needed polynomials can be written in terms of the Gegenbauer polynomials. The Gegenbauer polynomials  $C_n^{(I)}(x)$  are orthogonal on  $[-1,1]$  with respect to the weight  $(1-x^2)^{I-1/2}$ . With  $D_n^{(I)}(x) = \frac{1}{I} C_n^{(I)}$  and  $x = \cos \mathbf{q}$ ,  $D_n^{(I)}(\cos \mathbf{q})$  are orthogonal with respect to  $\sin^{2I} \mathbf{q}$  on  $[0, \mathbf{p}]$ . So, other than a scale factor,  $R_{n,a}(\cos \mathbf{q}) = D_n^{\left(\frac{a-1}{2}\right)}(\cos \mathbf{q})$ ,

Standard formulae (Abramowitz and Stegun chapter 22), imply that for  $I > 0$

$$\sum_{n=1}^{\infty} D_n^{(I)}(x) t^n = \frac{1}{I} \left( \frac{1}{(1-2xt+t^2)^I} - 1 \right), \quad D_0^{(I)} = \frac{1}{I},$$

and

$$\sum_{n=1}^{\infty} D_n^{(0)}(x) t^n = -\log(1-2xt+t^2)$$

and

$$\int_0^p (D_n^{(I)}(\cos \mathbf{q}))^2 \sin^{2I} \mathbf{q} d\mathbf{q} = \mathbf{p} \frac{2^{1-2I} \Gamma(n+2I)}{(n+I)\Gamma^2(I+1)\Gamma(n+1)} \text{ provided } n > 0 \text{ or } I > 0.$$

Writing  $(1-2xt+t^2) = (1-te^{iq})(1-te^{-iq})$ , along with the generating function, shows

$$D_n^{(0)}(x) = \frac{2}{n} \cos(n\mathbf{q}).$$

We want to determine the coefficient of  $V(n, \mathbf{m} c)$  of  $e^{i\mathbf{q}}$  in  $D_n^{(\mathbf{m}/2)}(\cos \mathbf{q})$ . Straightforward algebra provides the double generating function

$$\sum_{\mathbf{m}=0, m=0}^{\infty} (-1)^{\mathbf{m}} D_n^{(\mathbf{m}/2)}(x) t^{\mathbf{m}} y^{\mathbf{m}} = -2\log(y + \sqrt{1-2xt+t^2}),$$

where the sum includes all nonnegative integer pairs  $(\mathbf{m}, m)$  except  $\mathbf{m} = m = 0$ .

$$\sum_{\mathbf{m}=0, m=0, (\mathbf{m}, m) \neq (0,0)}^{\infty} (-1)^{\mathbf{m}} V(\mathbf{m}, \mathbf{m} c) t^{\mathbf{m}} y^{\mathbf{m}} = \frac{1}{2\mathbf{p}} \int_0^{2\mathbf{p}} -2\log\left(y + \sqrt{(1-te^{iq})(1-te^{-iq})}\right) e^{-i\mathbf{q}} d\mathbf{q}.$$

Put  $z = e^{i\mathbf{q}}$ .

$$\sum_{\mathbf{m}=0, m=0, (\mathbf{m}, m) \neq (0,0)}^{\infty} (-1)^{\mathbf{m}} V(\mathbf{m}, \mathbf{m} c) t^{\mathbf{m}} y^{\mathbf{m}} = \frac{1}{2\mathbf{p}i} \int -2\log\left(y + \sqrt{(1-tz)\left(1-\frac{t}{z}\right)}\right) \frac{dz}{z^{c+1}},$$

with the contour integral surrounding 0.

Noting that  $\sqrt{1+u} = 1 + \sum_{a=1}^{\infty} (-1)^{a+1} \frac{u^a}{2^{2a-1}} C_{a-1}$ , we have

$$\sqrt{(1-tz)(1-\frac{t}{z})} = \sum_{k=1}^{\infty} t^k \sum_{a+b=k, a \geq 1, b \geq 1} \frac{1}{2^{2a-1}} \frac{1}{2^{2b-1}} z^{a-b} C_{a-1} C_{b-1}.$$

Alternatively, let

$$f_p(a) = \frac{\Gamma(\frac{p}{2} + a)}{2} = \frac{\Gamma(p+2a)\Gamma(\frac{p+1}{2})}{4^a \Gamma(a+1)\Gamma(\frac{p+2a+1}{2})\Gamma(p)} \quad (50)$$

(via duplication formula for the gamma function), the coefficient in the Taylor series

$$(1-x)^{-p/2} = \sum_{a=0}^{\infty} x^a f_p(a) \quad .$$

It follows by equating coefficients in the generating functions that

$$D_m^{(p/2)}(\cos \mathbf{q}) = \sum_{c=-m}^m V(m, p, c) e^{i\mathbf{c}\mathbf{q}} \quad (51)$$

where the summation is only for  $m \equiv c \pmod{2}$  and

$$V(m, p, c) = \frac{2}{p} f_p\left(\frac{m+c}{2}\right) f_p\left(\frac{m-c}{2}\right) \text{ for } p > 0, \quad (52)$$

and, in the limit that  $p$  approaches 0,

$$V(m, 0, c) = \frac{1}{m} \mathbf{d}(|c|, m) \text{ so that } D_m^{(0)}(\cos \mathbf{q}) = \frac{2}{m} \cos(m\mathbf{q}) = \frac{1}{m} (e^{im\mathbf{q}} + e^{-im\mathbf{q}}) \text{ for } m > 0.$$

The normalization is

$$\int_0^p \left( D_m^{(p/2)}(\cos \mathbf{q}) \right)^2 \sin^p \mathbf{q} d\mathbf{q} = p \frac{2^{1-p} \Gamma(m+p)}{\left(m + \frac{p}{2}\right) \Gamma^2\left(\frac{p}{2} + 1\right) \Gamma(m+1)}, \quad (53)$$

again provided  $m > 0$  or  $p > 0$ .

Since the above quantities are undefined for  $m = 0, p = 0$ , we arbitrarily take

$$V(0, 0, c) = \mathbf{d}(c, 0) \text{ so that } D_0^{(0)} = 1, \text{ so}$$

$$\int_0^p \left( D_0^{(0)}(\cos \mathbf{q}) \right)^2 d\mathbf{q} = p.$$

Note  $f_0(j) = \mathbf{d}(j, 0)$  (the circle),  $f_1(j) = \frac{1}{4^j} \frac{(2j)!}{(j!)^2}$  (the sphere),  $f_2(j) = 1$  (the hypersphere,

as required for eq. (40)), and  $f_4(j) = j+1$ .

For  $p = 1$ ,  $V(m, 1, c) = \frac{2}{4^m} B_{m,c}$  (eq. (32)), and  $D_n^{(1/2)}(\cos \mathbf{q}) = 2P_n(\cos \mathbf{q})$  (eq. (30)).

**Moments for  $S_a$** 

Write  $M_j^{(p)} = \int_0^p \mathbf{q}^j \sin^p \mathbf{q} d\mathbf{q}$ . Via integration by parts and elementary calculations, we find

$$M_0^{(p)} = \frac{p-1}{p} M_0^{(p-2)}, M_0^{(0)} = p, M_0^{(1)} = 2, \text{ and hence}$$

$$M_0^{(p)} = \sqrt{p} \frac{\Gamma(\frac{p+1}{2})}{\Gamma(\frac{p}{2}+1)} \quad (54).$$

Similarly,  $M_1^{(p)} = \frac{p-1}{p} M_1^{(p-2)}$ ,  $M_1^{(p)} = \frac{p}{2} M_1^{(0)}$ , and hence

$$M_1^{(p)} = p^{3/2} \frac{\Gamma(\frac{p+1}{2})}{2\Gamma(\frac{p}{2}+1)},$$

and  $M_2^{(p)} = \frac{p-1}{p} M_2^{(p-2)} - \frac{2}{p^2} M_0^{(p-2)}$ , and hence

for  $p$  even:

$$M_2^{(p)} = \frac{\Gamma(\frac{p+1}{2})}{\Gamma(\frac{p}{2}+1)} \left( \frac{p^{5/2}}{3} - 2\sqrt{p} \left( \frac{1}{p^2} + \frac{1}{(p-2)^2} + \dots + \frac{1}{2^2} \right) \right)$$

for  $p$  odd:

$$M_2^{(p)} = \frac{\Gamma(\frac{p+1}{2})}{\Gamma(\frac{p}{2}+1)} \left( \frac{p^{5/2}}{2} - 2\sqrt{p} \left( \frac{1}{p^2} + \frac{1}{(p-2)^2} + \dots + \frac{1}{1^2} \right) \right).$$

Thus, the variance required for the right side of eq. (17), (or eq. (36)) is

$$\frac{1}{M_0^{(p)}} \left( M_2^{(p)} - \frac{(M_1^{(p)})^2}{M_0^{(p)}} \right) = 2 \sum_{m=1}^{\infty} \frac{1}{(p+2m)^2}, \text{ which is equivalent to}$$

for  $p$  even (using  $\frac{p^2}{24} = \frac{1}{2^2} + \frac{1}{4^2} + \frac{1}{6^2} + \dots$ ):

$$\frac{1}{M_0^{(p)}} \left( M_2^{(p)} - \frac{(M_1^{(p)})^2}{M_0^{(p)}} \right) = \frac{p^2}{12} - 2 \left( \frac{1}{2^2} + \frac{1}{4^2} + \dots + \frac{1}{p^2} \right), \quad (55)$$

for  $p$  odd (using  $\frac{p^2}{8} = \frac{1}{1^2} + \frac{1}{3^2} + \frac{1}{5^2} + \dots$ ):

$$\frac{1}{M_0^{(p)}} \left( M_2^{(p)} - \frac{(M_1^{(p)})^2}{M_0^{(p)}} \right) = \frac{p^2}{4} - 2 \left( \frac{1}{1^2} + \frac{1}{3^2} + \dots + \frac{1}{p^2} \right). \quad (56)$$

## Eigenvalues

The  $n$ th eigenvalue in dimension  $a$  is given by

$$\Lambda_n(s) = -\frac{1}{2} \int_0^p |\mathbf{q}|^s Q_n(\cos \mathbf{q}) w(\mathbf{q}) d\mathbf{q}$$

where  $w$  is given by eq. (48) and where  $Q_n(\cos \mathbf{q})$  is a multiple of  $D_n^{(\frac{a-1}{2})}$  satisfying

$$\int_0^p (Q_n(\cos \mathbf{q}))^2 w_a(\mathbf{q}) d\mathbf{q} = \frac{1}{\dim \mathbf{r}_n} = \frac{1}{\binom{n+a}{a} - \binom{n+a-2}{a}}.$$

From eq. (53) and (48),

$$\int_0^p \left( D_n^{(\frac{a-1}{2})}(\cos \mathbf{q}) \right)^2 w_a(\mathbf{q}) d\mathbf{q} = \frac{2^{2-a} \sqrt{p} \Gamma(n+a-1)}{\left(n + \frac{a-1}{2}\right) \Gamma\left(\frac{a}{2}\right) \Gamma\left(\frac{a+1}{2}\right) \Gamma(n+1)} = \frac{4\Gamma(n+a-1)}{(2n+a-1)\Gamma(a)\Gamma(n+1)},$$

where the second equality follows from the standard duplication formula,

$$\Gamma(2z) = \frac{1}{\sqrt{2p}} 2^{2z-1/2} \Gamma(z) \Gamma\left(z + \frac{1}{2}\right).$$

Thus,

$$\frac{Q_n(\cos \mathbf{q})}{D_n^{(\frac{a-1}{2})}(\cos \mathbf{q})} = \left( \frac{(2n+a-1)\Gamma(a)\Gamma(n+1)}{4\Gamma(n+a-1) \left( \binom{n+a}{a} - \binom{n+a-2}{a} \right)} \right)^{1/2} = \frac{\Gamma(a)\Gamma(n+1)}{2\Gamma(n+a-1)}.$$

Thus, it remains to find the coefficients in an orthogonal expansion of  $\mathbf{q}$ , i.e.,

$$\Lambda_n(s) = -\frac{1}{2} \int_0^p \mathbf{q} Q_n(\cos \mathbf{q}) w_a(\mathbf{q}) d\mathbf{q} = -\frac{\Gamma(a)\Gamma(n+1)}{4\Gamma(n+a-1)} \frac{\Gamma(\frac{a+1}{2})}{\Gamma(\frac{a}{2})\sqrt{p}} \sum_{c=-n}^n V(n, a-1, c) \int_0^p |\mathbf{q}|^s e^{i\mathbf{c}\mathbf{q}} \sin^{a-1} \mathbf{q} d\mathbf{q}$$

where again the summation is only over terms for which  $c \equiv n \pmod{2}$ . This also holds for  $a=1$ , since  $V$  has appropriate limiting behavior.

$$\text{In view of eq. (52) } V(n, a-1, c) = \frac{2}{a-1} f_{a-1}\left(\frac{n+c}{2}\right) f_{a-1}\left(\frac{n-c}{2}\right),$$

$$\text{and eq. (50) } f_{a-1}(r) = \frac{\Gamma(\frac{a-1}{2} + r)}{\Gamma(\frac{a-1}{2})\Gamma(r+1)}, \text{ (again using the duplication formula),}$$

$$\Lambda_n(s) = -2^{a-4} \frac{(a-1)}{p} \frac{\Gamma(n+1)}{\Gamma(n+a-1)} \sum_{c=-n}^n \frac{\Gamma(\frac{a-1+n+c}{2})\Gamma(\frac{a-1+n-c}{2})}{\Gamma(\frac{n+c}{2}+1)\Gamma(\frac{n-c}{2}+1)} \int_0^p |\mathbf{q}|^s e^{i\mathbf{c}\mathbf{q}} \sin^{a-1} \mathbf{q} d\mathbf{q},$$

where again the summation is only over terms for which  $c \equiv n \pmod{2}$ .

[Verified by riemds\_a.m for  $s=1$ .] This can be rearranged, via a binomial expansion for

$$\sin^{a-1} \mathbf{q} = \left(\frac{e^{i\mathbf{q}} - e^{-i\mathbf{q}}}{2i}\right)^{a-1} = \frac{1}{(2i)^a} \sum_h \binom{a-1}{h} (-1)^h e^{i(a-1-2h)\mathbf{q}}$$

and a change of variables  $c = b + h$ :

$$\Lambda_n(s) = -\frac{1}{8p\Gamma(n+a-1)} \sum_{|b| \leq a+n-1} \left( \sum_{|h| \leq a-1, b+h \leq n} i^h \binom{n}{n-b-h} \binom{a-1}{a-1-h} Z_{a,n}(b+h) \right) Y_s(b), \text{ where}$$

sums require  $b \equiv a+n-1$ ,  $h \equiv b+n \pmod{2}$ ,

$$Y_s(b) = \int_0^p |\mathbf{q}|^s e^{i\mathbf{q}b} d\mathbf{q},$$

and

$$Z_{a,n}(b+h) = (a-1)\Gamma\left(\frac{a-1+n+b+h}{2}\right)\Gamma\left(\frac{a-1+n-b-h}{2}\right), \text{ whose arguments are half-}$$

integer when  $a$  is even, and integer when  $a$  is odd. The factor  $(a-1)$  is absorbed into  $Z$  to ensure that behavior is finite for  $a=1$ . For  $s=1$ , the only nonzero terms are for  $n$  odd.

[Verified by riemds\_b.m for general  $s$  and  $n$ .]

Consider

$$S(a, n, b) = \sum_{|h| \leq a-1, b+h \leq n} i^h \binom{n}{n-b-h} \binom{a-1}{a-1-h} Z_{a,n}(b+h) \tag{57}$$

and the associated generating function



$$\hat{S}(\mathbf{a}, \mathbf{h}, \mathbf{b}) = \sum_{a, n, b} \frac{\mathbf{a}^a \mathbf{h}^n \mathbf{b}^b}{\Gamma(n+1)} S(a, n, b)$$

where the sums are over integers  $a \geq 1, n \geq 1$ , and all integers  $b$ . With

$$u = \frac{a-1}{2}, p = \frac{n+b}{2}, q = \frac{n-b}{2}, t = \frac{h}{2}; u, p, q, t \text{ integer if } a \text{ is odd; or half-integer if } a \text{ is even:}$$

$$\hat{S}(\mathbf{a}, \mathbf{h}, \mathbf{b}) = \sum_{t, u, p, q} \mathbf{a}^{2u+1} (\mathbf{h}\mathbf{b})^p \left( \frac{\mathbf{h}}{\mathbf{b}} \right)^q (-1)^t \frac{2u\Gamma(2u+1)}{\Gamma(u-t+1)\Gamma(u+t+1)} \frac{\Gamma(q-t+u)}{\Gamma(q-t+1)} \frac{\Gamma(p+t+u)}{\Gamma(p+t+1)},$$

where  $\max(-u, -p) \leq t \leq \min(u, q)$ . This reduces:

$$\hat{S}(\mathbf{a}, \mathbf{h}, \mathbf{b}) = \sum_{\substack{u \\ |t| \leq u} } \mathbf{a}^{2u+1} (-1)^t \frac{2u\Gamma(2u+1)\Gamma^2(u)}{\Gamma(u-t+1)\Gamma(u+t+1)} \frac{\mathbf{b}^{-t}}{\left(1 - \frac{\mathbf{h}}{\mathbf{b}}\right)^u} \frac{\mathbf{b}^{-t}}{(1 - \mathbf{h}\mathbf{b})^u},$$

$$\hat{S}(\mathbf{a}, \mathbf{h}, \mathbf{b}) = \sum_u \mathbf{a}^{2u+1} 2u\Gamma^2(u) \left( \frac{-\mathbf{b}^2 + 2 - \mathbf{b}^{-2}}{1 - \frac{\mathbf{h}}{\mathbf{b}} - \mathbf{h}\mathbf{b} + \mathbf{h}^2} \right)^u$$

where again the sum is over half-integers  $u \geq 0$ . From this, equating coefficients, we find the recursion relation:

$$\begin{aligned} & S(a, n, b) - nS(a, n-1, b+1) - nS(a, n-1, b-1) + n(n-1)S(a, n-2, b) \\ &= \frac{(a-3)(a-1)}{4} (-S(a-2, n, b-2) + 2S(a-2, n, b) - S(a-2, n, b+2)) \end{aligned}$$

[verified with riemds\_sanbr].

Taking

$$S(a, n, b) = \Gamma(n+1)\Gamma\left(\frac{a+1}{2}\right)\Gamma\left(\frac{a-1}{2}\right)T(a, n, b)$$

one finds

$$\begin{aligned} & T(a, n, b) - T(a, n-1, b+1) - T(a, n-1, b-1) + T(a, n-2, b) \\ &= -T(a-2, n, b-2) + T(a-2, n, b) - T(a-2, n, b+2) \end{aligned}$$

[verified with riemds\_tanbr].

Then,

$$T(a, n, b) = i^{n-b} \frac{b(a-1)}{\Gamma(n+1)} \frac{\Gamma\left(\frac{b+n}{2}\right)}{\Gamma\left(\frac{b-n}{2}+1\right)} \frac{\Gamma(a+n-1)}{\Gamma\left(\frac{a+n+b+1}{2}\right)\Gamma\left(\frac{a+n-b+1}{2}\right)},$$

provided  $a \geq 2$  and  $b \geq 0$ , and is 0 if  $b < n$  with  $n$  even ( $a$  odd), consistent with the pole in the denominator. This can be seen to satisfy the above recursion relation, and also to agree with eq. (57) for  $b = n + a - 1$  and  $b = n + a - 3$  [verified with `riemds_tanb`]. Thus,

$$\Lambda_n(s) = -\frac{\Gamma(n+1)\Gamma\left(\frac{a+1}{2}\right)\Gamma\left(\frac{a-1}{2}\right)}{8\mathbf{p}\Gamma(n+a-1)} \sum_{|b| \leq a+n-1} T(a,n,b)Y_s(b) \text{ or}$$

$$\Lambda_n(s) = -\frac{\Gamma^2\left(\frac{a+1}{2}\right)}{4\mathbf{p}} \sum_{0 \leq b \leq a+n-1} i^{n-b} \frac{\Gamma\left(\frac{b+n}{2}\right)}{\Gamma\left(\frac{b-n}{2}+1\right)\Gamma\left(\frac{a+n+b+1}{2}\right)\Gamma\left(\frac{a+n-b+1}{2}\right)} bY_s(b) + c.c. \quad (58)$$

with  $a+n+b \equiv 1 \pmod{2}$  in all sums [verified with `riemds_c`].

For analytic results, specialize to  $s=1$ . For  $a$  odd,  $n$  and  $b$  must be odd, and

$$Y_1(b) = \frac{\mathbf{p}i}{b} - \frac{2}{b^2}.$$

$$\sum_{0 \leq b \leq a+n-1} i^{n-b} \frac{\Gamma\left(\frac{b+n}{2}\right)}{\Gamma\left(\frac{b-n}{2}+1\right)\Gamma\left(\frac{a+n+b+1}{2}\right)\Gamma\left(\frac{a+n-b+1}{2}\right)} bY_1(b) + c.c. =$$

$$\frac{\Gamma(n)}{\Gamma(n+a)} \sum_{n \leq b \leq a+n-1} (-1)^{\frac{n-b}{2}} \binom{\frac{b+n}{2}-1}{n-1} \binom{a+n-1}{\frac{a+n+b-1}{2}} \left(-\frac{4}{b}\right), \text{ making use of the conjugate}$$

symmetry. From this and eq. (58),

$$\Lambda_n(1) = \frac{\Gamma(n)}{\mathbf{p}\Gamma(n+a)} \left(\Gamma\left(\frac{a+1}{2}\right)\right)^2 \sum_{n \leq b \leq a+n-1} \frac{(-1)^{\frac{n-b}{2}}}{b} \binom{\frac{b+n}{2}-1}{n-1} \binom{a+n-1}{\frac{a+n+b-1}{2}}. \quad (59)$$

For  $a=1$ , eq. (18) is recovered. For  $a=3$ , eq. (42) is recovered. For  $a=5$ ,

$$\Lambda_n(1) = \frac{64}{\mathbf{p}n^2(n+2)^2(n+4)^2}. \quad (60)$$

This suggests the formula

$$\Lambda_n(1) = \frac{2^{a-1}}{\mathbf{p}} \Gamma\left(\frac{a+1}{2}\right)^2 \frac{1}{n^2(n+2)^2(n+4)^2 \dots (n+a-1)^2}, \quad (61)$$

which may be written

$$\Lambda_n(1) = \frac{1}{4\mathbf{p}} \left( \frac{\Gamma\left(\frac{a+1}{2}\right)\Gamma\left(\frac{n}{2}\right)}{\Gamma\left(\frac{n+a+1}{2}\right)} \right)^2. \quad (62)$$

This appears to hold for not only for  $a$  odd but also for  $a$  even [riemds\_d].

For  $a$  even, eq. (62) can be rewritten without  $\Gamma$ -functions (using

$$\Gamma\left(\frac{1}{2} + c\right) = 2^{-c} \sqrt{\mathbf{p}} (1 \cdot 3 \cdot \dots \cdot (2c-1)) \text{ as}$$

$$\Lambda_n(1) = \frac{\mathbf{p}}{4^{n+a}} \left( \binom{a}{\frac{a}{2}} \binom{n-1}{\frac{n-1}{2}} \left( \frac{\left(\frac{a}{2}\right)! \left(\frac{n-1}{2}\right)!}{\left(\frac{n+a-1}{2}\right)!} \right) \right)^2 = \frac{\mathbf{p}}{4^{n+a}} \left( \frac{\binom{a}{\frac{a}{2}} \binom{n-1}{\frac{n-1}{2}}}{\binom{n+a-1}{\frac{n+a-1}{2}}} \right)^2.$$

For  $a = 2$ , this reduces to eq. (34). For  $a = 4$ , this becomes

$$\Lambda_n(1) = \frac{9\mathbf{p}}{4^n} \left( \frac{1}{(n+1)(n+3)} \binom{n-1}{\frac{n-1}{2}} \right)^2.$$

### Series for pi

The series for  $\mathbf{p}$  that follow from the Parseval relation (using the multiplicities (47), eq. (17), and eq. with  $p = a-1$ ) for  $a = 4$  is:

$$1 - \frac{80}{9\mathbf{p}^2} = 216 \sum_{n=2m+1} \frac{1}{2^{4n}} \frac{(n+2)(2n+3)}{(n+1)^3(n+3)^4} \left( \frac{n-1}{2} \right)^4,$$

and, for  $a = 2$  (equivalent to (38)),

$$1 - \frac{8}{\mathbf{p}^2} = 16 \sum_{n=2m+1} \frac{1}{2^{4n}} \frac{(2n+1)}{(n+1)^4} \left( \frac{n-1}{2} \right)^4.$$

In general, for  $a$  even,  $n$  and  $b$  must be odd, and  $Y_1(b) = \frac{\mathbf{p}i}{b} - \frac{2}{b^2}$ .

### Other symmetric spaces

The sphere  $S_a$  can be regarded as the set of rays in  $(a+1)$ -dimensional space. It has  $a$  parameters, and is acted on by  $G = \text{SO}(a+1)$ .  $G$  acts transitively on the sphere. The geodesics are obvious, namely, the trajectory taken between two given rays by a group action. The arc length distance is  $d(\mathbf{f}(\mathbf{a}), \mathbf{f}(\mathbf{b})) = \cos^{-1}(\mathbf{a}(\hat{z}) \cdot \mathbf{b}(\hat{z}))$ .

Consider the signed subspace defined by a  $k$ -tuple of vectors  $v_1, \dots, v_k$  in an  $n$ -dimensional space. The same subspace is defined by any nonsingular linear transformation of these vectors with positive determinant. ( $k=1, n=a+1$  corresponds to  $S_a$ , above). The dimension of the space is  $k(n-k)$ , as follows: To specify a  $k$ -dimensional subspace, choose  $k$  vectors in the  $n$ -dimensional space ( $nk$  dimensions). The space of interest is a quotient space of this  $k$ -fold product space by the general linear group on the  $k$  chosen vectors (any linear transformation of them leads to the same element of the symmetric space).

$nk - k^2 = k(n-k)$ . My “planesph.m” and “planesph\_inv.m” implement this mapping.

The distance between an element described by a set of unit vectors  $v_1, \dots, v_k$  and a second set of unit vectors  $w_1, \dots, w_k$  is  $d(v, w) = \cos^{-1}(\det v_j \bullet w_k)$ . Note that a space, and the same subspace with an odd permutation of the vectors, is considered maximally different, and just like sign inversion of one of the vectors. This is analogous to the fact that the antipodal points on a sphere are maximally different. One can also make a new symmetric space by identifying them with each other.

To carry out the above program, one needs to, decompose  $\cos^{-1}(\det v_j \bullet \mathbf{a}(v_k))$  in terms of irreducible representations of the group element  $\mathbf{a}$ . In the case of  $S_2$ , at eq. (23) and analogously for  $S_3$ , we used the fact that all but one of the matrix elements of an irreducible rotation have a dependence on the polar angle, via  $e^{if}$ . That angle could not influence the distance. But in the more general case, it is not yet clear whether the same logic applies. This should be testable empirically (at least if there is a dependence). A dependence seems likely, in that the distance between the index subspace and its image under  $\mathbf{a}$  should depend not only on how far the polar axis  $\hat{z}$  is moved, but also, on the movement of other vectors.

However, there is a short cut that allows one to see that these spaces are embeddable, if  $S_r$  is, for  $r = \binom{n}{k} - 1$ . This is because the  $k$ -spaces in an  $n$ -dimensional space can be mapped

into the 1-spaces in a space of dimension  $\binom{n}{k}$  via the antisymmetric tensor product. The

map preserves the above distance. This map is typically not onto. For example, for  $n=4$  and  $k=2$  the space of planes has 4 parameters, but is mapped into  $S_5$ , the five-parameter surface of a sphere in 6-dimensional space. Numerical experiments suggest (riemds.m, riemds\_subdim\_show.m) that indeed, not all of the embedding dimensions in  $S_5$  are needed for  $n=4$  and  $k=2$ . However, the embedding exponent still must be  $s=1$ , since this space is at least as complicated as  $n=3$  and  $k=1$ .

### More elegant setup, $G$ and $S$ distinct

We posit a subgroup  $H$  of  $G$ , and consider  $S$  to be the space of right cosets. The map  $f$  from  $G$  to  $S$  is the standard map from an element  $g$  to the coset  $gH$ .  $G$  acts transitively on  $S$ , and the stabilizer of any element of  $S$  is  $H$ . We allow  $d$  to act on  $G$ , and not just the coset space; diagonalizing  $d$  on  $G$  will be an equivalent problem.

The property (1) is replaced by the slightly more restrictive

$$d(\mathbf{g}\mathbf{b}, \mathbf{g}\mathbf{a}) = d(\mathbf{a}, \mathbf{b}) \text{ for } \mathbf{g} \in G \text{ because of the assumed symmetry of } S \quad (63)$$

and

$$d(\mathbf{a}\mathbf{h}, \mathbf{b}\mathbf{h}) = d(\mathbf{a}, \mathbf{b}) \text{ for } \mathbf{h} \in H \text{ because of the coset construction.} \quad (64)$$

Since the property (1) is not used until after eq. (12), we still have (from eqs. (5) and eq. (12)), for each irreducible representation  $\mathbf{r}$  of  $G$  :

$$\tilde{F}_{\mathbf{r}, \mathbf{r}}(m_1, m_2, n_1, m_2) = -\frac{\dim \mathbf{r}}{2} \left\langle f(d(0, \mathbf{g})) \overline{\mathbf{r}_{m_1}(\mathbf{g})} \right\rangle_{\mathbf{g} \in G}. \quad (65)$$

with  $\tilde{F}_{\mathbf{r}, \mathbf{r}}(m_1, m_2, n_1, n_2) = 0$  for  $m_2 \neq n_2$ . That is, the diagonalization (8) has  $\dim \mathbf{r}$  copies

$$\text{of a matrix } B_{\mathbf{r}} = -\frac{\dim \mathbf{r}}{2} \left\langle f(d(0, \mathbf{g})) \overline{\mathbf{r}(\mathbf{g})} \right\rangle_{\mathbf{g} \in G}.$$

In view of eqs. (63) and (64),  $d(0, \mathbf{g}) = d(0, \mathbf{h}^{-1}\mathbf{g}\mathbf{h})$  for  $\mathbf{g} \in G$  and  $\mathbf{h} \in H$ . Therefore,

$$\left\langle f(d(0, \mathbf{g})) \overline{\mathbf{r}(\mathbf{g})} \right\rangle_{\mathbf{g} \in G} = \left\langle f(d(0, \mathbf{h}\mathbf{g}\mathbf{h}^{-1})) \overline{\mathbf{r}(\mathbf{g})} \right\rangle_{\mathbf{g} \in G} = \left\langle f(d(0, \mathbf{h}\mathbf{g}\mathbf{h}^{-1})) \overline{\mathbf{r}(\mathbf{h}\mathbf{g}\mathbf{h}^{-1})} \right\rangle_{\mathbf{g} \in G}$$

and consequently,

$$B_{\mathbf{r}} = (\mathbf{r}(\mathbf{h}))^{-1} B_{\mathbf{r}} \mathbf{r}(\mathbf{h})$$

That is,  $\mathbf{r}(\mathbf{h})$  commutes with  $B_{\mathbf{r}}$  for any  $\mathbf{h} \in H$ . Now, consider the further reduction of  $\mathbf{r}$  to irreducible representations on  $H$ :

$$\mathbf{r} = k_1 \mathbf{x}_1 \oplus \dots \oplus k_{n(\mathbf{r})} \mathbf{x}_{n(\mathbf{r})}.$$

The above commutation relationship implies that  $B_{\mathbf{r}}$  is a block-diagonal matrix on the subspaces corresponding to each  $\mathbf{x}_r$ . If  $k_r = 1$ , it must be a multiple of an identity matrix of rank  $\dim \mathbf{x}_r$  within the subspace corresponding to  $\mathbf{x}_r$ . For  $k_r > 1$ , it is a matrix of rank  $k_r \dim \mathbf{x}_r$ , composed of  $k_r \times k_r$  blocks of arbitrary multiples of the identity matrix of rank  $\dim \mathbf{x}_r$ .

But also, in view of eq. (64),

$$B_{\mathbf{r}} = B_{\mathbf{r}} \mathbf{r}(\mathbf{h}) \text{ for any } \mathbf{h} \in H.$$

Therefore, the block matrix must be zero except within the space of  $\mathbf{x}_r$ , for which  $\mathbf{x}_r$  is the trivial (identity) representation on  $H$ .

In sum, there will only be contributions to the diagonalization for each irreducible representation  $\mathbf{r}$  of  $G$  for which the restriction to  $H$  contains at least one copy of the identity matrix. If the number of copies is 1, then there will be a set of  $\dim \mathbf{r}$  identical eigenvalues in the diagonalization. If there are  $k_r > 1$  copies, then it would appear that there can be up to  $k_r^2$  sets of  $\dim \mathbf{r}$  -tuples of identical eigenvalues.

Note however that in the case of  $G = S$  (with  $H$  the identity element), further reduction is possible. Every irreducible representation of  $G$  contains the identity representation on  $H$ , in  $k = \dim \mathbf{r}$  copies. But there are not  $k^2$  sets of  $\dim \mathbf{r}$  -tuples of identical eigenvalues, only  $k$  such sets. This is because  $\mathbf{r}(\mathbf{h})$  commutes with  $B_r$  for any  $\mathbf{h} \in G$ , in view of the more general property (1), and hence,  $B_r$  must be diagonal.

### Application of the more general formulation

The above formulation indicates which irreducible representations can contribute to the diagonalization for the more general symmetric spaces.

For the space of  $k$ -dimensional subspaces in an  $n$ -dimensional space, take  $G = \text{SO}(n)$  (with  $n = a+1$  to correspond to the discussion of hyperspheres  $S_a$ ) and  $H = \text{SO}(n) \times \text{SO}(n-k)$ .

Since the dimension of  $\text{SO}(n)$  is  $\frac{1}{2}n(n-1)$ , it follows that the dimension of the space of right cosets of  $H$  in  $G$  is  $k(n-k)$ .

Now we need to see how irreducible representations of  $G$  restrict to  $H$ .

## Appendix I: Fourier series for Legendre polynomials of cosine argument

We show by induction on  $n$  that

$$P_n(\cos \mathbf{q}) = \frac{1}{4^n} \sum_{a=-n}^n \frac{(n+a)!}{\left(\frac{n+a}{2}\right)!} \frac{(n-a)!}{\left(\frac{n-a}{2}\right)!} \cos(a\mathbf{q}), \quad (66)$$

which, along with equation (30), is equivalent to eq. (32). We use a recurrence formula for the Legendre polynomials,

$$P_{n+1}(x) = \frac{1}{n+1} ((2n+1)xP_n(x) - nP_{n-1}(x)) \quad (67)$$

along with

$$\cos(a\mathbf{q})\cos(\mathbf{q}) = \frac{1}{2} (\cos((a+1)\mathbf{q}) + \cos((a-1)\mathbf{q})). \quad (68)$$

Assuming that eq. (66) holds for all  $m \leq n$ , eqs. (67) and (68) imply that

$$B_{n+1,a} = \frac{1}{n+1} (2(2n+1)(B_{n,a+1} + B_{n,a-1}) - 16nB_{n-1,a}). \quad (69)$$

With  $u = n + a$  and  $v = n - a$ ,

$$B_{n,a} = \frac{u!}{\left(\frac{u}{2}\right)!} \frac{v!}{\left(\frac{v}{2}\right)!}.$$

Eq. (69) becomes

$$B_{n+1,a} = \frac{(u-1)!(v-1)!}{\left(\frac{u+1}{2}\right)! \left(\frac{v+1}{2}\right)!} \cdot \frac{1}{\frac{u+v}{2} + 1} \left( \frac{u+v+1}{2} (u(u+1)(v+1)^2 + v(v+1)(u+1)^2) - \frac{u+v}{2} (u+1)^2 (v+1)^2 \right),$$

which simplifies to

$$B_{n+1,a} = \frac{(u-1)!(v-1)!}{\left(\frac{u+1}{2}\right)! \left(\frac{v+1}{2}\right)!} (u(u+1)v(v+1)) = \frac{(u+1)!(v+1)!}{\left(\frac{u+1}{2}\right)! \left(\frac{v+1}{2}\right)!}, \quad (70)$$

and completes the induction.

## Appendix II: A combinatorial identity

In view of eq. (33), eq. (34) is equivalent to

$$-\frac{\mathbf{P}}{4} \sum_{q=n}^n \frac{(n+q)!(n-q)!}{4^n \binom{n+q}{2} \binom{n-q}{2}} z(n, q) = \frac{\mathbf{P}}{2^{2n+2}} C_m^2, \quad (71)$$

where, as before,  $n = 2m + 1$  and is the  $m$ th Catalan number  $C_m$  (eq. (35)),  $z(n, q) = 0$  unless  $q \equiv n \pmod{2}$ ,  $z(n, 1) = -\frac{1}{4}$ , and  $z(n, q) = \frac{1}{q^2 - 1}$ , otherwise. With  $q = 2r + 1$  and making

use of the fact that the summands depend only on  $|q|$ , this is equivalent to

$$\frac{1}{2} \frac{(2m+2)!(2m)!}{(m+1)!^2 m!^2} - \sum_{r=1}^m \frac{(2m+2r+2)!(2m-2r)!}{(m+r+1)!^2 (m-r)!^2} \frac{1}{2r^2+2r} = \frac{(2m)!^2}{(m+1)!^2 m!^2} = C_m^2. \quad (72)$$

We verify (72) by a telescoping, based on  $\frac{1}{2r^2+2r} = \frac{1}{2} \left( \frac{1}{r} - \frac{1}{r+1} \right)$ . Note that the initial term on the left of (72) is cancelled by the  $\frac{1}{r}$ -component of the  $r = 1$ -term in the summation. Thus,

$$\begin{aligned} & \frac{1}{2} \frac{(2m+2)!(2m)!}{(m+1)!^2 m!^2} - \sum_{r=1}^m \frac{(2m+2r+2)!(2m-2r)!}{(m+r+1)!^2 (m-r)!^2} \frac{1}{2r^2+2r} = \\ & \frac{1}{2(m+1)(2m+1)!^2} - \frac{1}{2} \sum_{r=1}^m \frac{1}{r} \left( \frac{(2m+2r+2)!(2m-2r)!}{(m+r+1)!^2 (m-r)!^2} - \frac{(2m+2r)!(2m-2r+2)!}{(m+r)!^2 (m-r+1)!^2} \right). \quad (73) \end{aligned}$$

We calculate

$$\begin{aligned} & \frac{1}{r} \left( \frac{(2m+2r+2)!(2m-2r)!}{(m+r+1)!^2 (m-r)!^2} - \frac{(2m+2r)!(2m-2r+2)!}{(m+r)!^2 (m-r+1)!^2} \right) = \\ & \frac{1}{r} \frac{(2m+2r)!(2m-2r)!}{(m+r+1)!^2 (m-r+1)!^2} \left( (2m+2r+2)(2m+2r+1)(m-r+1)^2 - (2m-2r+2)(2m-2r+1)(m+r+1)^2 \right) = \\ & \frac{1}{r} \frac{(2m+2r)!(2m-2r)!}{(m+r+1)!^2 (m-r+1)!^2} (4r(m+r+1)(m-r+1)) = \\ & 4 \frac{(2m+2r)!(2m-2r)!}{(m+r+1)!(m+r)(m-r+1)!(m-r)} = 4C_{m+r}C_{m-r}. \end{aligned}$$

Thus, we can rewrite eq. (73) as



$$\frac{1}{2} \frac{(2m+2)!(2m)!}{(m+1)!^2 m!^2} - \sum_{r=1}^m \frac{(2m+2r+2)!(2m-2r)!}{(m+r+1)!^2 (m-r)!^2} \frac{1}{2r^2 + 2r} = C_{2m+1} - 2 \sum_{r=1}^m C_{m+r} C_{m-r}. \quad (74)$$

Finally, the desired identity (72) follows from the autoconvolution property of the Catalan numbers, which can be written in the form

$$C_{2m+1} = C_m^2 + 2 \sum_{r=1}^m C_{m+r} C_{m-r}.$$

### Appendix III: The axial component of generalized spherical harmonics

[Supplanted via the use of Gegenbauer polynomials, above, with  $a = k + 1$ ]

We determine relationships among families of orthogonal polynomials  $p_n^{(k)}(\cos \mathbf{q})$ , orthogonal (but not necessarily orthonormal) with respect to the weight  $w_k(\mathbf{q}) = \frac{1}{\mathbf{p}} \sin^k \mathbf{q}$  on the interval  $\mathbf{q} \in [0, \mathbf{p}]$ . We choose  $p_n^{(0)}(\cos \mathbf{q}) = \cos n\mathbf{q}$ , and  $p_n^{(1)}(\cos \mathbf{q}) = P_n(\cos \mathbf{q})$ , where  $P_n(\cos \mathbf{q})$  is given by eq.(30).

Consider  $p^{(k)}$  to be a column vector composed of  $p_n^{(k)}(\cos \mathbf{q})$ . Orthogonality of these polynomials corresponds to

$$\frac{1}{\mathbf{p}} \int_0^{\mathbf{p}} p^{(k)} p^{(k)T} w_k(\mathbf{q}) d\mathbf{q} = D^{(k)}, \quad (75)$$

for some diagonal matrix  $D^{(k)}$ . Since

$$w_{k+2}(\mathbf{q}) = (\sin^2 \mathbf{q}) w_k(\mathbf{q}) = \left( \frac{1 - \cos 2\mathbf{q}}{2} \right) w_k(\mathbf{q}), \quad (76)$$

it follows that

$$\frac{1}{\mathbf{p}} \int_0^{\mathbf{p}} p^{(k)} p^{(k)T} w_{k+2}(\mathbf{q}) d\mathbf{q} = T^{(k)}, \quad (77)$$

for a matrix  $T_{m,n}^{(k)}$  whose only nonzero elements occur for  $m = n$ ,  $m = n + 2$ , or  $m = n - 2$ .

We work inductively, from  $k$  to  $k + 2$ , and attempt to find a matrix  $A^{(k+2)}$  of constants for which

$$p^{(k+2)} = p^{(k)} + A^{(k+2)} p^{(k+2)}, \quad (78)$$

i.e.,

$$p^{(k+2)} = (I - A^{(k+2)})^{-1} p^{(k)}. \quad (79)$$

Substituting this into eq. (75) yields

$$D^{(k+2)} = \int_0^p p^{(k+2)} p^{(k+2)T} w_{k+2}(\mathbf{q}) d\mathbf{q} = \int_0^p (I - A^{(k+2)})^{-1} p^{(k)} p^{(k)T} \left( (I - A^{(k+2)})^{-1} \right)^T w_{k+2}(\mathbf{q}) d\mathbf{q}, \quad (80)$$

or, using eq.(77),

$$(I - A^{(k+2)}) D^{(k+2)} (I - A^{(k+2)})^T = \int_0^p p^{(k)} p^{(k)T} w_{k+2}(\mathbf{q}) d\mathbf{q} = T^{(k+2)}. \quad (81)$$

Equating matrix entries leads to

$$D_{n,n}^{(k+2)} + (A_{n,n-2}^{(k+2)})^2 D_{n-2,n-2}^{(k+2)} = T_{n,n}^{(k+2)} \quad (82)$$

and

$$-A_{n+2,n}^{(k+2)} D_{n,n}^{(k+2)} = T_{n+2,n}^{(k+2)}. \quad (83)$$

**Example: k=0**

For  $k=0$ ,  $p_n^{(0)}(\cos \mathbf{q}) = \cos n\mathbf{q}$ . From eq. (77),

$$T_{n,n}^{(2)} = \frac{1}{p} \int_0^p \cos^2 n\mathbf{q} \sin^2 \mathbf{q} d\mathbf{q} = \frac{1}{p} \int_0^p \frac{1 + \cos 2n\mathbf{q}}{2} \frac{1 - \cos 2\mathbf{q}}{2} d\mathbf{q} = \begin{cases} \frac{1}{2}, n=0 \\ \frac{1}{8}, n=1 \\ \frac{1}{4}, n \geq 2 \end{cases}$$

and

$$T_{n+2,n}^{(2)} = \frac{1}{p} \int_0^p \cos(n+2)\mathbf{q} \cos n\mathbf{q} \sin^2 \mathbf{q} d\mathbf{q} = \frac{1}{p} \int_0^p \frac{\cos 2(n+1)\mathbf{q} + \cos 2\mathbf{q}}{2} \frac{1 - \cos 2\mathbf{q}}{2} d\mathbf{q} = \begin{cases} -\frac{1}{4}, n=0 \\ -\frac{1}{8}, n \geq 1 \end{cases}$$

From eqs. (82) and (83),  $D_{0,0}^{(2)} = \frac{1}{2}$  and  $A_{2,0}^{(2)} = \frac{1}{2}$ , and, for  $n \geq 1$ ,  $D_{n,n}^{(2)} = \frac{1}{8}$  and  $A_{n+2,n}^{(2)} = 1$ , consistent with eq. (40). Note that the normalization factor is different than in eq. (40), since here, we are integrating only over  $\mathbf{q}$ , and not the entire sphere.

**Example: k=1**

For  $k=1$ , we choose and  $p_n^{(1)}(\cos \mathbf{q}) = P_n(\cos \mathbf{q})$ , where  $P_n(\cos \mathbf{q})$  is given by eq.(30). From eq. (77),

## Acknowledgments

Thanks to John Velling for advice and Pascal Sebah for discussions related to series for  $\mathbf{p}$  .  
Supported in part by NIH EY9314.