Open problems related to Zernike polynomials

1er Encuentro de la Red Orthonet Logroño, La Rioja

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1 Introduction

The Zernike polynomials were named after Frits Zernike (1888 - 1966), a deutch physicist who won a Nobel prize for his invention of the 'phase contrast microscope'. He proposed these as a complete set of orthonormal polynomials, with respect to the plain Lebesgue measure in the unit disk $\mathbb{D} = \left\{(x, y) \in \mathbb{R}^2 / x^2 + y^2 \leq 1\right\}$, which also possess some additonal properties:

1. Variable separation in polar coordinates: $Z(\rho, \theta) = R(\rho)T(\theta)$
2. Rotational symmetry: $T(\theta)$ should be continuous, 2π-periodic and also $T(\theta + \alpha) = T(\theta)T(\alpha)$. For example, $T(\theta) = e^{ik\theta}, k \in \mathbb{Z}$, satisfies that.
3. The radial component $R(\rho)$ is a polynomial in ρ, such that $Z(\rho, \theta)$ is also a polynomial in cartesian coordinates.

The Zernike polynomials are an infinite family that fulfill the properties above.

There exist several manners of enumerating the Zernike polynomials. The most common one, is to use a double-index notation (n, m) with $n \in \mathbb{N}$, $|m| \leq n$ and $n - m$ even (for a fixed n, m vary in $\{-n, -n + 2, \ldots, n - 2, n\}$). In this way, they can be written explicitly as follows:

$$Z_n^m(\rho, \theta) = N_n^m R_n^m(\rho) T_n^m(\theta), \quad 0 \leq \rho \leq 1, 0 \leq \theta \leq 2\pi$$

N_n^m being a normalization constant, R_n^m is the radial part and T_n^m is the angular part, given by the following formulas:

$$N_n^m = \sqrt{\frac{2(n+1)}{1+\delta_{m,0}}}$$

$$R_n^{|m|} = (-1)^{(n-m)/2} \rho^m P_{(n-m)/2}^{(m,0)} (1-\rho^2)$$

with $P_k^{(\alpha,\beta)}$ the Jacobi orthogonal polynomials, and

$$T_n^m(\theta) = \begin{cases} \cos(m\theta) & \text{if } m \geq 0 \\ -\sin(m\theta) & \text{if } m < 0 \end{cases}$$

With these definitions, the Zernike polynomials $\{Z_n^m\}_{n,m}$ are in fact orthonormal in the unit disk $\mathbb{D}$:

$$\iint_{\mathbb{D}} Z_n^m(\rho,\theta) Z_s^r(\rho,\theta) \rho d\rho d\theta = \delta_{n,s} \delta_{m,r}$$

It is possible also to use an one-index notation, with $j \in \mathbb{N}$ (there are various ways of doing this), such that the conversion between both notations is given by:

$$j = \frac{1}{2}\left(n(n+2) + m\right)$$

$$n = \left\lceil \frac{1}{2}(-3 + \sqrt{9+8j}) \right\rceil, \quad m = 2j - n(n+2)$$

where $\lceil x \rceil$ represents the ceiling function, the smallest integer number greater or equal than x.

2 Discrete Orthogonality

In the way they have been defined, the Zernike polynomials are orthogonal for the continuous Lebesgue measure in the unit disk $\mathbb{D}$. But additionally, they also satisfy a discrete orthogonality, discovered in 2005 by Pap and Schipp [1], in the following way:

- For $N \in \mathbb{N}$, we take λ_j^N $(j = 1, \ldots, N)$ the zeros of the Legendre orthogonal polynomial of degree N; and define $\rho_j^N = \sqrt{\frac{1}{2}(1+\lambda_j^N)}$.
- We also consider the Christoffel numbers A_j^N corresponding to the interpolation at λ_j^N:

$$A_j^N = \int_{-1}^{1} \ell_j^N(x)dx, \quad \ell_j^N(x) \text{ is the Lagrange basic polynomial associated to } \lambda_j^N$$

- Define as well $N(4N+1)$ nodes $Q_{j,k}$, given in polar coordinates by the expression:

$$Q_{j,k} = \left(\rho_j^N, \frac{2\pi k}{4N+1}\right), \quad j = 1, \dots, N, \quad k = 0, \dots, 4N$$

- Finally, let us define the measure ν_N as:

$$\nu_N = \sum_{j=1}^{N} \sum_{k=0}^{N} \frac{A_j^N}{2(4N+1)} \delta_{Q_{j,k}}$$

  $\delta_{Q_{j,k}}$ being the Dirac delta at the node $Q_{j,k}$.

With the previous definitions, it results that $\nu_N \to \frac{1}{\pi} dA$, this is, the discrete measure ν_N tends to the plain measure of Lebesgue in the unit disk $\mathbb{D}$ when $N \to \infty$; and with respect to that measure, the Zernike polynomials are also orthogonal:

$$\int Z_n^m Z_s^r d\nu_N = \delta_{n,s} \delta_{m,r}$$

whenever $n, m, s, r \in \mathbb{Z}$ and in addition: $n + s + |r| \leq 2N - 1$, and $n + s + |m| \leq 2N - 1$.

3 Open Problems

Despite the continuous orthogonality of the Zernike polynomials seems to be a desirable property, in practice it becomes useless, as one normally makes use of the values of that polynomials in a finite and discrete set of points of the unit disk, say $P_k = (x_k, y_k) \in \mathbb{D}$, with $k = 1, \dots, N$. Also, a finite number of Zernike polynomials is used, namely the set of the $M + 1$ first of them: $\{Z_j(x, y)\}_{j=0,1,\dots,M}$.

Then, it is common to work with the collocation matrix, or evaluation matrix, of the $M + 1$ first Zernike polynomials (with the one-index notation) evaluated in a sample of N nodes of the unit disk.

$$A = \left(\ Z_j(x_i, y_i)\ \right)_{\substack{1 \leq i \leq N \\ 0 \leq j \leq M}} \in \mathcal{M}^{N \times (M+1)}(\mathbb{R})$$

$$A = \begin{pmatrix} Z_0(x_1, y_1) & Z_1(x_1, y_1) & \dots & Z_{M-1}(x_1, y_1) & Z_M(x_1, y_1) \\ Z_0(x_2, y_2) & Z_1(x_2, y_2) & \dots & Z_{M-1}(x_2, y_2) & Z_M(x_2, y_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ Z_0(x_N, y_N) & Z_1(x_N, y_N) & \dots & Z_{M-1}(x_N, y_N) & Z_M(x_N, y_N) \end{pmatrix}_{N \times (M+1)}$$

This matrix is of great practical importance, as it is used to solve some least squares problems, e.g. in order to obtain the coefficients of the Zernike polynomials in a linear combination.

In the following three open problems, the nodes $P_k = (x_k, y_k) \in \mathbb{D}$ might be given a priori, with a fixed and known distribution (e.g. those used by the commercial corneal topographers, which are regular or quasi-regular grids, in polar or cartesian coordinates), or alternatively it is possible to choose the most suitable distribution (for certain practical applications, it is possible to select the nodes that will be used). We can even assume that P_k's are angularly equally spaced.

3.1 Invertibility of the matrix A

The first open problem is, in the case of A being square (this is, we have the same number of nodes and of Zernike polynomials, $N = M+1$), decide whether the matrix A is invertible or not.

3.2 Condition number of matrix A

In the general situation, when A might be square or not, it would be of interest to estimate or bound the spectral condition number of the matrix A,

$$\kappa_2(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)},$$

where $\sigma_{\max}(A)$ and $\sigma_{\min}(A)$ are the largest and smallest singular values of A, respectively, or any other measure of numerical stability of this matrix.

3.3 Condition number of the matrix of derivatives

It is also useful for some practical applications to use the matrix of evaluations, but not of the Zernike polynomials directly, but of their partial derivatives:

$$B = \begin{pmatrix} \frac{\partial}{\partial x} Z_j(x_i, y_i) \\ \hline \frac{\partial}{\partial y} Z_j(x_i, y_i) \end{pmatrix}_{2N \times M}$$

and for the same previous reasons, it is important to estimate the condition number $\kappa_2(B)$.

References

[1] M. Pap and F. Schipp. Discrete orthogonality of Zernike functions. *Mathematica Pannonica*, 16(1):137–144, 2005.