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# Intrinsic shape invariants

Jérôme Houdayer

**Abstract**—Shape invariants are widely used in shape analysis. Usually they are build from rotational invariants based on coordinates systems. They are then transformed into translational invariants by fixing the center of gravity. Here, we propose a new approach by intrinsically defining an infinite family of invariants which are rotational and translational invariant from the beginning. This construction works in any dimension. Our invariants, which are true quadratic forms of the density form a basis of the quadratic invariants. Using their nice formulation, we can compute them analytically for simple shapes. We can also compute them from the 2D and 3D Zernike moments, and thus also express them as geometric moment invariants. From these invariants, we can define both a size dependent and a size independent distance between shapes. And last but not least, they can be measured for microscopic objects like proteins using small angle scattering experiments. We hope they can be usefull to reconstruct their original shape.

**Index Terms**—Shape analysis, Intrinsic invariants, Moment invariants, Shape distance.



## 1 INTRODUCTION

Shape invariants are quantities associated to shapes which are invariant under specific transformations. They are an important tool in a large variety of applications: object representation, recognition and retrieval, computer vision, medical imaging or molecular biology.

We will focus here on invariants by isometry, that is translations, rotations and mirror symmetry. There are other kinds of invariants, for examples those that change sign under mirror symmetry (skew invariants), those that are invariant by affine transformations, projections and so on.

The search for shape invariants by isometry began in 1962 with the work of Hu [1], where he introduced his famous seven 2D invariants. Those are geometric moment invariants (GMI) which means they are based on objects of the form  $\langle x^n y^m \rangle$  in 2D where  $\langle u \rangle = \int u \rho$  with  $\rho$  the density of the shape. This theory reached its full maturity with [2], [3]. The field diversified with the use of functional representation such as Zernike polynomials [4], [5] or Fourier-Mellin representations [6]. In 3D, the progress were slower due to the richer structure of the rotation group and lesser interest (3D data is less common). It started with GMI [7], which was later improved with [8], 3D Zernike were also used [9], [10] as well as polar radius representations [11]. Tensor methods were also introduced [12], [13]. A quite general solution was then achieved in [14].

The field is still very much active, see [15] concerning excessive enthousiasm. For a historical review see [16] and for a detailed presentation [17].

All these works use the same technique to build invariants: build a set of rotational invariants and make them translation invariants by fixing the center of gravity at the origin. Placing the shape in the coordinate system (position, orientation, scale) has been studied on its own in [18]. All those invariants thus share the same issues: the moments

are difficult to interpret as they depend on a coordinate system, because of that they are difficult to generalise in all dimensions. More importantly the invariants produced do not have a uniform dependence on the density (quadratic, quartic, ...). Note that a lot of invariants are said to be quadratic, but they are only before fixing the center of gravity (we will come back to this later). Why do we care for quadratic invariants ? Because of physics: if we build an experiment to measure the shapes of microscopic objects, the result will most probably be quadratic or at least with a definite dependence in the density. This is the case for small angle scattering (SAS) experiments (see for example [19]) which are the inspiration of this work.

Here we propose a new approach to shape invariants: we define intrinsic invariants that do not depend on a coordinate system. Because of this we can define them in any dimension. They are rotation and translation invariant from the beginning, so there is no fixing of the center of gravity. There have been some use of intrinsic descriptors for shapes, like shape distributions [20], [21] or integral invariants [22], but as far as we know nothing approaching true intrinsic invariants.

This paper is structured as follow. In Section 2, we define our invariants  $K_n$  and different tools to work with them. In Section 3, we show how to compute them from the density using 2D and 3D Zernike moments, and show that the  $K_n$  form a basis of quadratic invariants. In Section 4, we define two distances between shapes. In Section 5, we show how to compute our invariants for simple shapes. Finally, in Section 6, we show examples at low order to demonstrate the relations to GMI, in particular the Hu invariants. We finish by a conclusion.

## 2 INTRINSIC QUADRATIC SHAPE INVARIANTS

The theory presented here was started in [23] (following the breakthrough of [24]) in the context of small angle scattering experiments. Here, we present a much more developed theory. To do so, we have needed to change the notations, so the connection between the present work and [23] may

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be hard to follow. To make this article self contained, all relevant information from [23] is thus duplicated here with the new notations. Note that no knowledge of physics is required.

## 2.1 Notations

Before, we dive in our subject, we need to set some notations. We use standard notations for the multinomial coefficients  $\binom{n}{n_1, \dots, n_p} = n! / (n_1! \dots n_p!)$  and the kronecker symbol  $\delta_{nm}$  ( $\delta_{nn} = 1$  and  $\delta_{nm} = 0$  if  $n \neq m$ ).

We also use standard notations for the following functions:  $P_n$  is the Legendre polynomial,  $J_\nu$  the Bessel function,  $j_\nu$  the spherical Bessel function and the usual  $\Gamma$  function for which  $\Gamma(n+1) = n!$ . We also use the double factorial notation  $n!! = n(n-2) \dots$  so that  $(2n)!! = 2^n n!$  and  $(2n+1)!! = (2n+1)! / (2^n n!)$ . Finally, we also use  $\delta$  the Dirac's distribution.

The dimension of space is noted  $d$  and vectors are noted in bold characters  $\mathbf{r}$ . The corresponding length is noted in usual characters  $r = |\mathbf{r}|$ , and the direction of a vector is noted  $\hat{\mathbf{r}}$  so that  $\mathbf{r} = r \hat{\mathbf{r}}$ .

## 2.2 Usefull formulae

Some computations in this article are quite technical, we have gathered here a set of formulae we are going to use. This section can be skipped on a first read: it is only usefull as a reference. In this section all references to equation numbers refer to [25]. Using, Eq. 3.621.5, we have

$$\int_0^1 x^{2n+d} \sqrt{1-x^2}^{d-1} dx = \frac{\Gamma(n + \frac{d+1}{2}) \Gamma(\frac{d+1}{2})}{2(n+d)!}, \quad (1)$$

and from Eq. 3.715.21, we have

$$\int_0^\pi e^{ix \cos \theta} (\sin \theta)^d d\theta = 2^{d/2} \sqrt{\pi} \Gamma\left(\frac{d+1}{2}\right) \frac{J_{d/2}(x)}{x^{d/2}}. \quad (2)$$

In particular

$$\int_{\mathbb{S}^{d-1}} e^{i\mathbf{q} \cdot \mathbf{r}} d\hat{\mathbf{q}} = (2\pi)^{d/2} \frac{J_{d/2-1}(qr)}{(qr)^{d/2-1}}. \quad (3)$$

Bessel functions have some useful properties. From Eqs. 8.472.3, 8.440, 8.442.1 and 8.442.2, we have

$$\frac{d}{dz} (z^\nu J_\nu(z)) = z^\nu J_{\nu-1}(z). \quad (4)$$

$$J_\nu(x) = \sum_{n=F0}^{\infty} \frac{(-1)^n}{n! \Gamma(\nu+n+1)} \left(\frac{x}{2}\right)^{2n+\nu}. \quad (5)$$

$$J_\nu^2(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(\frac{x}{2}\right)^{2(\nu+n)} \frac{\Gamma(2\nu+2n+1)}{\Gamma^2(\nu+n+1) \Gamma(2\nu+n+1)}, \quad (6)$$

$$J_\nu(x) J_\nu(\lambda x) = \lambda^\nu \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(\frac{x}{2}\right)^{2(\nu+n)} \mu_n^\nu(\lambda), \quad (7)$$

with

$$\mu_n^\nu(\lambda) = \sum_{k=0}^n \binom{n}{k} \frac{\lambda^{2k}}{\Gamma(\nu+k+1) \Gamma(\nu+n-k+1)}. \quad (8)$$

Using Eq. 8.442.1 again, we have

$$J_{n-k}(x) J_{n+k}(x) = \sum_{l=n}^{\infty} (-1)^l \Theta_l^{nk} \left(\frac{x}{2}\right)^{2l}, \quad (9)$$

$$j_{n-k}(x) j_{n+k}(x) = \sum_{l=n}^{\infty} (-1)^l \theta_l^{nk} \left(\frac{x}{2}\right)^{2l}, \quad (10)$$

with

$$\Theta_l^{nk} = \frac{(-1)^n}{(2l)!} \binom{2l}{l-n} \binom{2l}{l-k}, \quad (11)$$

$$\theta_l^{nk} = \frac{(-1)^n 4^l}{(2(l+k)+1)!! (2(l-k)+1)!!} \binom{2l+1}{l-n}. \quad (12)$$

Finally, there is a nice expansion for  $J_\nu(qx)$ . From, Eq. 8.532.1, we get for  $0 \leq x \leq 2$

$$\frac{J_\nu(qx)}{(qx)^\nu} = 2^\nu \Gamma(\nu) \sum_{k=0}^{\infty} (\nu+k) \frac{J_{\nu+k}^2(q)}{q^{2\nu}} C_k^\nu \left(1 - \frac{x^2}{2}\right), \quad (13)$$

where  $C_k^\nu$  is the Gegenbauer polynomial. This formula has the nice property of separating the variables  $q$  and  $x$ .

## 2.3 Quadratic invariants

We will consider shapes in  $d$ -dimensional Euclidean space  $\mathbb{R}^d$ . A shape will be described through its density  $\rho$ . We will restrict ourselves to finite shapes, meaning that  $\rho(\mathbf{r}) = 0$  for large enough  $r$ . We consider only the case  $\rho$  real, but it may be negative.

We call  $M$  the total mass of the shape given by

$$M = \int_{\mathbb{R}^d} \rho(\mathbf{r}) d\mathbf{r}. \quad (14)$$

We suppose that  $M$  is finite but we make no other assumption on  $M$  so it may be negative or even null.

We now consider the set  $\mathcal{I}$  of the invariants  $Q$  by isometry (i.e. rotations, translations and mirror symmetry) which can be written

$$Q = \iint_{\mathbb{R}^d} \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) g_Q(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2, \quad (15)$$

where  $g_Q$  is a continuous function. Since  $Q$  is invariant by translation, we can restrict  $g_Q$  to depend only on  $\mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1$  and since it is invariant by rotation it may only depend on  $r_{12} = |\mathbf{r}_{12}|$ . Hence we can write

$$Q = \int_0^\infty p(x) g_Q(x) dx, \quad (16)$$

where  $p$  is the pair distance distribution function (PDDF) of  $\rho$  given by

$$p(x) = \iint_{\mathbb{R}^d} \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) \delta(x - r_{12}) d\mathbf{r}_1 d\mathbf{r}_2. \quad (17)$$

Note that this definition does not encompass quadratic invariants such as  $\int \rho^2$  which is related to  $p^{(d-1)}(0)$  and would require  $g_Q$  to be a distribution.

We call the function  $g_Q$  the *generator* of the quadratic invariant  $Q$ . Our goal here is to build a basis to represent  $g_Q$  and thus a basis of  $\mathcal{I}$ .

## 2.4 Relation to geometric moment invariants

Before we start, we can remark that  $\mathcal{I}$  contains all GMI which are quadratic. Indeed geometric moments are of the form  $\int \rho P$  for some polynomial  $P$ , so that a quadratic GMI  $Q$  takes the form

$$\begin{aligned} Q &= \sum_{i=0}^N \alpha_i \int_{\mathbb{R}^d} \rho(\mathbf{r}_1) P_{1,i}(\mathbf{r}_1) d\mathbf{r}_1 \int_{\mathbb{R}^d} \rho(\mathbf{r}_2) P_{1,i}(\mathbf{r}_2) d\mathbf{r}_2 \\ &= \iint_{\mathbb{R}^d} \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) g_Q(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2, \end{aligned} \quad (18)$$

where  $N$  is some integer,  $\alpha_i$  are real numbers and the  $P_{*,i}$  are polynomials and

$$g_Q(\mathbf{r}_1, \mathbf{r}_2) = \sum_{i=0}^N \alpha_i P_{1,i}(\mathbf{r}_1) P_{2,i}(\mathbf{r}_2), \quad (19)$$

which is continuous, so that  $Q \in \mathcal{I}$  according to Eq. 15.

Note that the GMI of the litterature are usually not quadratic even if they seem to be at first sight. For example, consider the second Hu invariant [1] in 2D: as a rotational invariant it is given by

$$I_{02} I_{20} = \langle x^2 \rangle^2 + 4 \langle xy \rangle^2 - 2 \langle x^2 \rangle \langle y^2 \rangle, \quad (20)$$

where  $\langle u \rangle = \int \rho(x, y) u dx dy$ . Note that to save space, we have omitted obvious symmetric terms: here  $\langle x^2 \rangle^2$  implies the term  $\langle y^2 \rangle^2$ . This a nice quadratic form on  $\rho$ . Its translation invariant form is found by replacing  $x$  by  $x - \langle x \rangle / M$  and  $y$  by  $y - \langle y \rangle / M$ . This gives (again omitting symmetric terms)

$$\begin{aligned} I_{02} I_{20} &= \frac{1}{M^2} \left( \langle x \rangle^4 - 2M \langle x \rangle^2 \langle x^2 \rangle + M^2 \langle x^2 \rangle^2 \right. \\ &\quad + 2 \langle x \rangle^2 \langle y \rangle^2 + 2M \langle x^2 \rangle \langle y \rangle^2 - 8M \langle x \rangle \langle y \rangle \langle xy \rangle \\ &\quad \left. + 4M^2 \langle xy \rangle^2 - 2M^2 \langle x^2 \rangle \langle y^2 \rangle \right), \end{aligned} \quad (21)$$

which is not quadratic in  $\rho$  but quartic.

## 2.5 The $H_n$ invariants

To build a basis of  $\mathcal{I}$ , we introduce our first set of invariants for  $n = 0, 1, 2, \dots$

$$H_n = \iint_{\mathbb{R}^d} \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) r_{12}^{2n} d\mathbf{r}_1 d\mathbf{r}_2. \quad (22)$$

The  $H_n$  are obviously in  $\mathcal{I}$  and their generators are the  $x^{2n}$ , namely we have

$$H_n = \int_0^\infty p(x) x^{2n} dx. \quad (23)$$

By construction, we have

$$H_0 = M^2, \quad (24)$$

$$H_1 = 2M^2 R_g^2, \quad (25)$$

where  $R_g$  is the radius of gyration of the shape. We will also use another size descriptor in the following, namely  $D_{\max}$  which is the diameter of the shape, i.e. the upper bound on the distances inside the shape. Or said otherwise the support of  $p$  is  $[0, D_{\max}]$ .

A remark on the value of  $M$ . If  $M = 0$ ,  $R_g$  is infinite but  $H_1$  is finite and not null in general. Our theory has no problem with the case  $M = 0$ . Nevertheless, when  $M \neq 0$ , it may be practical to set it to one, this is equivalent to dividing all  $H_n$  by  $M^2$  so that  $H_0 = 1$ . Likewise for  $p$ :  $\int p = M^2$  but if we normalise  $M$  to 1 then  $\int p = 1$ .

## 2.6 Questions of size

When we compare shapes, the relative size of the shapes may be relevant or not. To accomodate both possibilities, we will introduce rescaled version  $\bar{\rho}$  of  $\rho$  which depends on a size parameter  $D > 0$ :

$$\bar{\rho}(\mathbf{r}, D) = D^d \rho(D \mathbf{r}). \quad (26)$$

We will note  $\bar{X}(\rho) = X(\bar{\rho})$  for any functional of  $\rho$ . For example, we have made sure that  $\bar{M} = M$ . To take advantage of this definition, it is usefull to understand the size behavior of the different quantities we have introduced

$$\bar{p}(x, D) = D p(D x), \quad (27)$$

$$\bar{H}_n(D) = H_n / D^{2n}, \quad (28)$$

$$\bar{R}_g(D) = R_g / D, \quad (29)$$

$$\bar{D}_{\max}(D) = D_{\max} / D. \quad (30)$$

It is important to understand that *all* functional equations in this article are still valid when we add bars to all their functionals of  $\rho$ . For exmple  $\bar{H}_1 = 2\bar{M}^2 \bar{R}_g^2$ .

We can finally introduce a size invariant form  $\tilde{\rho}$  of  $\rho$  by setting  $D$  to its preferred value, namely  $D = D_{\max}$

$$\tilde{\rho}(\mathbf{r}) = \bar{\rho}(\mathbf{r}, D_{\max}). \quad (31)$$

Again we note  $\tilde{X}(\rho) = X(\tilde{\rho})$ , in particular  $\tilde{D}_{\max} = 1$ . Again *all* functional equations in this article are still valid when we add tildes to all their functionals of  $\rho$ . For example,  $\tilde{H}_1 = 2\tilde{M}^2 \tilde{R}_g^2$ .

## 2.7 The SAS profile

Since the PDDF  $p(x)$  is in general very difficult to compute, our previous definitions do not allow us to compute our invariants in practical cases. We will thus use the following: we define the  $d$ -dimensional SAS profile by

$$I(q) = \frac{1}{\mathcal{A}_d} \int_{\mathbb{S}^{d-1}} d\hat{\mathbf{q}} |\mathcal{F}(\rho)(\mathbf{q})|^2, \quad (32)$$

where  $\mathbb{S}^{d-1}$  is the unit sphere of dimension  $d-1$  (imbedded in  $\mathbb{R}^d$ ),  $\mathcal{A}_d = 2\pi^{d/2} / \Gamma(d/2)$  is the measure of its surface (i.e.  $\mathcal{A}_2 = 2\pi$  and  $\mathcal{A}_3 = 4\pi$ ),  $\mathbf{q} = q\hat{\mathbf{q}}$  and  $\mathcal{F}(\rho)(\mathbf{q})$  is the Fourier transform of  $\rho$  given by

$$\mathcal{F}(\rho)(\mathbf{q}) = \int_{\mathbb{R}^d} \rho(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}} d\mathbf{r}. \quad (33)$$

In 3D,  $I(q)$  is essentially the output profile of the small angle scattering (SAS) experiments, hence the name.

As before, we define a  $\bar{I}(\rho) = I(\bar{\rho})$ . The scaling law for  $I$  is then

$$\bar{I}(q, D) = I(q/D). \quad (34)$$

In particular  $\bar{I}(0) = I(0) = M^2$ .

If we develop the norm in  $I(q)$ , we get

$$\begin{aligned} I(q) &= \frac{1}{\mathcal{A}_d} \iint_{\mathbb{R}^d} d\mathbf{r}_1 d\mathbf{r}_2 \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) \int_{\mathbb{S}^{d-1}} e^{i\mathbf{q}\cdot\mathbf{r}_{12}} d\hat{\mathbf{q}} \\ &= \int_0^\infty p(x) g_I(qx) dx, \end{aligned} \quad (35)$$

where we have defined (see Eq. 3)

$$g_I(z) = 2^{d/2-1} \Gamma(d/2) \frac{J_{d/2-1}(z)}{z^{d/2-1}}, \quad (36)$$

where  $J_n$  is the Bessel function. Thus  $I(q) \in \mathcal{I}$  and  $g_I(qx)$  is the generator of  $I(q)$ .

Finally, we can relate  $I(q)$  to the  $H_n$  by developing  $g_I$  (using Eq. 5), and obtain

$$I(q) = \Gamma\left(\frac{d}{2}\right) \sum_{n=0}^{\infty} \frac{(-1)^n}{n! \Gamma(n + d/2)} \left(\frac{q}{2}\right)^{2n} H_n. \quad (37)$$

## 2.8 The $K_n$ invariants

We will now build a generating set  $K_n$  for  $\mathcal{I}$ . We will decompose  $g_Q$  on a polynomial family. In order to do this, we will restrict ourselves to shapes with  $D_{\max} \leq 1$ , so that  $g_Q$  is defined on  $[0, 1]$ . Since  $g_Q(x)$  is continuous on  $[0, 1]$ , then  $g_Q(\sqrt{x-1}/2)$  is continuous on  $[-1, 1]$ , we can thus decompose it with the Legendre polynomials  $P_n$

$$g_Q\left(\frac{\sqrt{x-1}}{2}\right) = \sum_{n=0}^{\infty} \alpha_n P_n(x), \quad (38)$$

with uniform convergence. Hence

$$g_Q(x) = \sum_{n=0}^{\infty} \alpha_n U_n(x), \quad (39)$$

where

$$U_n = P_n(1 - 2x^2), \quad (40)$$

$$\alpha_n = \int_0^1 g_Q(x) T_n(x) dx, \quad (41)$$

$$T_n(x) = 2x(2n+1)P_n(1-2x^2), \quad (42)$$

and

$$\int_0^1 U_n(x) T_m(x) dx = \delta_{nm}. \quad (43)$$

Note that  $U_0 = 1$  and thus  $K_0 = M^2$ . From this, we have for  $Q \in \mathcal{I}$  and  $D_{\max} \leq 1$

$$Q = \sum_{n=0}^{\infty} \alpha_n K_n, \quad (44)$$

with

$$K_n = \int_0^1 p(x) U_n(x) dx. \quad (45)$$

Hence the  $K_n$  form a generating set of  $\mathcal{I}$  restricted to  $D_{\max} \leq 1$ . We will see later on, that they are independent and thus form a basis of  $\mathcal{I}$ .

From this, we also get for  $0 \leq x \leq 1$

$$p(x) = \sum_{n=0}^{\infty} K_n T_n(x), \quad (46)$$

$$I(q) = \sum_{n=0}^{\infty} K_n S_n(q), \quad (47)$$

$$S_n(q) = \int_0^1 T_n(x) g_I(qx) dx, \quad (48)$$

$$g_I(qx) = \sum_{n=0}^{\infty} S_n(q) U_n(x). \quad (49)$$

Finally, we can relate the  $K_n$  to the  $H_n$  by writing

$$U_n(x) = \sum_{k=0}^n u_{nk} x^{2k}, \quad (50)$$

which gives

$$K_n = \sum_{k=0}^n u_{nk} H_k. \quad (51)$$

Using standard representation of  $P_n$ , we get

$$u_{nk} = (-1)^k \binom{n}{k} \binom{n+k}{k}. \quad (52)$$

We can also reverse this relation with

$$H_n = \sum_{k=0}^n v_{nk} K_k, \quad (53)$$

$$v_{nk} = (-1)^k \frac{n!^2 (2k+1)}{(n-k)! (n+k+1)!}. \quad (54)$$

We will see later on (after Eq. 59) where this last equation comes from.

For larger shapes (i.e. with  $D_{\max} > 1$ ), we choose a  $D \geq D_{\max}$  and we can use the barred versions of the equations of this section (since  $\bar{D}_{\max} = D_{\max}/D \leq 1$ ).

## 2.9 The $K_n^d$ invariants: a variation on the $K_n$

This section is only relevant for the SAS experiments (and demonstration of Eq. 54). It can be skipped on the first read.

The choice of the  $U_n$  is not unique and different choices lead to different definitions of the  $K_n$ . We will now make a choice dependent on the dimension and will note all the corresponding quantities with a  $d$  exponent.

To proceed, we rewrite  $g_I$  using Eq. 13. Starting from this equation at  $\nu = d/2$ , we differentiate it relatively to  $x$  using Eq. 4, and deduce for  $0 \leq x \leq 1$

$$g_I(qx) = \sum_{n=0}^{\infty} S_n^d(q) U_n^d(x), \quad (55)$$

with

$$S_n^d(q) = 2^d \Gamma^2\left(1 + \frac{d}{2}\right) \frac{J_{n+d/2}^2(q)}{q}, \quad (56)$$

$$U_n^d(x) = \frac{2n+d}{d^2} \frac{1}{x^{d-1}} \frac{d}{dx} \left(x^d C_n^{d/2}(1-2x^2)\right), \quad (57)$$

where  $C_n^\lambda$  is the Gegenbauer polynomial. This is identical to Eq. 49, we thus define  $K_n^d$  using Eq. 45 with  $U_n^d$ , and we recover Eqs. 46 to 49. We can define  $\alpha_n^d$  using Eq. 41, but it

is difficult to say if Eq. 39 converges in this case, we thus cannot tell whether the  $K_n^d$  form a generating set of  $\mathcal{I}$ . We believe this to be the case if we restrict ourselves to shapes with an intrinsic dimension larger than  $d$ .

To work with the  $K_n^d$ , we need to know more of the  $U_n^d$ . From [25] (Eq. 8.932.1), we find that

$$u_{nk}^d = \frac{\Gamma\left(\frac{d+1}{2}\right)}{d!} (-1)^k \binom{n}{k} \frac{(2n+d)(2k+d)(n+d+k-1)!}{n! \Gamma\left(k + \frac{d+1}{2}\right)}. \quad (58)$$

Note that these numbers are always rational. We can by the way check that  $U_0^d = u_{00}^d = 1$  as it should.

To compute the  $v_{nk}^d$ , we develop Eq. 47 with Eq. 6, we can thus express the  $H_n$  from the  $K_n^d$ , that is Eq. 53 with

$$v_{nk}^d = (-1)^k \frac{d d!! n! \binom{2n+d}{n-k}}{2^n (2n+d)(2n+d)!}. \quad (59)$$

That is the point where we can prove Eq. 54. Indeed Eq. 52 is very similar to Eq. 58 at  $d = 1$ , we can then deduce Eq. 54 from Eq. 59 at  $d = 1$ .

The case  $d = 3$  is of particular interest for the SAS experiments as Eq. 47 with  $K_n^d$  and  $S_n^d$  is used to fit the experimental data [23].

In this case, we can write  $S_n^3(q) = 9j_{n+1}^2(q)/q^2$  where  $j_n$  is the spherical Bessel function and  $T_n^3$  has been computed in [23], here is the result in our notations

$$T_n^3(x) = \frac{72}{2n+3} x^2 - 36 \sum_{k=0}^{n+1} \frac{(-1)^k x^{2k+3}}{(k+1)(2k+1)} \binom{n+1}{k} \binom{n+k+1}{k}. \quad (60)$$

To go from  $K_n^d$  to  $K_n$ , we use Eqs. 53 and 51 and obtain

$$K_n = \sum_{l=0}^n A_{nl}^d K_l^d, \quad (61)$$

with

$$A_{nl}^d = \sum_{k=l}^n u_{nk}^d v_{kl}^d. \quad (62)$$

It happens that, for  $d = 3$ , the  $A_{nl}^3$  can be written in closed form. Indeed for  $n \geq l$  we have

$$A_{nl}^3 = \frac{9\zeta_{nl}}{(2n-1)(2n+1)(2n+3)(2l+3)}, \quad (63)$$

with  $\zeta_{nn} = 2n-1$ ,  $\zeta_{n,n-1} = 2(2n-1)$ ,  $\zeta_{n,n-2} = 2n-5$  and  $\zeta_{nl} = -8$  otherwise. We do not have a demonstration for this in general, but we have checked it up to  $n = 100$ . In any cases, the  $A_{nl}$  are bounded so that this transformation is a smooth one and does not lead to a loss of precision.

### 3 COMPUTATION OF THE INVARIANTS

We will now see how we can evaluate the  $H_n$  and the  $K_n$  from the density  $\rho$ . To do this, we will compute  $I(q)$  from the Zernike moments of the density. The  $d$ -dimensional Zernike polynomials form a polynomial orthogonal basis of the unit  $d$ -dimensional ball, so we will fit our shape into the unit ball by using  $\bar{\rho}(\mathbf{r}, D)$ . The following computation is probably feasible in any dimension, but we will focus on 2D and 3D.

#### 3.1 In two dimensions

In 2D, one can compute the  $H_n$  from the 2D Zernike moments. This is important as it allows us to numerically compute our invariants in many situations in 2D.

The 2D complex Zernike polynomials form an orthogonal basis on the unit disk  $\mathbb{D}$ . They are given by

$$Z_n^m(\mathbf{r}) = R_n^m(r) e^{im\theta}, \quad (64)$$

$$R_n^m(r) = \sum_{k=0}^{\frac{n-|m|}{2}} \frac{(-1)^k (n-k)!}{k! \left(\frac{n+m}{2} - k\right)! \left(\frac{n-m}{2} - k\right)!} r^{n-2k}. \quad (65)$$

here  $n$  and  $m$  are integers,  $n \geq 0$ ,  $n \geq m \geq -n$  and  $n-m$  even. Here the chosen normalisation is  $\|Z_n^m\|_2 = \sqrt{\pi/(n+1)}$ .

We first rescale our shape so that it fits inside the unit disk. Namely we choose  $D$  such that  $\bar{\rho}(\mathbf{r}, D)$  has its support inside the unit disk. We can then write

$$\bar{\rho}(\mathbf{r}, D) = \sum_{n=0}^{\infty} \sum_{m=-n}^n c_n^m Z_n^m(\mathbf{r}), \quad (66)$$

where the  $c_n^m$  are the 2D Zernike moments of  $\bar{\rho}(\mathbf{r}, D)$  given by

$$c_n^m = \frac{n+1}{\pi} \int_{\mathbb{D}} \bar{\rho}(\mathbf{r}, D) Z_n^{m*}(\mathbf{r}) d\mathbf{r}. \quad (67)$$

Now, we can use the 2D plane wave expansion

$$e^{i\mathbf{q} \cdot \mathbf{r}} = \sum_{l=-\infty}^{\infty} i^l J_l(qr) e^{il(\theta_q - \theta_r)}, \quad (68)$$

where  $J_n$  is the Bessel function and this well known relation on  $R_n^m$

$$\int_0^1 r R_n^m(r) J_m(qr) dr = (-1)^{(n-m)/2} \frac{J_{n+1}(q)}{q}, \quad (69)$$

to get the Fourier transform of  $Z_n^m$

$$\hat{Z}_n^m(\mathbf{q}) = 2\pi i^m (-1)^{(n-m)/2} e^{im\theta_q} \frac{J_{n+1}(q)}{q}, \quad (70)$$

still with  $n-m$  even.

Plugging this in the barred version of Eq. 32, one gets

$$\bar{I}(q, D) = \frac{4\pi^2}{q^2} \sum_{n=0}^{\infty} \sum_{k=0}^n J_{n+k+1}(q) J_{n-k+1}(q) F_{nk}^2, \quad (71)$$

with

$$F_{nk}^2 = (-1)^k \epsilon_k \sum_{m=k-n}^{n-k} c_{n+k}^m c_{n-k}^{-m}, \quad (72)$$

where  $n-k-m$  even and  $\epsilon_0 = 1$  and  $\epsilon_k = 2$  for  $k \geq 1$ .

Finally, using Eq. 9 and identifying with Eq. 37 gives

$$\bar{H}_l(D) = -\pi^2 l^2 \sum_{n=0}^l \sum_{k=0}^n \Theta_{l+1}^{n+1,k} F_{nk}^2, \quad (73)$$

with  $\Theta_l^{nk}$  given by Eq. 11. From this, we can deduce

$$\bar{K}_m(D) = \pi^2 \sum_{n=0}^m \sum_{k=0}^n F_{nk}^2 \Omega_m^{nk}, \quad (74)$$

with

$$\Omega_m^{nk} = -\sum_{l=n}^m l!^2 u_{ml} \Theta_{l+1}^{n+1,k}. \quad (75)$$

*Important practical note:* To obtain accurate  $K_n$ , one should *not* compute them from the  $H_n$ . Eq. 74 must be used instead. For this, it is important to compute the  $\Omega_m^{nk}$  exactly (they are rationals) and convert them to floating point numbers afterwards.

### 3.2 In three dimensions

In 3D the computation is analogous using the 3D Zernike moments. It has first be done in [23], for completeness we sketch the computation here. The 3D complex Zernike polynomials form an orthogonal basis on the 3D unit ball  $\mathbb{B}$ . They are given by

$$Z_{nl}^m(\mathbf{r}) = R_{nl}(r)Y_l^m(\hat{\mathbf{r}}), \quad (76)$$

$$R_{nl}(r) = r^l \sum_{\nu=0}^k (-1)^{k+\nu} \frac{\binom{2k}{k} \binom{k}{\nu} \binom{2(k+l+\nu)+1}{2k}}{4^k \binom{k+l+\nu}{k}} r^{2\nu}, \quad (77)$$

where  $n, l$  and  $m$  are integers  $n \geq l \geq 0$ ,  $-l \leq m \leq l$ ,  $n-l$  even and  $k = (n-l)/2$ .  $Y_l^m$  are the usual complex spherical harmonics which form an orthonormal polynomial basis on the unit sphere. Here the chosen normalisation is  $\|Z_{nl}^m\|_2 = 1/\sqrt{2n+3}$ .

We choose  $D$  such that  $\bar{\rho}(\mathbf{r}, D)$  fits inside the unit ball and we can write

$$\bar{\rho}(\mathbf{r}, D) = \sum_{n=0}^{\infty} \sum_{l=0}^n \sum_{m=-l}^l c_{nl}^m Z_{nl}^m(\mathbf{r}), \quad (78)$$

where the  $c_{nl}^m$  are the 3D Zernike moments of  $\bar{\rho}(\mathbf{r}, D)$  given by

$$c_{nl}^m = (2n+3) \int_{\mathbb{B}} \bar{\rho}(\mathbf{r}, D) Z_{nl}^{m*}(\mathbf{r}) d\mathbf{r}. \quad (79)$$

Using the 3D plane wave expansion

$$e^{i\mathbf{t}\cdot\mathbf{x}} = 4\pi \sum_{l=0}^{\infty} i^l j_l(tx) \sum_{m=-l}^l Y_l^m(\hat{\mathbf{t}}) Y_l^{m*}(\hat{\mathbf{x}}),$$

where  $j_n$  is the spherical Bessel function, and

$$\int_0^1 x^2 R_{nl}(x) j_l(tx) dx = (-1)^{(n-l)/2} \frac{j_{n+1}(t)}{t}, \quad (80)$$

one easily finds that the Fourier transform of  $Z_{nl}^m$  is

$$\hat{Z}_{nl}^m(\mathbf{q}) = 4\pi i^l (-1)^{(n-l)/2} Y_l^m(\hat{\mathbf{q}}) \frac{j_{n+1}(q)}{q}. \quad (81)$$

Plugging this in the barred version of Eq. 32, one gets

$$\bar{I}(q, D) = \frac{4\pi}{q^2} \sum_{n=0}^{\infty} \sum_{k=0}^n j_{n+k+1}(q) j_{n-k+1}(q) F_{nk}^3, \quad (82)$$

with

$$F_{nk}^3 = (-1)^k \epsilon_k \sum_{l=0}^{n-k} \sum_{m=-l}^l (-1)^m c_{n+k,l}^m c_{n-k,l}^{-m}, \quad (83)$$

with  $n+k-l$  even and  $\epsilon_0 = 1$  and  $\epsilon_k = 2$  for  $k \geq 1$ .

Finally, using Eq. 10 and identifying with Eq. 37 gives

$$\bar{H}_l(D) = -\frac{\pi(2l+1)!}{4^l} \sum_{n=0}^l \sum_{k=0}^n \theta_{l+1}^{n+1,k} F_{nk}^3, \quad (84)$$

where  $\theta_l^{n,k}$  is given by 12. From this, we can deduce

$$\bar{K}_m(D) = \pi \sum_{n=0}^m \sum_{k=0}^n F_{nk}^2 \omega_m^{nk}, \quad (85)$$

with

$$\omega_m^{nk} = -\sum_{l=n}^m \frac{(2l+1)!}{4^l} u_{ml} \theta_{l+1}^{n+1,k}. \quad (86)$$

The remark after Eq. 75 also applies in 3D.

### 3.3 The $K_n$ form a basis of $\mathcal{I}$

We will now show that the  $H_n$  are independent in 3D, but this easily generalises to any dimension.

It is easy to see from Eq. 84 that  $H_k$  only depends on the Zernike coefficients  $c_{nl}^m$  with  $2n \leq k$ .

If we suppose that the  $H_n$  are algebraically dependent, this means that there exists a non trivial algebraic relation  $X(H_0, \dots, H_k) = 0$  for some  $k$  which stands for any value of the  $c_{nl}^m$ . But we can change the value of  $H_k$  without changing the  $H_0, \dots, H_{k-1}$  by changing the value of the  $c_{2k-1,l}^m$  and  $c_{2k,l}^m$  so that  $X$  cannot depend on  $H_k$  and by recursion on any  $H_n$ , which is a contradiction. Hence the  $H_n$  are algebraically independent.

Since the  $K_n$  are related to the  $H_n$  through a reversible linear transformation they also are independent. We can thus deduce that the  $K_n$  form a basis of  $\mathcal{I}$  (when restricted to  $D_{\max} \leq 1$ ).

We can also deduce that the  $K_n$  (resp.  $H_n$ ) form a basis for finite order quadratic GMI (those involving the  $c_n^m$  or  $c_{nl}^m$  up to a maximum  $n$  value).

## 4 DISTANCES BETWEEN SHAPES

We will now show how to compute a distance between two shapes, using our invariant basis  $K_n$ . We would like to have two kinds of distances: a size dependent one and a size independent one.

### 4.1 Norms on the PDDF

To build a distance, we will start by building a norm on the PDDF. To do this, we remark that from Eqs. 46 and 42 for  $D_{\max} \leq 1$

$$p(x) = 2x \sum_{n=0}^{\infty} (2n+1) K_n U_n(x). \quad (87)$$

Squaring this and integrating, we hence get for  $D_{\max} \leq 1$  (using Eq. 43)

$$\int_0^1 \frac{p^2(x)}{2x} dx = \sum_{n=0}^{\infty} (2n+1) K_n^2. \quad (88)$$

So we define a norm for  $p$  (for any  $D_{\max}$ ) which we call the  $U$ -norm by

$$\|p\|_U^2 = \int_0^{\infty} \frac{p^2(x)}{2x} dx. \quad (89)$$

Hence  $\|\bar{p}\|_U = D\|p\|_U$ . Thus, for  $D \geq D_{\max}$

$$\|p\|_U^2 = \frac{1}{D^2} \|\bar{p}\|_U^2 = \frac{1}{D^2} \sum_{n=0}^{\infty} (2n+1) \bar{K}_n^2(D), \quad (90)$$

independently of  $D$ . It is important to remark that the convergence of this sum is better when  $D$  is smaller. Indeed from Eqs. 51 and 28, we see that  $\bar{K}_n^2(D)/D^2$  goes to zero at large  $D$  as  $1/D^2$ . So the larger the  $D$ , the smaller the  $\bar{K}_n^2(D)/D^2$  and the more terms we need for the same precision.

We can interpret the  $U$ -norm in the following way: let  $p_2$  be the distribution of the squares of the distances in the object. A simple change of variables gives  $p_2(x) = p(\sqrt{x})/(2\sqrt{x})$  and a simple computation shows that the  $U$ -norm on  $p$  is the usual norm on  $p_2$ .

## 4.2 Distances

From the  $U$ -norm, we can derive a distance between PDDFs and hence a distance between shapes. The distance between two PDDFs  $p$  and  $q$  is given by

$$\begin{aligned} d^2(p, q) &= \|p - q\|_U^2 \\ &= \frac{1}{D^2} \sum_{n=0}^{\infty} (2n+1) (\bar{K}_n(p, D) - \bar{K}_n(q, D))^2, \end{aligned} \quad (91)$$

independently of  $D$ , as long as  $D \geq D_{\max}(p)$  and  $D \geq D_{\max}(q)$ . Deriving from a norm, this is a true distance in the mathematical sense.

To lighten notations, we introduce

$$\begin{aligned} \Delta(D, \rho, \sigma_\rho, \mu, \sigma_\mu) &= \\ \frac{1}{D^2} \sum_{n=0}^{\infty} (2n+1) (\bar{K}_n(\rho, \sigma_\rho D) - \bar{K}_n(\mu, \sigma_\mu D))^2, \end{aligned} \quad (92)$$

independently of  $D$  as long as  $D \geq D_{\max}(\rho)/\sigma_\rho$  and  $D \geq D_{\max}(\mu)/\sigma_\mu$ .

Given two shapes with densities  $\rho$  and  $\mu$ , we can define two interesting distances. To do this we will suppose that their densities are normalized, that is  $M(\rho) = M(\mu) = 1$  (i.e. the  $K_n$  are normalised so that  $K_0 = 1$ ).

We can first define a size dependent distance  $d_D$  given by

$$d_D^2(\rho, \mu) = \|p_\rho - p_\mu\|_U^2 = \Delta(D, \rho, 1, \mu, 1). \quad (93)$$

We also want a size independent distance. To do this, we use resized versions of  $\rho$  and  $\mu$  namely  $\bar{\rho}(\alpha)$  and  $\bar{\mu}(\beta)$ . Hence

$$\begin{aligned} d_D^2(\bar{\rho}(\alpha), \bar{\mu}(\beta)) &= \Delta(D, \bar{\rho}(\alpha), 1, \bar{\mu}(\beta), 1) \\ &= \Delta(D, \rho, \alpha, \mu, \beta). \end{aligned} \quad (94)$$

To choose  $\alpha$  and  $\beta$ , we can remark that the first term in  $\Delta$  (at  $n = 0$ ) is always null since  $K_0 = 1$ . We can choose  $\alpha$  and  $\beta$  to also cancel the second term (at  $n = 1$ ). This corresponds to  $\bar{K}_1(\rho, \alpha D) = \bar{K}_1(\mu, \beta D)$ , which can be obtained with  $\alpha = R_g(\rho)$  and  $\beta = R_g(\mu)$ . We can thus define a size independent distance  $d_1$  by

$$\begin{aligned} d_1^2(\rho, \mu) &= d_D^2(\bar{\rho}(R_g(\rho)), \bar{\mu}(R_g(\mu))) \\ &= \Delta(D, \rho, R_g(\rho), \mu, R_g(\mu)). \end{aligned} \quad (95)$$

We want to stress that in all cases, a zero distance does not mean identical shapes but only identical PDDF. The  $\bar{K}_n$  simply do not hold enough information for a true distance between shapes, they only contain the same information as  $p$ .

## 4.3 Distances in practice

To use these distances in practice, one needs to have for each shape, a  $D \geq D_{\max}$  (the smaller the better) and the corresponding  $\bar{K}_n$ . We will suppose that the shapes are normalised, that is  $\bar{K}_0 = 1$ . We know that  $\bar{H}_1 = 2M^2 R_g^2/D^2$  and that  $\bar{H}_1 = \frac{1}{2}(1 - \bar{K}_1)$ . Thus we can get the radius of gyration

$$R_g = \frac{D}{\lambda}, \quad (96)$$

with

$$\lambda = \frac{2}{\sqrt{1 - \bar{K}_1}} \quad (97)$$

To use the distances, we will have to limit us to a finite number of terms. As they are all positive, the more we can take, the more precise the result.

If we have two shapes  $\rho$  and  $\mu$  such that  $D_\rho \leq D_\mu$  then

$$d_D^2(\rho, \mu) = \Delta(D_\mu, \rho, 1, \mu, 1). \quad (98)$$

And if we suppose that  $\lambda_\rho \leq \lambda_\mu$  then

$$d_1^2(\rho, \mu) = \Delta\left(\lambda_\mu, \rho, \frac{D_\rho}{\lambda_\rho}, \mu, \frac{D_\mu}{\lambda_\mu}\right). \quad (99)$$

## 4.4 Navigating through the $\bar{K}_n$

You will need to change the value of  $D$  in  $\bar{K}_n(D)$  to accomodate the  $D \geq D_{\max}$  constraints required to compute distances. To do this, we have from Eqs. 53, 51 and 28

$$\bar{K}_n(\alpha D) = \sum_{l=0}^n S_{nl} \left(\frac{1}{\alpha^2}\right) \bar{K}_l(D), \quad (100)$$

where  $S_{nl}$  is a polynomial of degree  $n$  given by

$$S_{nl}(x) = \sum_{k=l}^n u_{nk} v_{kl} x^k. \quad (101)$$

we can compute from the definitions

$$u_{nk} v_{kl} = (-1)^{k+l} \frac{2l+1}{n+k+1} \binom{n+k+1}{n-k, k-l, k+l+1}. \quad (102)$$

There is a difficulty here: These coefficients diverge quite fast as  $n$  increases. Nevertheless the polynomials  $S_{nl}$  are essentially bounded on  $[0, 1]$ , so that the transformation of Eq. 100 is smooth for  $\alpha > 1$ . To use it, we need to be able to compute the  $S_{nl}$  precisely, to do this, we can for example compute the roots of  $S_{nl}$  using multiple precision (all those roots happen to be reals in  $[0, 1]$ ) and use them to evaluate the  $S_{nl}$ .

It is important to note that Eq. 100 cannot be used for  $\alpha < 1$  as the  $S_{nl}$  diverge very fast for  $x > 1$ . We thus need to take the original  $D$  as small as possible so we only need  $\alpha > 1$ .



## 5 COMPUTATION OF THE $\tilde{H}_n$ FOR SIMPLE SHAPES

In this section, we show how the  $H_n$  can be computed for simple geometric shapes. The point of this computation is to provide reference points. Coupled with distance evaluation, it can be used to find the nearest simple shape from a given shape.

The aim here is to compute  $D_{\max}$  and the  $\tilde{H}_n$ , since all other quantities are easily derived from there.

*Important remark:* when computing  $\tilde{H}_n$  for specific shapes, we will set  $M = 1$ . Constant factors are then irrelevant, so we will compute up to a constant factor. At the end we normalise the  $\tilde{H}_n$  using the fact that  $\tilde{H}_0 = 1$ .

### 5.1 Using the PDDF (segment)

The natural approach to compute  $H_n$  is to use the PDDF and Eq. 23. As an example, we will consider the case of a segment (which we call  $\mathbb{L}$ ) of constant density (normalisation is irrelevant as we will set  $\tilde{H}_0 = 1$  at the end) and of length  $l$ . By definition, we have for  $0 \leq x \leq l$

$$p_{\mathbb{L}}(x) \propto \int_0^l \int_0^l \delta(x - |x_2 - x_1|) dx_1 dx_2 \propto l - x. \quad (103)$$

Now using Eq. 23, we obtain

$$H_n(\mathbb{L}) \propto \int_0^l (l - x)x^{2n} dx \propto \frac{l^{2n+2}}{(n+1)(2n+1)}. \quad (104)$$

It is now an easy task to compute  $D_{\max}$  and the  $\tilde{H}_n$

$$D_{\max}^2(\mathbb{L}) = l^2, \quad \tilde{H}_n(\mathbb{L}) = \frac{1}{(n+1)(2n+1)}. \quad (105)$$

Computing Eq. 103 was already painful for such a simple shape. Indeed, computing the PDDF rapidly becomes a daunting task even for simple shapes like a disk or a cube. And we then still need to integrate Eq. 23.

This method of computation is not up to the task, and we will not go further this way. Another path must be found.

### 5.2 Using the autocorrelation function (ball)

The difficulty with the previous method is that it forces the use of spherical coordinates which are rarely adapted to the shape of interest. Here is a trick to prevent this. Remember that we note  $x = |\mathbf{x}|$ . Starting from Eq. 17, we can write

$$\begin{aligned} p(x) &= \iint_{\mathbb{R}^d} \rho(\mathbf{r}_1)\rho(\mathbf{r}_2)\delta(x - |\mathbf{r}_2 - \mathbf{r}_1|)d\mathbf{r}_1d\mathbf{r}_2 \\ &= \iint_{\mathbb{R}^d} \rho(\mathbf{r}_1)\rho(\mathbf{y} + \mathbf{r}_1)\delta(x - y)d\mathbf{r}_1d\mathbf{y} \\ &= \int_{\mathbb{R}^d} \gamma(\mathbf{y})\delta(x - y)d\mathbf{y}, \end{aligned} \quad (106)$$

where we have introduced  $\gamma$  the autocorrelation function

$$\gamma(\mathbf{x}) = \int_{\mathbb{R}^d} \rho(\mathbf{y})\rho(\mathbf{y} - \mathbf{x})d\mathbf{y}. \quad (107)$$

Now we can rewrite Eq. 23

$$\begin{aligned} H_n &= \int_0^\infty dr r^{2n} \int_{\mathbb{R}^d} \gamma(\mathbf{x})\delta(r - x)d\mathbf{x} \\ &= \int_{\mathbb{R}^d} \gamma(\mathbf{x})x^{2n}d\mathbf{x} \end{aligned} \quad (108)$$

Hence to compute  $H_n$ , we first need to compute  $\gamma$  using Eq. 107. For shapes with constant density (density 1 inside and density 0 outside) this is simply the volume of the intersection of the shape with a translated copy of itself. Note that constant factors are also irrelevant in  $\gamma$  and will also be dropped. We continue the computation with Eq. 108 using any suitable coordinate system.

We will now treat the example of the  $d$ -dimensional ball (noted  $\mathbb{B}^d$ ). In this case,  $\gamma$  depends only on the radial coordinate  $r$ .  $\gamma(r)$  is the volume of the intersection of two unit  $d$ -dimensional balls whose centres are at a distance  $r$ . It is simpler to compute its derivative. Indeed, it is the inner volume of the  $d - 2$  dimensional sphere which is the intersection of the surface of the balls. The radius of this intersection is easily found to be  $\sqrt{4 - r^2}/2$  and we get

$$\gamma'(r) \propto \sqrt{4 - r^2}^{d-1}, \quad (109)$$

for  $0 \leq r \leq 2$ . Now we have (using Eq. 1)

$$\begin{aligned} H_n(\mathbb{B}^d) &\propto \int_0^\infty r^{2n+d-1}\gamma(r)dr \\ &\propto \frac{1}{2n+d} \int_0^\infty r^{2n+d}\gamma'(r)dr \\ &\propto \frac{4^n}{2n+d} \int_0^1 r^{2n+d}\sqrt{1-r^2}^{d-1}dr \\ &\propto \frac{4^n}{(2n+d)(n+d)!} \Gamma\left(n + \frac{d+1}{2}\right). \end{aligned} \quad (110)$$

We thus get

$$D_{\max}^2(\mathbb{B}^d) = 4r^2, \quad \tilde{H}_n(\mathbb{B}^d) = \frac{dd!\Gamma\left(n + \frac{d+1}{2}\right)}{(2n+d)(n+d)!\Gamma\left(\frac{d+1}{2}\right)}. \quad (111)$$

In particular, we recover the segment for  $d = 1$ . Moreover, for the disk  $d = 2$  and the usual ball  $d = 3$ , we have

$$\tilde{H}_n(\mathbb{B}^2) = \frac{(2n+1)!!}{2^{n-1}(n+1)(n+2)!}, \quad (112)$$

$$\tilde{H}_n(\mathbb{B}^3) = \frac{18}{(n+2)(n+3)(2n+3)}. \quad (113)$$

### 5.3 Linear transformations (ellipsoidal shapes)

It is often practical to use a linear transformation to compute  $\gamma$  more easily. If  $t$  is an invertible linear transformation then we have

$$\begin{aligned} \gamma_\rho(\mathbf{x}) &= \int_{\mathbb{R}^d} \rho(\mathbf{y})\rho(\mathbf{y} - \mathbf{x})d\mathbf{y} \\ &\propto \int_{\mathbb{R}^d} \rho(t\mathbf{y}')\rho(t\mathbf{y}' - t\mathbf{x})d\mathbf{y}' \\ &\propto \gamma_{\rho \circ t}(t^{-1}\mathbf{x}). \end{aligned} \quad (114)$$

And we can compute  $H_n$  with

$$H_n \propto \int_{\mathbb{R}^d} \gamma_{\rho \circ t}(\mathbf{x})(t\mathbf{x})^{2n}d\mathbf{x}. \quad (115)$$

We do not need to compute  $t^{-1}$ . In general, there are no simple expression for transforming  $D_{\max}$ .

In particular, the following case is particularly useful for ellipsoidal shapes: if  $t(x_1, \dots, x_d) = (a_1x_1, \dots, a_dx_d)$  with

$a_i > 0$  and  $\rho \circ t$  depends only on the radial coordinate  $r$  then

$$H_n(\rho) \propto \int_{\mathbb{R}^d} \gamma_{\rho \circ t}(r) (a_1^2 x_1^2 + \dots + a_d^2 x_d^2)^n dx_1 \dots dx_d. \quad (116)$$

To compute this, we proceed as follow, we define

$$Z = \int_{\mathbb{R}^d} x_1^{2n_1} x_2^{2n_2} \dots x_d^{2n_d} e^{-x^2} d\mathbf{x}, \quad (117)$$

where  $\mathbf{x} = (x_1, \dots, x_d)$  and  $x = |\mathbf{x}|$ . We compute  $Z$  once in Cartesian coordinates and once in spherical coordinates. Comparing the two gives

$$\int_{\mathbb{S}^{d-1}} x_1^{2n_1} \dots x_d^{2n_d} d\hat{\mathbf{x}} = \frac{2\Gamma(n_1 + \frac{1}{2}) \dots \Gamma(n_d + \frac{1}{2})}{\Gamma(n_1 + \dots + n_d + \frac{d}{2})}. \quad (118)$$

Now, for any function  $f$ , we have

$$\int_{\mathbb{R}^d} x_1^{2n_1} \dots x_d^{2n_d} f(x) d\mathbf{x} = \frac{2\Gamma(n_1 + \frac{1}{2}) \dots \Gamma(n_d + \frac{1}{2})}{\Gamma(n_1 + \dots + n_d + \frac{d}{2})} \mathcal{A}_d \int_{\mathbb{R}^d} x^{2(n_1 + \dots + n_d)} f(x) d\mathbf{x}. \quad (119)$$

In particular for  $a_i > 0$

$$\int_{\mathbb{R}^d} (a_1^2 x_1^2 + \dots + a_d^2 x_d^2)^n f(x) d\mathbf{x} = (\max a_i)^{2n} E_n(a_1, \dots, a_d) \int_{\mathbb{R}^d} x^{2n} f(x) d\mathbf{x}, \quad (120)$$

with

$$E_n(a_1, \dots, a_d) = \frac{\Gamma(\frac{d}{2})}{2^n \Gamma(n + \frac{d}{2})} \frac{1}{(\max a_i)^{2n}} \sum_{\sum n_i = n} \binom{n}{n_1 \dots n_d} a_1^{2n_1} \dots a_d^{2n_d} (2n_1 - 1)!! \dots (2n_d - 1)!!. \quad (121)$$

We can now compute  $H_n$ :

$$H_n(\rho) \propto (\max_i a_i)^{2n} E_n(a_1, \dots, a_d) H_n(\rho \circ t). \quad (122)$$

In this case  $D_{\max}(\rho) = (\max_i a_i) D_{\max}(\rho \circ t)$ .

So, for any shape  $\mathbb{X}$  with spherical symmetry (namely  $\mathbb{X}$  depending only on  $r$ ), we can use this technique to elongate the shape by a factor  $a_i > 0$  depending on the axis, to make it ellipsoidal, we call this new shape  $t\mathbb{X}$ . We then get

$$D_{\max}^2(t\mathbb{X}) = (\max a_i^2) D_{\max}^2(\mathbb{X}), \quad (123)$$

$$\tilde{H}_n(t\mathbb{X}) = E_n(a_1, \dots, a_d) \tilde{H}_n(\mathbb{X}), \quad (124)$$

For example, the full 3D ellipsoid  $t\mathbb{B}^3$  is given by

$$D_{\max}^2(t\mathbb{B}^3) = 4 \max(a^2, b^2, c^2), \quad (125)$$

$$\tilde{H}_n(t\mathbb{B}^3) = \frac{18E_n(a, b, c)}{(n+2)(n+3)(2n+3)}. \quad (126)$$

## 5.4 Orthogonal factorisation (cuboid, cylinder)

We now consider the case where the density of the object can be factorised between  $p$  orthogonal subsets of coordinates. For example, this is the case for right cylinders or right cuboids. We suppose that we divide our  $d$  dimensional Cartesian coordinates in  $p$  orthogonal sets  $\mathbf{x} = (x_1, \dots, x_p)$  and that the density function can be factorised  $\rho(\mathbf{x}) = \rho_1(x_1) \dots \rho_p(x_p)$ . In this case, it is easy to see that

$$\gamma_\rho(\mathbf{x}) = \gamma_{\rho_1}(x_1) \dots \gamma_{\rho_p}(x_p) \quad (127)$$

and we have

$$\begin{aligned} H_n(\rho) &= \int \gamma_\rho(\mathbf{x}) x^{2n} d\mathbf{x} \\ &= \int \gamma_{\rho_1}(x_1) \dots \gamma_{\rho_p}(x_p) (x_1^2 + \dots + x_p^2)^n dx_1 \dots dx_p \\ &= \sum_{\sum_i n_i = n} \binom{n}{n_1 \dots n_p} H_{n_1}(\rho_1) \dots H_{n_p}(\rho_p), \end{aligned} \quad (128)$$

and

$$D_{\max}^2(\rho) = D_{\max}^2(\rho_1) + \dots + D_{\max}^2(\rho_p). \quad (129)$$

Orthogonal factorisation is useful to get the cuboid  $t\mathbb{C}^d$  of size  $(a_1, \dots, a_d)$  which factorises into segments:

$$D_{\max}^2(t\mathbb{C}^d) = \sum_i a_i^2, \quad \tilde{H}_n(t\mathbb{C}^d) = C_n(a_1, \dots, a_d), \quad (130)$$

where

$$C_n(a_1, \dots, a_d) = \frac{1}{(a_1^2 + \dots + a_d^2)^n} \sum_{\sum_i n_i = n} \binom{n}{n_1 \dots n_d} \frac{a_1^{2n_1} \dots a_d^{2n_d}}{(n_1 + 1)(2n_1 + 1) \dots (n_d + 1)(2n_d + 1)}. \quad (131)$$

In particular, for the  $d$ -cube  $\mathbb{C}^d$ , we have

$$D_{\max}^2(\mathbb{C}^d) = da^2, \quad \tilde{H}_n(\mathbb{C}^d) = C_n(1, \dots, 1). \quad (132)$$

From this, one can easily get the results for the square  $\mathbb{C}^2$ , the rectangle  $t\mathbb{C}^2$ , the usual cube  $\mathbb{C}^3$  and the usual rectangular cuboid (or rectangular parallelepiped)  $t\mathbb{C}^3$ .

This technique is also usefull for the right cylinders  $\mathbb{X} \times \mathbb{L}$  where  $\mathbb{X}$  is the base shape of the cylinder. In this case

$$D_{\max}^2(\mathbb{X} \times \mathbb{L}) = D_{\max}^2(\mathbb{X}) + l^2, \quad (133)$$

$$\begin{aligned} \tilde{H}_n(\mathbb{X} \times \mathbb{L}) &= \left( \frac{1}{1 + \varepsilon^2} \right)^{2n} \\ &= \sum_{k=0}^n \binom{n}{k} \frac{\varepsilon^{2k}}{(n-k+1)(2(n-k)+1)} \tilde{H}_k(\mathbb{X}), \end{aligned} \quad (134)$$

with  $\varepsilon = D_{\max}(\mathbb{X})/l$ . Using this general formula, one can explicitly get a variety of cylinders. For example, the full right circular cylinder  $\mathbb{B}^2 \times \mathbb{L}$  of radius  $r$  and length  $l$  is given, with  $\sigma = r/l$  (and thus  $\varepsilon = 2\sigma$ ), by

$$D_{\max}^2(\mathbb{B}^2 \times \mathbb{L}) = 4r^2 + l^2, \quad (135)$$

$$\tilde{H}_n(\mathbb{B}^2 \times \mathbb{L}) = \frac{\left(\frac{1}{1+4\sigma^2}\right)^n \sum_{k=0}^n \binom{n}{k} 2^{k+1}(2k+1)!!\sigma^{2k}}{(n-k+1)(2(n-k)+1)(k+1)(k+2)!}. \quad (136)$$

### 5.5 Using the SAS profile (sphere, spherical shell)

To finish our computations of simple shapes, we look at another way to compute the  $H_n$ . We can compute the SAS profile using Eq. 32 and use Eq. 37 to compute the  $H_n$ . For example, we can get the sphere  $\mathbb{S}^d$  (imbedded in  $\mathbb{R}^{d+1}$ ), using Eq. 3, we easily find that

$$I_{\mathbb{S}^d}(q) = \left| \int_{\mathbb{S}^d} e^{i\mathbf{q}\cdot\mathbf{r}} d\hat{\mathbf{r}} \right|^2 = (2\pi)^{d+1} \frac{J_{(d-1)/2}^2(q)}{q^{d-1}}. \quad (137)$$

We develop using Eq. 6 and compare to Eq. 37 (at  $d+1$ ), we thus get

$$H_n(\mathbb{S}^d) \propto \frac{4^n \Gamma(n + \frac{d}{2})}{(n+d-1)!}. \quad (138)$$

Hence

$$D_{\max}^2(\mathbb{S}^d) = 4r^2, \quad \tilde{H}_n(\mathbb{S}^d) = \frac{d! \Gamma(n + \frac{d}{2})}{2(n+d-1)! \Gamma(1 + \frac{d}{2})}. \quad (139)$$

In particular, for the circle  $\mathbb{S}^1$  and the usual sphere  $\mathbb{S}^2$ , we have

$$\tilde{H}_n(\mathbb{S}^1) = \frac{1}{4^n} \binom{2n}{n}, \quad \tilde{H}_n(\mathbb{S}^2) = \frac{1}{n+1}, \quad (140)$$

We can get a second elementary shape with this approach: the spherical shell  $\mathbb{A}^d$  ('A' stands for annulus). It is a unit ball with a centred spherical hole of radius  $\lambda$ . Computing  $I_{\mathbb{A}^d}$  proceeds as follow (using Eqs. 3 and 4)

$$\begin{aligned} I_{\mathbb{A}^d}(q) &= \left| \int_{\lambda}^1 r^{d-1} dr \int_{\mathbb{S}^{d-1}} e^{i\mathbf{q}\cdot\mathbf{r}} d\hat{\mathbf{r}} \right|^2 \\ &= \frac{(2\pi)^d}{q^d} \left( J_{d/2}^2(q) + \lambda^d J_{d/2}^2(\lambda q) \right. \\ &\quad \left. - 2\lambda^{d/2} J_{d/2}(q) J_{d/2}(\lambda q) \right), \end{aligned} \quad (141)$$

Using Eqs. 6 and 7, we obtain

$$H_n(\mathbb{A}^d) \propto H_n(\mathbb{B}^d) \sigma_n^d(\lambda), \quad (142)$$

$$\sigma_n^d(\lambda) = 1 + \lambda^{2(n+d)} \quad (143)$$

$$- 2\lambda^d \frac{(n+d)! \Gamma^2(n + \frac{d}{2} + 1)}{(2n+d)!} \mu_n^{d/2}(\lambda), \quad (144)$$

with  $\mu_n^d$  given by Eq. 8. Finally, this gives

$$D_{\max}^2(\mathbb{A}^d) = 4r^2, \quad \tilde{H}_n(\mathbb{A}^d) = \frac{\sigma_n^d(\lambda)}{(1-\lambda^d)^2} \tilde{H}_n(\mathbb{B}^d). \quad (145)$$

The special value  $\lambda = 0$  gives the ball back and the limit  $\lambda \rightarrow 1$  gives the sphere  $\mathbb{S}^{d-1}$ .  $\sigma_n^d$  can be written (see Eq. 143)

$$\begin{aligned} \sigma_n^d(\lambda) &= 1 + \lambda^{2(n+d)} \\ &\quad - 2\lambda^d \frac{(n + \frac{d}{2})!^2}{(2n+d)!} \sum_{k=0}^n \binom{n}{k} \binom{n+d}{k + \frac{d}{2}} \lambda^{2k}. \end{aligned} \quad (146)$$

In odd dimension, the fractional factorials  $\alpha!$  are to be understood as  $\Gamma(\alpha + 1)$  (and likewise for binomials). In dimension  $d = 3$ , an alternative derivation (brute force computation of  $\gamma$ , not shown) gives this somewhat simpler formula

$$\begin{aligned} \sigma_n^3(\lambda) &= 1 + \lambda^{2n+6} - 2(\lambda_+^{2n+6} - \lambda_-^{2n+6}) \\ &\quad + 2 \frac{n+3}{n+1} \lambda_+^2 \lambda_-^2 (\lambda_+^{2n+2} - \lambda_-^{2n+2}), \end{aligned} \quad (147)$$

where  $\lambda_{\pm} = (1 \pm \lambda)/2$ .

### 5.6 Other simple shapes (torus, cone, truncated cone)

There are probably other shapes that can be computed with the techniques presented here.

Another approach is also possible for shapes known analytically. One could try, using automatic algebra system to analytically compute the Zernike moments and deduce  $H_n$  from there. This will typically give an analytical formula for each  $H_n$  up to some maximum  $n$ , but not the  $n$  dependence itself.

This is particularly well adapted to shapes with cylindrical symmetry, such as the torus, the cone or the truncated cone, since the Zernike polynomials have good rotational properties.

## 6 EXAMPLES

In this section, we will give the first  $H_n$  as GMI in 2D and 3D. We do not show the  $K_n$  because their expressions are much longer, but they can easily be retrieved from Eqs. 51 and 52. As before, we note the geometric moments  $\langle u \rangle = \int \rho u$ , and to save (much) space, we do not write obvious symmetric terms. For example, in  $H_4$  in 3D, the term  $\langle x^3 y^2 \rangle \langle x z^2 \rangle$  represents 6 terms obtained by permutating the coordinates  $x, y$  and  $z$ .

Contrary to usual GMI formulae, the one showed here are already translation invariant. They do not need to be centralised for that.

### 6.1 Examples in two dimensions

Here are the first few  $H_n$  in 2D. To obtain their expression, we use Eq. 73 and then use the Cartesian expression of the 2D Zernike polynomials to derive the geometric moment expression.

$$\begin{aligned} H_0 &= M^2, \\ H_1 &= 2M \langle x^2 \rangle - 2 \langle x \rangle^2, \\ H_2 &= 2M \langle x^4 \rangle + 4M \langle x^2 y^2 \rangle - 8 \langle x^3 \rangle \langle x \rangle \\ &\quad - 8 \langle x^2 y \rangle \langle y \rangle + 6 \langle x^2 \rangle^2 + 4 \langle x^2 \rangle \langle y^2 \rangle + 8 \langle xy \rangle^2, \\ H_3 &= 2M \langle x^6 \rangle + 6M \langle x^4 y^2 \rangle - 12 \langle x^5 \rangle \langle x \rangle \\ &\quad - 12 \langle x^4 y \rangle \langle y \rangle - 24 \langle x^3 y^2 \rangle \langle x \rangle + 30 \langle x^4 \rangle \langle x^2 \rangle \\ &\quad + 6 \langle x^4 \rangle \langle y^2 \rangle + 48 \langle x^3 y \rangle \langle xy \rangle + 36 \langle x^2 y^2 \rangle \langle x^2 \rangle \\ &\quad - 20 \langle x^3 \rangle^2 - 24 \langle x^3 \rangle \langle xy^2 \rangle - 36 \langle x^2 y \rangle^2, \\ H_4 &= 2M \langle x^8 \rangle + 8M \langle x^6 y^2 \rangle + 12M \langle x^4 y^4 \rangle \\ &\quad - 16 \langle x^7 \rangle \langle x \rangle - 16 \langle x^6 y \rangle \langle y \rangle - 48 \langle x^5 y^2 \rangle \langle x \rangle \\ &\quad - 48 \langle x^4 y^3 \rangle \langle y \rangle + 56 \langle x^6 \rangle \langle x^2 \rangle + 8 \langle x^6 \rangle \langle y^2 \rangle \end{aligned}$$

$$\begin{aligned}
& + 96 \langle x^5 y \rangle \langle xy \rangle + 120 \langle x^4 y^2 \rangle \langle x^2 \rangle \\
& + 72 \langle x^4 y^2 \rangle \langle y^2 \rangle + 192 \langle x^3 y^3 \rangle \langle xy \rangle \\
& - 112 \langle x^5 \rangle \langle x^3 \rangle - 48 \langle x^5 \rangle \langle xy^2 \rangle \\
& - 240 \langle x^4 y \rangle \langle x^2 y \rangle - 48 \langle x^4 y \rangle \langle y^3 \rangle \\
& - 160 \langle x^3 y^2 \rangle \langle x^3 \rangle - 288 \langle x^3 y^2 \rangle \langle xy^2 \rangle \\
& + 70 \langle x^4 \rangle^2 + 120 \langle x^4 \rangle \langle x^2 y^2 \rangle + 12 \langle x^4 \rangle \langle y^4 \rangle \\
& + 160 \langle x^3 y \rangle^2 + 192 \langle x^3 y \rangle \langle xy^3 \rangle + 216 \langle x^2 y^2 \rangle^2 .
\end{aligned}$$

## 6.2 Examples in three dimensions

To get the expressions of the  $H_n$  in 3D, we use Eq. 84, and use the Cartesian expression of the 3D Zernike polynomials. For  $H_0$ ,  $H_1$  and  $H_2$  the expressions are the same in two and three dimensions. Note that they do not mean the same thing:  $\langle x^2 \rangle$  represents two terms in 2D and three in 3D. For higher order, the expression of  $H_n$  in 3D "contains" the one in 2D.

$$\begin{aligned}
H_3 = & \text{"2D"} + 12M \langle x^2 y^2 z^2 \rangle - 24 \langle x^2 y^2 z \rangle \langle z \rangle \\
& + 12 \langle x^2 y^2 \rangle \langle z^2 \rangle + 48 \langle x^2 yz \rangle \langle yz \rangle \\
& - 24 \langle x^2 y \rangle \langle yz^2 \rangle - 48 \langle xyz \rangle^2 , \\
H_4 = & \text{"2D"} + 24M \langle x^4 y^2 z^2 \rangle - 48 \langle x^4 y^2 z \rangle \langle z \rangle \\
& - 96 \langle x^3 y^2 z^2 \rangle \langle x \rangle + 24 \langle x^4 y^2 \rangle \langle z^2 \rangle \\
& + 96 \langle x^4 yz \rangle \langle yz \rangle + 192 \langle x^3 y^2 z \rangle \langle xz \rangle \\
& + 144 \langle x^2 y^2 z^2 \rangle \langle x^2 \rangle - 48 \langle x^4 y \rangle \langle yz^2 \rangle \\
& - 96 \langle x^3 y^2 \rangle \langle xz^2 \rangle - 384 \langle x^3 yz \rangle \langle xyz \rangle \\
& - 288 \langle x^2 y^2 z \rangle \langle x^2 z \rangle - 96 \langle x^2 y^2 z \rangle \langle z^3 \rangle \\
& + 24 \langle x^4 \rangle \langle y^2 z^2 \rangle + 192 \langle x^3 y \rangle \langle xyz^2 \rangle \\
& + 288 \langle x^2 yz \rangle^2 + 144 \langle x^2 y^2 \rangle \langle x^2 z^2 \rangle .
\end{aligned}$$

## 6.3 Relations to the Hu invariants

Using the geometric moments expressions of our invariants in 2D, we identify their relations to the first Hu invariants [1]:

$$\begin{aligned}
H_1 & = 2MI_{11}, \\
H_2 & = 4I_{11}^2 + 2MI_{22} + 2I_{20}I_{02}, \\
H_3 & = 18I_{11}I_{22} + 2MI_{33} - 2I_{30}I_{03} \\
& \quad - 18I_{21}I_{21} + 6(I_{31}I_{02} + I_{13}I_{20}).
\end{aligned}$$

Of course Hu invariants are not quadratic (except  $I_{11}$ ), so we can reproduce only selected combinations of them, namely one per order, which is  $H_n$ .

## 7 CONCLUSION

In this article, we propose a new approach to shape invariants. Instead of focusing on rotational invariants and then making them also translation invariant by fixing the centre of mass, we use intrinsic functional of the density which are rotation and translation invariant from the beginning.

We have build a set of invariants, the  $K_n$  which are independent of coordinate systems and even independent of the dimension of the space. They are quadratic forms of the density and form a basis of the vector space  $\mathcal{I}$  which in

particular contains all quadratic geometric moment invariants (in any dimension).

Due to their intrinsic definition, we could achieve a lot of analytical results. In particular, we can compute them analytically (through the  $H_n$ ) for simple shapes, we can relate them to the 2D and 3D Zernike moments, so that we can compute them in many situations. We can also express them as geometric moment invariants. Finally, they are related to small angle scattering experiments so that they can be measured experimentally for microscopic objects like proteins.

These invariants allow the definition of two distances between shapes. A size dependent one and a size independent one. Equipped with these distances, one can easily compare shapes independently of position and orientation (and optionally size), which is usefull in many applications.

We hope in a near future, to extend this theory to quartic invariants and beyond, providing a complete set of invariants in all dimensions which can be explicitly computed from Zernike moments thus generating all geometric moment invariants.

Finally, in the context of SAS in particular, it would be interesting to be able to reconstruct the shape from the invariants. Clearly some information is missing, but we hope that it is sufficient to get usefull results.

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