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Complete Modal Representation with Discrete Zernike Polynomials - Critical Sampling in Non Redundant Grids

Rafael Navarro¹ and Justo Arines²

¹ICMA, Consejo Superior de Investigaciones Científicas & Universidad de Zaragoza

²Universidade de Santiago de Compostela
Spain

1. Introduction

Zernike polynomials (ZPs) form a complete orthogonal basis on a circle of unit radius. This is useful in optics, since a great majority of lenses and optical instruments have circular shape and/or circular pupil. The ZP expansion is typically used to describe either optical surfaces or distances between surfaces, such as optical path differences (OPD), wavefront phase or wave aberration. Therefore, applications include optical computing, design and optimization of optical elements, optical testing (Navarro & Moreno-Barriuso, 1999), wavefront sensing (Noll, 1978)(Cubalchini, 1979), adaptive optics (Alda & Boreman, 1993), wavefront shaping (Love, 1997) (Vargas-Martin et al., 1998), interferometry (Kim, 1982)(Fisher et al., 1993)(van Brug, 1997)(Chen & Dong, 2002), surface metrology topography (Nam & Rubinstein, 2008), corneal topography (Schwiegerling et al., 1995)(Fazekas et al., 2009), atmospheric optics (Noll, 1977) (Roggemann, 1996), etc. This brief overview shows that the modal description provided by ZPs was highly successful in a wide variety of applications. In fact, ZPs are embedded in many technologies such as optical design software, large telescopes, ophthalmology, communications, etc.

The modal representation of a function (wavefront, OPD, surface, etc.) over a circle in terms of ZPs is:

$$W(\rho, \theta) = \sum_{n,m} c_n^m Z_n^m(\rho, \theta) \quad (1)$$

where c_n^m are the coefficients of the expansion; (ρ, θ) are polar coordinates with origin at the pupil centre. The radial coordinate is normalized to the physical (real) radius of the circle $\rho = r/R$, since the ZPs are orthogonal only within a circle of unit radius. The usefulness and importance of ZPs is associated to two main properties, completeness and orthogonality (Mahajan, 2007). However, in real applications one is constrained to work with discrete (sampled) arrays of data rather than with continuous functions, and then the discrete (sampled) Zernike polynomials loose these two essential properties, namely orthogonality and completeness (Wang & Silva, 1980)(Navarro et al., 2009). For this reason different authors have proposed alternative basis functions, such as Fourier series, splines or Chebyshev-polynomials (Ares & Royo, 2006)(Soumelidis, 2005).

The estimation of the coefficients of the Zernike expansion is still an open problem, which has attracted the interest of many researchers. In particular, different studies had shown the decisive influence of the type of sampling pattern on the quality of the reconstructions (Voitsekhovich, 2001)(Diaz-Santana et al., 2005)(Pap & Shipp, 2005). For instance, orthogonal discrete ZPs were introduced for wavefront fitting (Malacara et al., 1990) (Fisher et al., 1993); random patterns provided enhanced performance (Soloviev & Vdovin, 2005); and Albrecht grids have the property of keeping the orthogonality of ZPs (Rios et al., 1997). Nevertheless, apart of the lack of completeness and orthogonality of discrete ZPs, there is an additional issue, which affect several important applications, such as optical design (ray tracing), wavefront sensing and surface metrology. In all these applications the modal description of the wavefront is not reconstructed from wavefront samples but from (measure or computation of) wavefront slopes (Southwell, 1980) (Bará, 2003) (Liang et al., 1994) (Solomon, 1998) (Primot, 2003). The third problem arises because in order to reconstruct the wavefront, one fit the data (slopes) to the slopes, i.e. partial derivatives, of ZPs, and these partial derivatives are not orthogonal even for the ideal continuous polynomials.

In summary, there are three different problems that one has to face when implementing practical applications (either numerical or experimental): (1) Lack of completeness of ZPs; (2) Lack of orthogonality of ZPs and (3) Lack of orthogonality of ZP derivatives. To overcome these limitations, the general standard procedure is to apply a strong oversampling (redundancy) and reconstruct the wavefront by standard least squares fit. The advantage of a strong redundancy is to minimize the reconstruction noise, but it has two main disadvantages. When one reconstructs fewer modes than measures, then there is a high probability of having cross coupling and aliasing in the modal wavefront estimation (Herrmann, 1981). In addition, oversampling necessarily implies that the wavefront reconstruction is not invertible. This means that it is not possible to recover the initial measures (or samples) from the reconstructed wavefront. This complicates or can even preclude some applications involving iterative processes, inverse problems, etc.

Our goal in this work was to study these three problems and provide practical solutions, which are tested and validated through realistic numerical simulations. Our approach was to start studying and eventually solve the problem of completeness (both for ZPs and ZPs derivatives), because if we can guarantee completeness, then it is straightforward to apply Gram-Schmidt (or related method) to obtain an orthonormal basis over the sampled circular pupil (Upton et al., 2004). Furthermore, completeness in the discrete domain, means that Eq.1 can be expressed as a matrix-vector product, where the matrix is square and has an inverse. This means that we have the same number of samples and coefficients and that we should be able to pass one set to the other and viceversa. However, orthogonality becomes important, especially for large matrices, because in that case the inverse transform (matrix) is equal to its transpose, which guarantees numerical stability of matrix inversion. Our approach to guarantee completeness is based on the intuitive idea of avoiding any redundancy in the sampling pattern. This means that the coordinates of the sampling points never repeat: that is $\theta_i \neq \theta_k$ and $\rho_i \neq \rho_k \forall i, k$ in the sampling grid. We confirmed empirically, with different sampling patterns (regular, random and randomly perturbed regular), that these non-redundant sampling schemes keep completeness of both ZPs and ZP derivatives. This permits to work with invertible square matrices, which can be orthogonalized through the classic QR factorization. In the following Sections, we first overview the basic theory (Section 2); then we obtain the orthogonal modes for both the

discrete Zernike and the Zernike derivatives transforms for different sampling patterns (Section 3); in Section 4 we describe the implementation and results of realistic computer simulations; and the main conclusions are given in Section 5.

2. Theory

Zernike polynomials are separable into radial polynomial and an angular frequency. According to the ANSI Z80.28 standard the general expression is:

$$Z_n^m(\rho, \theta) = \begin{cases} N_n^m R_n^{|m|}(\rho) \cos m\theta & \text{for } m \geq 0 \\ -N_n^m R_n^{|m|}(\rho) \sin m\theta & \text{for } m < 0 \end{cases} \quad (2)$$

where the radial polynomial is:

$$R_n^{|m|}(\rho) = \sum_{s=0}^{(n-|m|)/2} \frac{(-1)^s (n-s)!}{s! [0.5(n+|m|)-s]! [0.5(n-|m|)-s]!} \rho^{n-2s} \quad (3)$$

and orthonormality is guaranteed by the normalization factor N :

$$N_n^m = \sqrt{\frac{2(n+1)}{1+\delta_{m0}}} \quad (4)$$

where δ_{m0} is the Kronecker delta function. The radial order n is integer positive, and the angular frequency m can only take values $-n, -n+2, -n+4, \dots, n$. For practical implementation, sampled signals and discrete polynomials, we shall use vector-matrix formulation, and hence it is useful to merge n and m indexes into a single one $j = (n(n+2)+m)/2$ (ANSI Z80.28 standard).

2.1 Critical sampling and invertible transform

The classical problem to represent a function as an expansion such as that of Eq. 1 is to obtain the coefficients $c_n^m = c_j$. The orthogonality of ZPs implies that we can compute the coefficients as the projections (inner product) of the function W on each basis function:

$$c_n^m = \int_0^1 \int_0^{2\pi} W(\rho, \theta) Z_n^m(\rho, \theta) \rho d\theta d\rho \quad (5)$$

but this expression can be hardly applied when we only have a discrete set of samples of W , and the discrete polynomials are not orthogonal.

The discrete version of Eq. 1 is $\mathbf{w} = \mathbf{Z}\mathbf{c}$. Now, $\mathbf{w}$ is a column vector whose components are the I samples of $W(\rho, \theta)$; $\mathbf{c}$ is another column vector formed by J expansion coefficients $c_j = c_n^m$; and $\mathbf{Z}$ is a matrix, $Z_{i,j}$, whose columns are sampled Zernike polynomials. Matrix $\mathbf{Z}$ is rectangular, but for a given sampling pattern, the number of coefficients (modes) has to be less or equal to the number of samples ($J \leq I$). The case $J = I$ corresponds to critical sampling. To obtain the coefficients one can solve $\mathbf{w} = \mathbf{Z}\mathbf{c}$ for $\mathbf{c}$, but for doing that $\mathbf{Z}$ must have an inverse so that one can apply $\mathbf{c} = \mathbf{Z}^{-1}\mathbf{w}$. The inverse $\mathbf{Z}^{-1}$ exists only if (1) it is square (critical

sampling) and (2) its determinant $\text{Det}(\mathbf{Z}) \neq 0$. In other words the rank of this $I \times J$ matrix has to be $\text{Rank}(\mathbf{Z}) = I = J$. As we will see below, $\text{Rank}(\mathbf{Z}) < I$ for most common sampling patterns, and $\mathbf{Z}^{-1}$ does not exist. The standard way to overcome this problem is to apply a strong oversampling to the wavefront W and estimate a number of coefficients much lower than the number of samples ($J \ll I$). Provided that, $\text{Rank}(\mathbf{Z}) \geq J$, then the coefficients can be estimated computing the Moore-Penrose pseudoinverse of $\mathbf{Z}$:

$$\hat{\mathbf{c}} = (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \mathbf{w} \quad (6)$$

This is a standard (linear) least squares fit. The tilde means estimated, since the wavefront expansion is approximated. This estimation is optimal under a least squares criterion (minimum RMS error). However it may not be exact due to mode coupling and aliasing (Herrmann, 1980) (Herrmann, 1981) and always requires a highly redundant sampling. As a consequence, Eq. 6 is not invertible, in the sense that one recovers estimates $\hat{\mathbf{w}} = \mathbf{Z}\hat{\mathbf{c}}$ rather than the true original samples $\mathbf{w}$. In Section 3 we show that non redundant patterns keep completeness of the ZPs basis, which permits to work with critical sampling, and guarantee the existence of both direct and inverse transforms:

$$\mathbf{w} = \mathbf{Z}\mathbf{c} \quad \text{and} \quad \mathbf{c} = \mathbf{Z}^{-1}\mathbf{w} \quad (7)$$

2.2 Critical sampling of Zernike polynomial derivatives

There is a variety of applications where the measurements (samples) are slopes or gradient of the surface (surface metrology) or wavefront (numerical ray tracing or wavefront sensing) (Wyant & Creath, 1992) (Welsh et al., 1995). In the last case, the original samples at points (ρ_i, θ_i) , $i = 1, \dots, I$ are transverse aberrations, proportional to the wavefront slopes, components of the wavefront gradient:

$$(x'_i, y'_i) = f'/R \nabla W(\rho_i, \theta_i) \quad (8)$$

where R is the total pupil radius and f' is the focal length of the lens (or microlens array) of the measuring instrument (Navarro & Moreno-Barriuso, 1999). To recover the wavefront W one has to integrate the gradient, and to this end it is convenient to apply some expansion of W in terms of some derivable basis functions. For circular pupils, Zernike polynomials (ZPs) seem an appropriate basis even though ZP derivatives are not orthogonal. In terms of ZPs derivatives, we can express the gradient of W as a column vector, and using the expansion of Eq. 1 we arrive to the expression of a normalized i -th measure vector $\mathbf{m}_i$, formed by the normalized measurements along the x and y axes:

$$\mathbf{m}_i = R_{pup} / f' \begin{pmatrix} x'_i \\ y'_i \end{pmatrix} = \sum_{j=1}^J c^j \begin{pmatrix} Z'_X{}^j \\ Z'_Y{}^j \end{pmatrix} \quad (9a)$$

where $Z'_X{}^j$, $Z'_Y{}^j$ are the partial derivatives of the j -th ZP at point i . It is important to note that we exclude the constant piston term $j = 0$ since the partial derivatives are zero. For the complete set of samples in vector-matrix notation we obtain:

$$\mathbf{m} = \begin{pmatrix} \mathbf{Z}'_X \\ \mathbf{Z}'_Y \end{pmatrix} \mathbf{c} = \mathbf{D}\mathbf{c} \quad (9b)$$

This expression $\mathbf{m} = \mathbf{D}\mathbf{c}$ is similar to the discrete version of Eq. 1 ($\mathbf{w} = \mathbf{Z}\mathbf{c}$) before, but now the columns of matrix $\mathbf{D}$ are concatenated partial derivatives of ZPs. This means that $\mathbf{D}$ has double $2I$ rows. As in the preceding Subsection, the usual strategy is to apply a strong oversampling, $J \ll I$, and then compute the least squares solution, i.e. the pseudo inverse, so that the coefficients are estimated as $\hat{\mathbf{c}} = (\mathbf{D}^T \mathbf{D})^{-1} \mathbf{D}^T \mathbf{m}$. Again, in case that we could guarantee completeness, it would be possible to apply critical sampling, so that $\mathbf{D}$ is square $J = 2I$; as before, completeness means that $\text{Det}(\mathbf{D}) \neq 0$ or equivalently $\text{Rank}(\mathbf{D}) = 2I = J$.

It is worth remarking that critical sampling in this case means to recover double number of modes than sampling points, $J=2I$, simply applying $\mathbf{c} = \mathbf{D}^{-1}\mathbf{m}$. This possibility is plausible since we have two measures (two partial derivatives in $\mathbf{m}_i$) at each point, provided that there is no redundancy (Navarro et al., 2011). This would be similar to the Hermite interpolation, where one has the function and its first derivative at each point and recovers $J=2I$ coefficients. Regarding completeness, the intuitive hypothesis is that if the original basis $\mathbf{Z}$ is complete, and able to represent any continuous (derivable) function W within a circular support, then we would expect that the set formed by their derivatives $\mathbf{D}$ should provide a complete representation for the derivatives (gradient) of W . As shown in the next Section, this hypothesis was verified empirically for a variety of families of non redundant sampling patterns.

2.3 Orthogonalization

As we said above, our main empirical finding was that different types of non redundant sampling patterns on the circle keep completeness of both the discrete ZPs and discrete (sampled) derivatives. However, orthogonality is lost in both cases after sampling. One of the most important problems caused by the lack of orthogonality is a bad condition number of matrix $\mathbf{Z}$ (or $\mathbf{D}$), which makes the inversion ($\mathbf{Z}^{-1}$ or $\mathbf{D}^{-1}$) to be numerically instable (Navarro et al., 2011) (Zou & Rolland, 2006). The consequence is noise amplification when one tries to estimate the coefficients, using either $\mathbf{c} = \mathbf{Z}^{-1}\mathbf{w}$ or $\mathbf{c} = \mathbf{D}^{-1}\mathbf{m}$. The condition number (CN), ratio between the highest and lowest singular value of the matrix, is the main metric for the expected numerical instability, and also provides an initial prediction of the level of expected noise amplification when passing from the measures (samples) to the coefficients. The ideal value is $\text{CN} = 1$ since then the noise amplification factor is 1 as well; that is no amplification. Orthogonality implies that the inverse matrix equals its transpose. As matrix transpose is a trivial transform, thus for orthogonal matrices $\text{CN} = 1$. If that is not the case, CN tends to increase with the size of the matrix. For the typical sizes used in practical applications it can take huge values (from 10^2 up to 10^5 in the cases analyzed in the next Section), which means that the numerical implementation with real data will be ineffective.

The Gram-Schmidt orthogonalization (and further enhanced versions) method permits us to decompose the initial matrix into a product $\mathbf{Z} = \mathbf{Q}\mathbf{R}$ (also known as QR factorization), where $\mathbf{Q}$ is the matrix formed with the new orthonormal basis vectors, so that $\mathbf{Q}^{-1} = \mathbf{Q}^T$; and $\mathbf{R}$ is an upper triangular matrix passing from the $\mathbf{Q}$ to the $\mathbf{Z}$ basis. (Of course we can apply $\mathbf{D} = \mathbf{Q}_d \mathbf{R}_d$ as well). If the initial matrix was square and $\text{Det}(\mathbf{Z}) \neq 0$ (complete basis), then we can express both the $\mathbf{Q}$ direct and inverse transform (the Discrete Zernike Transform):

$$\mathbf{w} = \mathbf{Q}\mathbf{c}_q \text{ and } \mathbf{c}_q = \mathbf{Q}^T \mathbf{w} \quad (10a)$$

and similarly for the Zernike derivatives:

$$\mathbf{m} = \mathbf{Q}_d \mathbf{c}_d \text{ and } \mathbf{c}_d = \mathbf{Q}_d^T \mathbf{m} \quad (10b)$$

Note that $\mathbf{Q}$ and $\mathbf{Q}_d$ are new basis, and the new coefficients will be different. To pass from former to the new basis we simply apply $\mathbf{R} : \mathbf{c}_q = \mathbf{R} \mathbf{c}$ and $\mathbf{c}_d = \mathbf{R}_d \mathbf{c}$ respectively. Also, we can pass from $\mathbf{Q}_d$ to $\mathbf{Q} : \mathbf{c}_d = \mathbf{R}_d \mathbf{R}^{-1} \mathbf{c}_q$ and vice versa. This is a crucial point because the condition number of matrix $\mathbf{R}$ is the same as that of the initial basis $\mathbf{Z}$. If we want to recover the original coefficients $\mathbf{c}$, then we have to invert $\mathbf{R} : \mathbf{c} = \mathbf{R}^{-1} \mathbf{c}_q$ and then we will have the deleterious effects of noise amplification again. In other words, orthogonalization makes sense only if the new $\mathbf{Q}$ basis has a clear physical meaning and the coefficients of the transform $\mathbf{c}_q$ are useful to us. In the case of $\mathbf{Z}$ and $\mathbf{Q}$, the physical meaning of $\mathbf{R}$ is to pass from the continuous to the discrete domain. When we adopt the $\mathbf{Q}$ basis we are giving up knowing the wavefront outside the sampling points. That is, we can recover the exact values of the samples from the coefficients $\mathbf{c}_q$, but we can not interpolate between them. In order to interpolate, to know the continuous wavefront, then we have to apply $\mathbf{R}^{-1}$ with the potential danger of noise amplification. In other words, we get an important gain: an exact and fully invertible transform, with a maximum number of coefficients (critical sampling), which in turns minimizes the effects of spectral overlapping and avoids noise amplification. The cost is the constraint to work within the discrete domain, without trying to reconstruct a continuous version of the wavefront. This (somehow optional) cost is fully assumable in most applications where the final interpolation is not necessary. In fact this is totally equivalent to the discrete Fourier transform (DFF) in signal processing, where one always work within the discrete domain.

In the case of the Zernike derivatives basis, the physical meaning of $\mathbf{R}_d$ is different because now, that basis change implies two transforms: passing from the continuous to the discrete domain, but also differentiating to pass from the wavefront to the derivatives. This means that the range of applications of the $\mathbf{Q}_d$ basis is lower. It can be highly useful to have a complete orthogonal basis for spot diagrams, but $\mathbf{Q}_d$ is not a particularly useful basis for wavefront sensing or applications where the main goal is to integrate.

Finally, we want to remark that the DZT basis $\mathbf{Q}$ is going to change not only with the number of samples I , but also with the sampling scheme. For each sampling scheme, we will have a different $\mathbf{Z}$ matrix and hence a different basis change operator $\mathbf{R}$ and sampling-distinctive direct $\mathbf{Q}$ and inverse $\mathbf{Q}^T$ discrete Zernike transform DZT.

3. Construction of orthogonal basis

In this Section we apply the above theory to construct the complete basis and to obtain orthogonal modes.

3.1 Complete sampling patterns

Our starting point is to analyze the rank of matrix $\mathbf{Z}$ (and $\mathbf{D}$) for different regular sampling patterns chosen among the most used in the literature (redundant) and types of non redundant patterns proposed here. The rank measures the dimension of the subspace covered by the basis functions, so that the case $\text{Rank}(\mathbf{Z}) = I$ means that the basis is complete. The rank was computed always for critical sampling (square matrix) and for different numbers of sampling points.

3.1.1 Non redundant sampling patterns: Random, perturbed and regular

Random patterns (i) were generated as follows. Each sampling point is obtained by adding a random displacement to the coordinates of the previous sampling element. These displacements have a Gaussian distribution with zero mean and standard deviation equal to the diameter of the sampling element. Non-overlapping between samples and total inclusion of the sampling element into the measured pupil were imposed. Several masks were generated and compared in terms of the condition number of the $\mathbf{Z}$ matrix obtained for each of them, in order to choose the best realization.

The perturbed regular sampling patterns (ii) were implemented by adding small random Cartesian displacements $(\varepsilon_x, \varepsilon_y)$ to the sampling points of regular grids. These perturbations have a Gaussian distribution with zero mean, and their magnitude is determined by the standard deviation σ . We have performed simulations with perturbations ranging from 10^{-8} to 10^{-2} in pupil radius (R) units. To be effective we found that σ has to be equal or greater than $10^{-3} R$.

Finally, we designed regular (deterministic) non redundant sampling patterns (iii). Regular sampling patterns are commonly obtained by convolution of the function to be sampled with a Dirac comb. Let us start with the angular coordinate. To sample the interval $[0, \theta_{\max}]$ with I equally spaced samples, the interval will be $\delta\theta = \theta_{\max}/(I-1)$. Now, we could apply a similar sampling to ρ . If the comb is 2D (2-dimensional) we obtain a pure polar sampling, which is redundant in both coordinates. A way to avoid redundancy is to apply 1D Dirac combs to both coordinates; or in other words to make ρ proportional to θ and set $\theta_{\max} = 2\pi N_c$. In this way we obtain a rolled 1D pattern, which is a spiral with N_c cycles covering a circular area with radius $\rho_{\max} \propto \theta_{\max}$. To completely avoid redundancy, we have to be careful with the periodicity of the angular variable, i.e. we need to guarantee that the number of samples per cycle $NSPC = 2\pi/\delta\theta$ is non integer. The difference between polar and spiral patterns is that the former is a purely 2-dimensional whereas the spiral is obtained by rolling a 1D pattern. Despite their different nature, both can adequately cover a circular domain. The linear spiral, however, has the problem that the density of samples per unit of area is high at the centre and decreases towards the edge. One way to avoid that problem is to use an array of spirals to form an helical pattern (Mayall & Vasilevskis, 1960). Here, however, the goal was to avoid redundancy, and we implemented different spirals controlling the density of samples. The general expression for the radial coordinate was $\rho(\theta) = \sqrt[p]{\theta/\theta_{\max}}$, which ensures that $\rho \leq 1$. For $p = 2$ we obtain the Fermat or parabolic spiral, in which the density of samples is nearly constant when the angle is sampled uniformly. We also tried other values of p . In particular for $p = 4$ the density of samples shows a quadratic increase of density towards the periphery, which improves the orthogonality, and hence the condition number for inverting the transform.

For the Fermat spiral, constant density of samples occurs, in a first approximation, when the total number of cycles is proportional to the square root of the number of samples $N_c \approx \sqrt{I/\pi}$. Usually N_c is chosen to be integer, but in some cases this could result in a redundant sampling. If that happens (see below) we add $1/2$ to break periodicity: Thus, we have different cases $N_c = \text{int}(\sqrt{I/\pi})$ or $N_c = \text{int}(\sqrt{I/\pi}) + 0.5$ where "int" means nearest integer. In terms of the number of cycles $\delta\theta = 2\pi N_c/(I-1)$. By definition, the radial coordinate ρ is never repeated, and with the additional condition that the sampling is not

periodic in 2π (i.e. the number of samples per cycle is not integer, $NSPC = 2\pi/\delta\theta = (I-1)/N_c \neq i$), then we avoid any redundancy in both radial and angular coordinates. The examples implemented here correspond to maximum orders of ZPs $n = 7$ and $n = 12$, and represent the two possible cases of N_c integer or non integer. In the first case we have $J = I = 36$; then $N_c = 3$, $\delta\theta = 0.5386$ radians and $NSPC = 11.667$. Since this is not an integer number, the sampling is non redundant. In the second example, $N = 12$ and $I = J = 91$. If we choose an integer value $N_c = 5$, $\delta\theta = 0.349$ but then we will have $NSPC = 18$ and the sampling would be periodic in θ , i.e. redundant. We can avoid that redundancy by adding 0.5 cycles so that $N_c = 5.5$, then $\delta\theta = 0.384$ radians and $NSPC = 16.36$.

Finally, the last sample of the spiral has to strictly meet the condition $\rho_I < 1$ to avoid partial occlusion of the marginal samples by the pupil. One possible criterion is to keep the area covered by this last sample equal to the average. As an approximation, here we impose the radial distance of the last sample to the pupil edge to be equal to half the width of the last cycle: $1 - \rho_I = 1/2(\rho_I - \rho_{I-NSPC})$; solving for $\rho_I = 2/3 + 1/3\rho_{I-NSPC}$; and in terms of N_c :

$\rho_I = 2/3 + 1/3\sqrt{(N_c - 1)/N_c}$. (In the examples $\rho_{I=36} = 0.9388$ for $I = 36$ and $\rho_{I=91} = 0.9682$ respectively.) Now, the sampling grid is fully determined by $\theta_i = \delta\theta/k + (i-1)\delta\theta$ with $i = 1, 2, \dots, I$ and $\rho_i = \rho_I\sqrt{\theta_i/\theta_I}$. Therefore, given a maximum order N of Zernike polynomials, we

want as many samples as Zernike modes, $I = J = 1 + N(N+3)/2$; then assign a number of cycles (first option N_c integer when $NSPC$ is non integer; or add 0.5 to avoid periodicity if $NSPC$ integer). Finally choose a value for k to have the spiral sampling completely determined. The above computation of the number of cycles N_c and last value of ρ corresponds to the Fermat spiral, $p=2$, but the same analysis can be applied for different spirals. We found that $p=2$ was optimal to get homogeneous density, but $p=4$ was optimal in terms of minimum condition number.

Figure 1 shows some of the sampling patterns analyzed here, for the case of $I = 91$ samples (order $n = 12$), hexagonal (H91), hexagonal perturbed (HR91), hexapolar (HP91), random (R91), spiral (S91) and spiral with quadratic density (SQ91). The ranks obtained for the different patterns are summarized in Table 1. Three (left) columns correspond to three standard (redundant) patterns (square, hexagonal and hexapolar), and three (right) columns to the non-redundant patterns proposed here (hexagonal perturbed, random and spirals). Only random and spiral patterns permit to set an arbitrary number of samples which provides total flexibility to match the number of samples to any (maximum) order n of Zernike polynomials. This is the reason why some rows in Table 1 are incomplete. The 2D regular patterns considered here are centred at the origin (i.e. they include the central sample) and they can only match determined orders, except for the case $n=7$ ($I=36$), where we had to remove the central sample, otherwise we had 37 samples. This Table shows that non-redundant patterns (except for the case perturbed hexapolar not included in Table) provide maximum rank (completeness), whereas regular 2D patterns yield lower ranks. Among them, square and hexagonal seem equivalent, but the hexapolar shows the lowest value for 36 samples.

In summary, the completeness of sampled Zernike polynomial basis is strongly dependent on sampling pattern. The above results support the relationship between redundancy, low efficiency of sampling and lack of completeness. Taking into account the symmetry of ZPs where radial and angular parts are separable, polar (or hexapolar) sampling schemes are expected to have the highest redundancy in the Z matrix, which is confirmed by the lower

values both in rank and condition number of $\mathbf{Z}$. Non-polar sampling (square, hexagonal) has an intermediate level of redundancy, which can be improved by introducing small perturbations to the regular sampling grid. On the other hand either fully random or spiral patterns seem to guarantee completeness. The later has the advantage of being deterministic and regular. Nevertheless, completeness does not ensure an accurate inversion in practice.

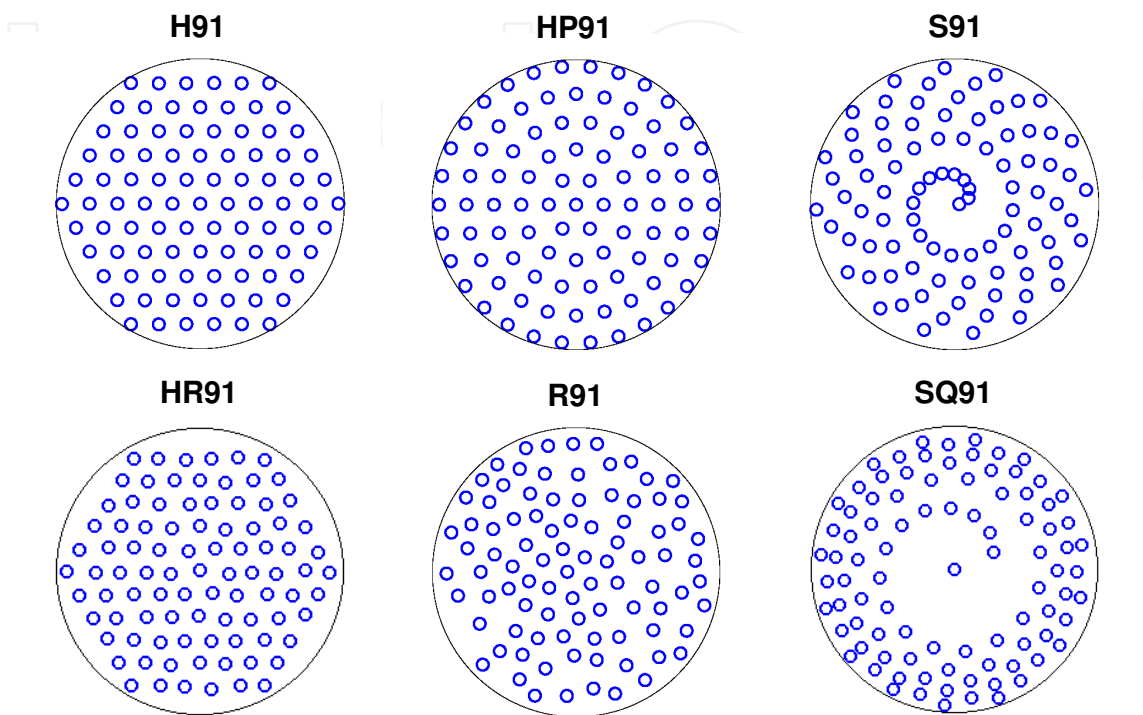


Fig. 1. Examples of sampling patterns with 91 points providing singular $\mathbf{Z}$ (hexagonal and hexapolar) and invertible (hexagonal perturbed, random and spirals).

The same non redundant sampling patterns, which guarantee completeness of the ZPs, namely random, perturbed regular, and spirals (especially Fermat and quadratic ones), do also guarantee completeness of the $\mathbf{D}$ basis (Navarro et al., 2011). In other words, the 2 sampled partial derivatives of ZPs form a complete basis for the set of measurements $\mathbf{m}$. The size of the matrix is $2IxJ$ with $2I = J$. For the particular case of $I = 91$ and critical sampling, $J = 182$ and $\mathbf{D}$ is a 182×182 square matrix. The rank was always maximum, 182 for this case and for all non-redundant samplings. Surprisingly, the rank was much lower (by a factor of two approximately) and always lower than I for the rest of redundant sampling patterns: for example the rank was $89 < I$ for the hexagonal case. This suggests the possibility of implementing wavefront sensing with critical sampling to recover $2J$ modes of the wavefront.

	Square	Hexagonal	Hexapolar	Random	Perturbed	Spirals
$I=36$ ($n=7$)	34	34	30	36	36	36
$I=91$ ($n=12$)	-	87	88	91 (H)	91	91
$I=120$ ($n=14$)	112	-	-	120 (Sq)	120	120

Table 1. Rank of matrix $\mathbf{Z}$ for different sampling schemes (rows) and number of samples (columns). Square (Sq), Hexagonal (H).

The main limitation is that the condition number of **Z** (and **D**) strongly increases with matrix size. For $I=36$, CN is between 10^3 and 10^2 for the complete sampling patterns, and increases up to 10^5 for S1, 10^4 for random and keeps above 10^2 for quadratic spiral S2, all the cases with $I=91$. The high CN (obtained for the S1 and random sampling grids) mean that the estimation of $\mathbf{Z}^{-1}$ (or $\mathbf{D}^{-1}$) could be highly noisy, getting worse in general as the number of samples increases. In fact, when I is of the order of 10^2 or higher, matrix inversion will be numerically instable, so that completeness alone is insufficient for effective practical implementation. In this context, orthogonalization is the way to optimize CN and matrix inversion.

3.2 Orthogonal modes

In the next paragraph we analyze the resulting orthonormal basis functions after applying the QR factorization. The Zernike modes are highly significant in optics since each mode corresponds to a type of aberration: piston ($n=0, m=0$), tilt ($n=1, m=\pm 1$), defocus ($n=1, m=0$), and so on. Each mode corresponds to a Zernike polynomial defined on a continuous circle of unit radius. Sampled polynomials do not form an orthogonal basis anymore, but if we apply a complete (non redundant) critical sampling scheme and apply orthogonalization, then the resulting columns of matrix **Q** will be the new Zernike modes in the discrete domain (see figure 2).

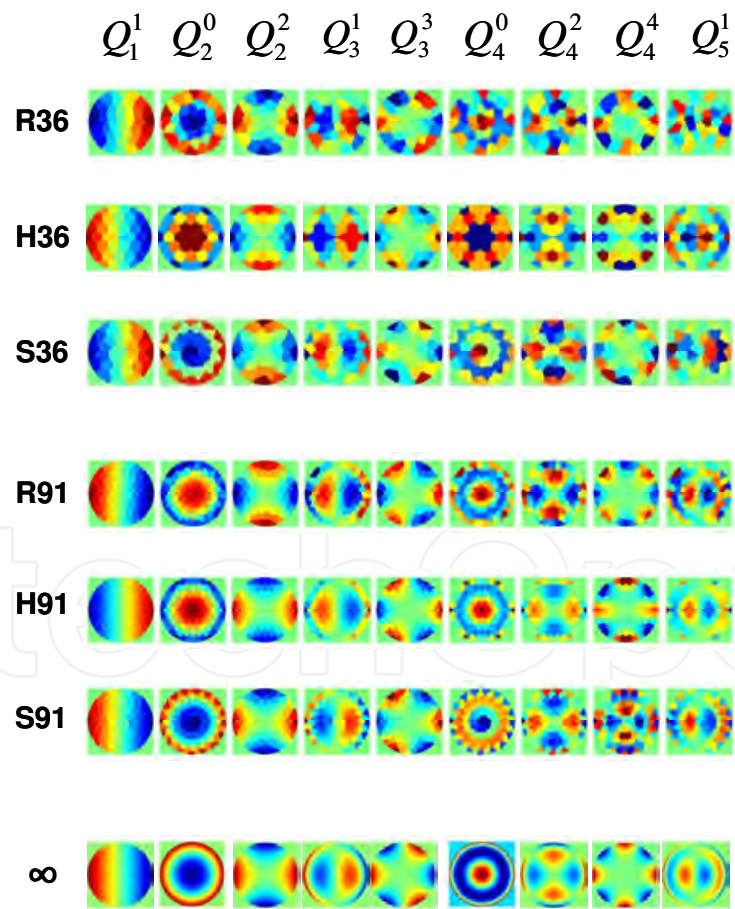


Fig. 2. a (left). Modes ($m \geq 0$) of the DZT for different sampling schemes: random (R), perturbed hexagonal (H) and spiral (S). The three upper rows correspond to $I = 36$ samples and the three lower rows to $I = 91$. Bottom row represents the continuous ($I = \infty$) Zernike modes.

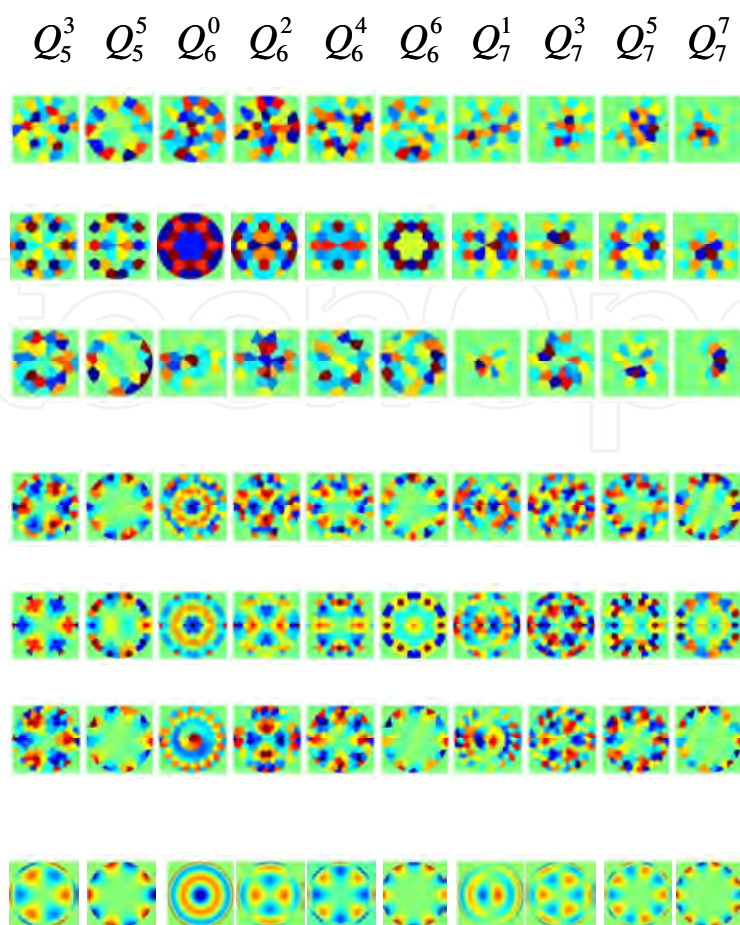


Fig. 2. b (right).

3.2.1 Discrete wavefront modes

Figure 2 compares the resulting discrete modes of the orthonormal DZT for the three types of non redundant sampling patterns: random, R, perturbed hexagonal (with perturbation $\sigma = 10^{-3}$) H and Fermat spiral, S. The three upper rows correspond to 36 ($n \leq 7$) samples, and the lower rows to 91 ($n \leq 12$) samples. The bottom row (∞ number of samples) shows the original continuous Zernike polynomials. (For the case H36 the central sample was removed, otherwise we would have 37 sampling points). Only modes with non-negative angular frequency ($m \geq 0$) are shown up to radial order $n=7$. If we compare the discrete and continuous (bottom row) modes we can see clear differences. Many times we observe change of polarity (sign reversals) of different modes, depending on the sampling pattern and number of samples. For instance, tilt, Q_1^1 shows a sign reversal for random and spiral patterns for the low sampling rate (36), but for 91 samples there are no reversals (except for the hexagonal one). In general, similarities between discrete and continuous modes increase with the number of samples (as expected). The differences tend to increase with the order of polynomials. This is patent for the highest order modes $n=7$ in the upper rows.

These discrete Zernike modes do change with the sampling pattern, which has physical consequences. For example, the spherical aberration of a standard (continuous) lens (Z_4^0 , bottom row in Fig. 2) is different from that of a segmented mirror. If one has a mirror with 36 hexagonal facets the spherical aberration looks different: Q_4^0 for H36. The same applies

for defocus, astigmatism and the rest of aberration modes. In fact, the aberration modes change both with the sampling type and the sampling rate, especially the highest orders. In other words, the $\mathbf{Q}$ basis may have a real physical meaning as wave aberration modes of segmented (or faceted) optical systems, such as compound eyes, large telescopes, lenslet arrays, spatial light modulators, etc.

3.2.2 Discrete modes of wavefront gradient

The same analysis can be applied to the partial derivatives (gradient) of the wavefront to obtain the complete orthogonal basis $\mathbf{Q}_d$. As we said before, the physical nature of the gradient modes is totally different, as the gradient is proportional to the transverse aberrations. These are the coordinates x'_i, y'_i of the impact of rays, normal to the wavefront. For this reason, $\mathbf{Q}_d$ contains the modes of the spot diagrams, which are the initial set of raw data in many optical computations (ray tracing) and measurements (wavefront sensing, etc.) Spot diagrams are essentially discrete in nature as they contain a finite number of spots. As before, we can obtain the modes for any non redundant pattern, but as we explain below, we obtained a much higher performance (lower CN) for the quadratic spiral (or spiral 2), with $p = 4$, so that the density of samples increases towards the periphery with ρ^2 . Figure 3 shows the spot diagram modes for that spiral sampling and $I = 91$. The three columns represent the initial basis $\mathbf{D}$ (left); the same basis, but after normalizing the ZP derivatives (center), as an intermediate stage in the orthonormalization process, $\mathbf{D}_n$; and the final orthonormal modes, $\mathbf{Q}_d$ (right). The axis of the plots were adjusted for visualization, being an scaling factor of 10^2 between the axis used for representing $\mathbf{D}$ and those used for $\mathbf{D}_n$ and $\mathbf{Q}_d$. The plot of the column of $\mathbf{D}$ corresponding to the pair (8,8) is incomplete, some of the impact rays were not represented because they are out of range, causing the difference in the aspect with the plot of $\mathbf{D}_n$.

4. Implementation and results of computer simulations

We implemented the above sampling patterns and basis functions and conducted different realistic computer simulations to test the possibilities of practical application.

4.1 Wavefronts

In the simulations we used ocular wavefront aberration data taken from an experimental data set used in a recent study (Arines et al., 2009). We implemented the different sampling patterns proposed so far, always with $I = 91$ samples. Two types of initial wavefronts having either 91 or 182 Zernike modes (non zero coefficients) were tested. Coefficients for higher orders were assumed to be zero. Different levels of noise (0%, 1%, 3% and 5%) were added to the initial samples. The metric used was always RMS errors (differences) or values. First of all, we compared standard least squares estimation (Eq. 6) and the inverse DZT ($\mathbf{Q}^T$) (Eq. 10a) to estimate the continuous and discrete coefficients (first and second rows in Table 2). From them, we reconstructed the wavefront (3rd and 4th rows). For the sake of simplicity, we only show results for regular (unperturbed) hexagonal (H), random (R) and spiral (S) patterns. The original RMS wavefront was $2.5 \mu\text{m}$.

The results by standard least squares ($\mathbf{c} - \hat{\mathbf{c}}_Z$, first row,) are bad for the hexagonal pattern, even for the ideal case (left columns). The result is better for complete sampling schemes (R and S), but even then, the results are strongly affected by aliasing due to the presence of

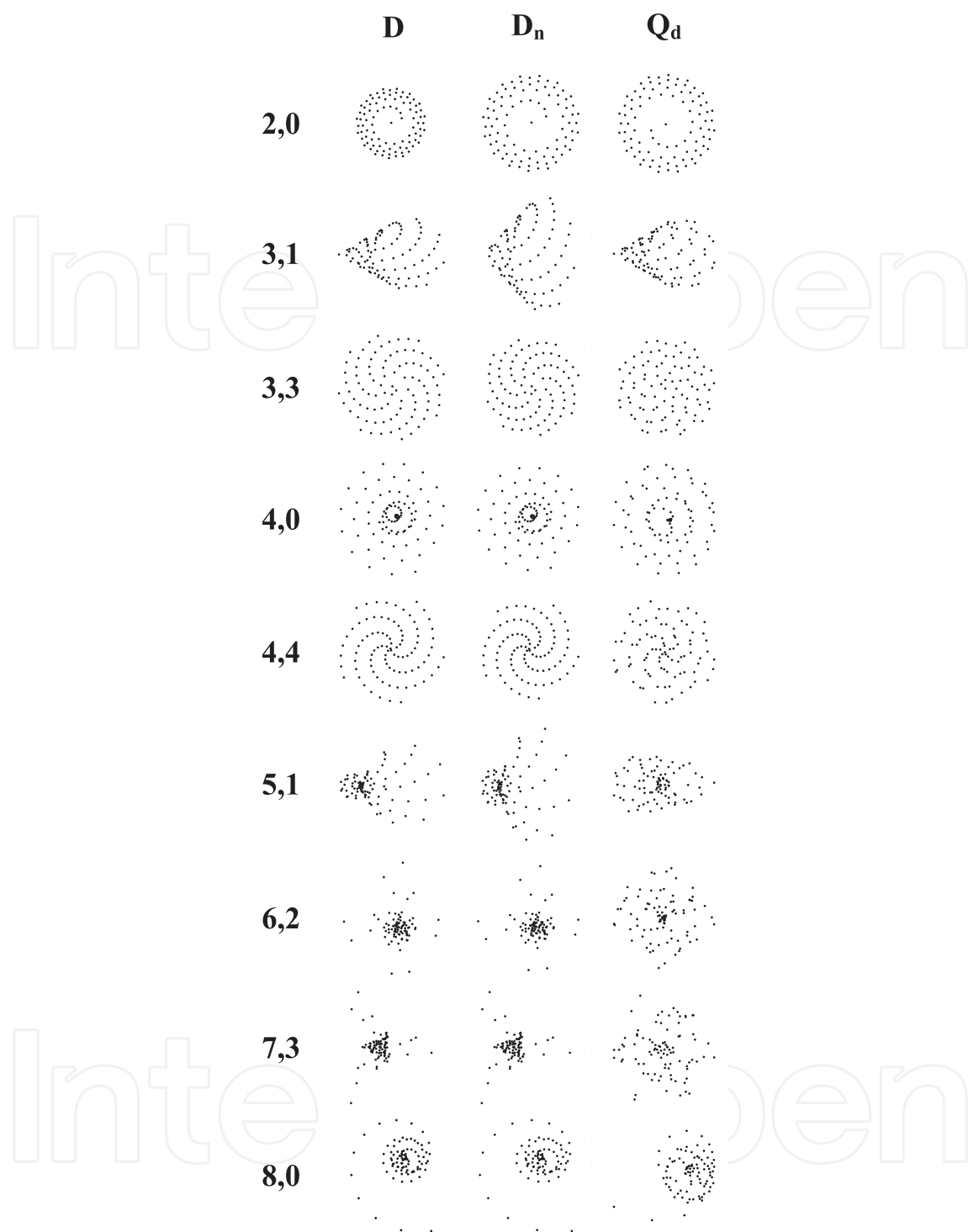


Fig. 3. Initial (**D**), normalized (**D_n**) and orthonormal modes (**Q_d**) of wavefront gradient (spot diagram) for the quadratic spiral of 91 samples. Pair numbers are the (n,m) index of ZPs.

higher order modes (i.e. undersampling; central columns). The right column shows huge errors in the presence of noise. Therefore, the standard method of Eq. 6 can not be applied with critical sampling in practice. This is the reason why standard modal estimation requires redundancy with $I \gg J$. Using the DZT (and the non redundant schemes R and S), the results (second row in Table 2) are greatly improved (the errors are now residual, of the

order of 10^{-14} μm). Note that now we applied matrix $\mathbf{R}$ to the continuous original coefficients to compute the RMS error in the discrete $\mathbf{Q}$ basis. Using the DZT, the error also increases with the presence of higher order modes and noise, but improves by one (182 modes, central columns) or three (noise, right columns) orders of magnitude compared to the standard method. If we now reconstruct the wavefront from the estimated coefficients, we observe that the standard method (third row in Table 2) is affected by both aliasing and noise, but the DZT, $\mathbf{Q}$ transform (bottom row in Table 2) is basically unaffected, and hence the initial measurements are recovered with high fidelity.

	91 modes; 0% noise			182 modes; 0% noise			91 modes; 3% noise		
RMS error	H	R	S	H	R	S	H	R	S
$\mathbf{c} - \hat{\mathbf{c}}_{\mathbf{Z}}$	2.717	4.3×10^{-6}	1.6×10^{-6}	2.53	0.066	0.003	1.6×10^4	2.0×10^3	1.2×10^3
$\mathbf{Rc} - \hat{\mathbf{c}}_{\mathbf{Q}}$		3.1×10^{-14}	1.1×10^{-14}		3.8×10^{-4}	3.8×10^{-4}		0.61	0.64
$\mathbf{w} - \mathbf{Z}\hat{\mathbf{c}}_{\mathbf{Z}}$	2.4×10^{-8}	2.0×10^{-10}	1.3×10^{-10}	4.5×10^{-5}	1.5×10^{-10}	1.3×10^{-10}	0.13	2.7×10^{-7}	9.5×10^{-8}
$\mathbf{w} - \mathbf{Q}\hat{\mathbf{c}}_{\mathbf{Q}}$		2.1×10^{-14}	1.1×10^{-14}		1.5×10^{-14}	1.4×10^{-14}		1.8×10^{-14}	1.4×10^{-14}

Table 2. RMS errors obtained with standard ($\mathbf{Z}$) and discrete ($\mathbf{Q}$) Zernike basis for coefficients ($\mathbf{c}$) and in wavefront ($\mathbf{w}$) for hexagonal (H), random (R) and Fermat spiral (S) sampling patterns. All values are in micrometers.

4.2 Wavefront reconstruction from wavefront slopes

The problem of wavefront reconstruction from its slopes is totally different, since here the reconstruction requires to integrate the gradient. If we apply $\mathbf{Q}_a^T$ we are not integrating, and therefore to recover the wavefront coefficients, we have to apply either $\mathbf{R}_a^{-1}$ or $\mathbf{D}^{-1}$ directly. This means that we have especial care with the condition number of these matrices to avoid excessive noise amplification. We studied the problem of potential noise amplification in two ways. First, we obtained the singular value decomposition of matrix $\mathbf{D}$ as a metric to predict the amplification of noise. The condition numbers obtained for the square 182×182 $\mathbf{D}$ matrices ($I = 91$) improve progressively: ∞ for H (hexagonal); 4.3×10^7 for P (perturbed H); 1.6×10^7 for S1 (homogeneous sampling spiral); 4×10^6 for R (random); and 1.71×10^5 for S2 (quadratic sampling spiral). This has important consequences. In the presence of noise, noise amplification will preclude to work with critical sampling, but on the other hand we should expect that spiral S2 is going to provide better reconstructions. To have a more realistic estimation of the performance, including the effects of noise amplification, we conducted a series of computer simulations. Now the task is to reconstruct different number of modes, starting from $J = 1$ (maximum redundancy) and progressively increasing up to the critical value $J = 2I$ (zero redundancy). Now we will use standard least squares ($\hat{\mathbf{c}} = (\mathbf{D}^T \mathbf{D})^{-1} \mathbf{D}^T \mathbf{m}$), except for the last case (critical sampling) where $\mathbf{D}$ is square. We applied the QR factorization to $\mathbf{D}$ to improve its condition number (typically by a factor of 2.) Our criterion for the best reconstruction is that of minimum RMS reconstruction error. We used the same data set as before, but now we always considered wavefronts with 182 Zernike modes. This means that now we only have the effect of noise, while we assume that the number of modes 182 is large enough to avoid aliasing (spectral overlapping.) Now the

initial wavefront has an RMS value of $0.54 \mu\text{m}$ ($\sim 1 \lambda$). For each condition, 30 different measurements $\mathbf{m}$ were simulated using the expression $\mathbf{m}_k = \mathbf{D}\mathbf{c} + \mathbf{n}_k$ for the k -th realization, where $\mathbf{n}_k$ is a column vector containing (Gaussian zero-mean) random noise. Then we computed the mean and standard deviation (error bars) over the 30 realizations. The noise variance was adjusted to simulate different levels of signal-to-noise ratio (SNR) from 1 to ∞ (zero noise). We computed the SNR as $\text{SNR} = \langle |\mathbf{m}| \rangle / \langle \sigma_{\mathbf{m}} \rangle_k$ the ratio between the average absolute measurements value among all the noise-free measurements, and the mean standard deviation of the noise (where k refers to the different realizations).

The results for the different sampling patterns are plotted in Figure 4, for the case of $\text{SNR} = 30$. That SNR is within the range of typical values in ocular aberrometers (Rodriguez et al., 2006). The vertical axis represents the RMS difference between the original (ideal) wavefront and that reconstructed from the noisy measurements; and the horizontal axis represents the number of modes J considered in the matrix $\mathbf{D}$. As we can see, all the sampling patterns show a similar performance for $J \leq 62$, but for $J > 62$ the noise amplification increases rapidly for the redundant H pattern. This particular line ends when we reach the maximum rank of $\mathbf{D}$. For the non redundant sampling patterns (R, P, S1 and S2) the effect of noise amplification becomes patent for higher values of J ; as J increases S2 shows the best behaviour. For this sampling pattern, and $\text{SNR} = 30$, the optimal performance is obtained for $J \approx 122$, significantly greater than $I = 91$. This optimal number of modes (best reconstruction) is roughly double than 62 obtained for standard redundant patterns. For the ideal noise free case ($\text{SNR} = \infty$) the best reconstruction corresponds to $J = \text{Rank}(\mathbf{D})$. This is $J = 89$ for standard (hexagonal) and $J = 182$ for non redundant sampling patterns respectively. The results for different $\text{SNR} = 1, 10, 30, 100$ and ∞ , confirm the same type of behaviour as in Fig. 4. As the SNR increases, then the absolute minimum is lower and moves to the right (the optimum value of J increases) and conversely. Random and spiral curves are better in all cases and tend to show a rather flat valley indicating that the optimal value of number of modes, J is not critical. This behaviour is opposite to standard and perturbed sampling grids where the minimum is much more marked. This means that the number of modes is critical and that the least squares fit is less robust. Finally, the quadratic spiral S2 always provides the best reconstruction.

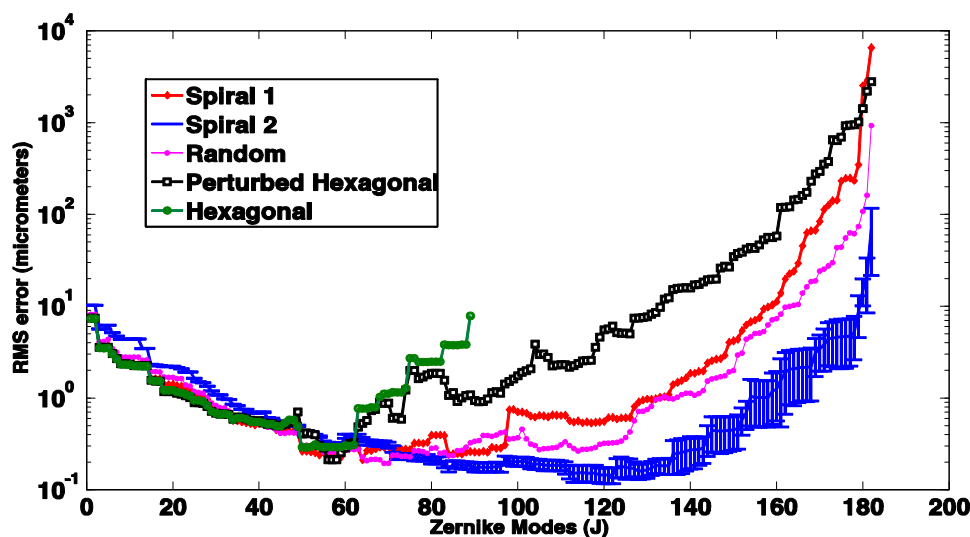


Fig. 4. RMS error of the reconstructed wavefront for different sampling patterns.

5. Conclusion

In conclusion, the non redundant sampling grids proposed above are found to keep completeness of discrete Zernike polynomials within the circle. This has important consequences both in theoretical and practical aspects. Now it is feasible to implement direct and inverse discrete Zernike transforms (DZT) for these sampling patterns. Furthermore, we found that when the discrete ZPs basis is complete, then the basis formed by their (equally sampled) gradients is complete as well. This is true for all non redundant grids tested so far, but spiral 2, with a quadratic increase of sampling density from the centre to the periphery, seems to be especially well adapted to the symmetry of ZPs. In fact, it provides the lowest CN. On the other hand, orthogonality is lost either by sampling or by differentiation in all cases studied. We can recover this property and construct an orthogonal basis $\mathbf{Q}$, through QR factorization, but at the cost of losing some information contained in $\mathbf{R}$. In the case of the DZT, the $\mathbf{Q}$ basis implies to work in the discrete domain. Thus, we lose the interpolation ability of continuous polynomials. In the case of gradients, we lose the information both for interpolation and for integration. It is possible to apply $\mathbf{R}^{-1}$ but then there is the concern of noise amplification.

There are many practical implications of completeness. For standard redundant sampling grids, and realistic values of the SNR of the input data, the optimal number of modes providing the best reconstruction is about $J = I/2$. In wavefront sensing or ray tracing, where one has two measures at each point, J can be somewhat higher (0.6 or 0.7 times I). Our results suggest that by using non redundant sampling patterns, one can reconstruct double number of modes. This has a double effect in improving the reconstruction by decreasing the reconstruction error due to noise, but also due to potential spectral overlapping. Furthermore, both completeness and lower redundancy can help to save costs in many applications, ranging from numerical ray tracing to modal wavefront control by deformable mirrors (adaptive optics). In the first case one can save computing time, and in the second case one can save mechanical actuators.

We believe that the discrete orthogonal modes of Figures 2 and 3, for discrete wavefronts and for spot diagrams, respectively, have a clear physical meaning for optical systems, measurements or computations which are discrete intrinsically. Fig. 2 shows examples of wave aberration modes in segmented optics (arrays of facets, mirrors, microlenses, etc.) with determined geometries (hexagonal, random, or spiral). It is clear that these aberration modes change both with the array geometry and with the number of facets (samples), especially higher orders. The physical meaning of the modes of spot diagrams (Fig. 3) is even more obvious, since ray tracing or wavefront gradient measurements are essentially discrete.

Regarding practical applications, sampling grids with inhomogeneous densities, such as quadratic spiral, or random (irregular) are difficult to implement in conventional monolithic microlens arrays used in Hartmann-Shack sensors, segmented mirrors, etc. However there are highly flexible and re-configurable (almost in real time) devices such as liquid crystal spatial light modulators (Arines et al. 2007) or laser ray-tracing methods (Navarro & Moreno-Barriuso, 1999) which can easily implement almost any possible sampling grid.

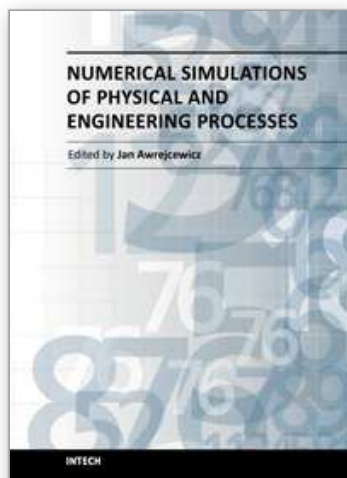
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