



Holodiagrams using Mahalanobis distance

H. Rabal^{a,*}, N. Cap^a, C. Criado^b, N. Alamo^c

^a Centro de Investigaciones Ópticas (CONICET La Plata-CIC), Facultad de Ingeniería (UID-OPTIMO), Universidad Nacional de la Plata, P.O. Box 3, 1897, Gonnet, La Plata, Argentina

^b Departamento de Física Aplicada I, Universidad de Málaga, 29071 Málaga, Spain

^c Departamento de Álgebra, Geometría y Topología, Universidad de Málaga, 29071, Málaga, Spain

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ABSTRACT

We propose the generalization of the Holodiagram concept that has demonstrated many useful properties in optics, to include other metric measurement, namely the Mahalanobis distance, thus involving several other optical possible uses. So, besides being useful in the study of decision and classification problems it can be used in geometric solutions involving Fermat's principle in a rather wide range of situations.

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1. Introduction

In 1969 Abramson [1] proposed the use of a diagram, named by him the Holodiagram (HD), to optimize the use of the limited coherence length in holography of relatively large objects.

The concept soon proved to encompass several other optical phenomena and some generalizations have been proposed that involve the solutions of reflection and refraction in arbitrary surfaces [2–7], both for isotropic and birefringent materials.

Although the HD itself does not provide any new information, it presents the Fermat principle in a graphic way that gives insight in the existence of previously unknown situations, such as a spherical surface inside crystals that conjugates by reflection a point to a different one, the loci of the surfaces that limit refraction by internal reflection or the existence of non deviation interfaces between two birefringent materials.

Some generalizations to include non spherical wavefronts, both in reflection and refraction were also developed [8,9] and the existence and geometry of Generalized Fresnel Zone Plates for rather general surfaces were found.

In this work we introduce a generalization that replaces the Euclidean distance implicit in the HD by the more general Mahalanobis distance [10] and compare the results with optical geometrical properties.

We shortly review the mean aspects of the already known HDs and the concept of Mahalanobis distance. Then the concept of

Mahalanobis based HD (MHD) is proposed and some rather general possible applications are suggested. Two variations are possible for the HD: the locus of points where the sum S of the distances to two fixed points called foci is a constant and the locus of the points where the difference D of the distances is a constant. We are going to show these loci through plots of $\cos(kS)$ or $\cos(kD)$ so that they will appear as fringes, the geometry and spacing of which will indicate the corresponding properties. We are going to show also the sensitivity to the changes in the variables in both cases.

2. Theory

Abramson's HD is a plot of the loci of equal sum of (Euclidean) distances to two fixed points F_1 and F_2 . It can be shown as the $\cos(kS)$ in the shape of fringes. Along one of such fringes the total distance $D_1 + D_2$ is a constant so that changing the variables along it does not modify the value of S , while the normal to the fringes is the direction where the change of the variables produces the maximum variation in S . These properties make the HD an appropriate tool for graphically solving variational problems in optics, namely finding points that obey Fermat's Principle or the geometry of the interference fringes, among others. The concept describes also the case of virtual sources or images, that can be modified to include refraction, Snell's law, partial coherence and can also be generalized to wavefronts other than spherical.

In the ellipse, the sum of the (Euclidean) distances between a point on the curve and two fixed points F_1 and F_2 named foci is the same value for all points.

The ellipse permits the finding of stationary points when a certain solution requires the fulfilling of an additional condition or

* Corresponding author.

E-mail addresses: hrabal@ing.unlp.edu.ar (H. Rabal), lilic@ciop.unlp.edu.ar (N. Cap), c.criado@uma.es (C. Criado).

constrain. Stationary optical path of light via Fermat's principle from a point to another being reflected in a mirror is one example.

The loci of equal path difference of light in a point coming from two coherent light sources at F_1 and F_2 , depicted by hyperbolas, defines interference (Young) fringes.

Holodiagrams have been motivated by using the Moiré effect [1] between two families of curves, representing the families of loci where weighted distance to a point is a constant. As Moiré patterns form group in the mathematical sense, it is, given two families of curves additive and subtractive Moiré give rise to new families from which the original ones can be re obtained fulfilling the group conditions, Holodiagrams, when described as Moiré patterns also behave in this way.

In 1936 P.C. Mahalanobis defined a distance based in statistical considerations that takes into account the standard deviation of the variables and their mutual correlations.

It reduces to Euclidean distance when the variables are uncorrelated and the standard deviations are equal. This distance concept is usually used to establish similarities between statistical variables of already classified samples and an unknown one but its application to Holodiagrams for general purpose classification and optimization operations will be soon proposed [11].

Mahalanobis distance is a concept that was born in the realm of statistics. It can be schematically described in the following way.

Let us assume a set of points characterized by two parameters

$$x = (x_1, x_2),$$

from which we know a random sample of N points, and we want to estimate the probability that a given point belongs to that set.

It seems natural to estimate that that probability should be proportional to the Euclidean distance from that point to the vector of the means

$$\mu = (\mu_1, \mu_2),$$

that is

$$d(x, \mu) = \sqrt{(x_1 - \mu_1)^2 + (x_2 - \mu_2)^2}.$$

The Standard deviations σ_1 and σ_2 of the random variables should be taken into account and to weight the distribution of each variable by means of the reciprocal of the corresponding standard deviation.

In this way we have
$$d(x, \mu) = \sqrt{\left(\frac{x_1 - \mu_1}{\sigma_1}\right)^2 + \left(\frac{x_2 - \mu_2}{\sigma_2}\right)^2}.$$

Finally, we should also take into account the possibility that the random variables could be correlated, so that an adequate measurement could be:

$$d(x, \mu) = \sqrt{(x - \mu)\Sigma^{-1}(x - \mu)^T}$$

where

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{21} & \sigma_2^2 \end{pmatrix}.$$

This is the Mahalanobis definition that for any two points takes the form:

$$d(x, y) = \sqrt{(x - y)\Sigma^{-1}(x - y)^T}$$

It is easy to verify that this definition fulfills the characteristic properties of a distance and that it can be easily generalized to a space with N random variables for any $N > 2$.

For $N=2$ the distance can be written in terms of the correlation coefficient $r = \sigma_{12}/\sigma_1\sigma_2$ thus taking the form:

$$d(x, y) = \sqrt{\frac{1}{1 - r^2} \left(\left(\frac{x_1 - y_1}{\sigma_1}\right)^2 + \left(\frac{x_2 - y_2}{\sigma_2}\right)^2 - 2r \left(\frac{x_1 - y_1}{\sigma_1}\right) \left(\frac{x_2 - y_2}{\sigma_2}\right) \right)}$$

Formally, the Mahalanobis distance from a group of values with mean vector μ is defined as

$$D_M(x) = \sqrt{(x - \mu)^T S^{-1}(x - \mu)}.$$

where

$$\mu = (\mu_1, \mu_2, \mu_3, \dots, \mu_N)^T$$

is a vector formed by the mean values of the variables $x = (x_1, x_2, x_3, \dots, x_N)^T$ and S is their covariance matrix.

Mahalanobis distance is used in analysis of clusters, in classification techniques by choosing the mean vector that is in the closest neighborhood to a test point, in supervised learning, to detect outliers in linear regressions, as a measure of leverage, etc.

In two dimensions, Mahalanobis distance can be written:

$$D^2 = \frac{1}{1 - r^2} \left(\left(\frac{x - \bar{x}}{s_1}\right)^2 + \left(\frac{y - \bar{y}}{s_2}\right)^2 - 2r \left(\frac{x - \bar{x}}{s_1}\right) \left(\frac{y - \bar{y}}{s_2}\right) \right)$$

where s_1 and s_2 are the standard deviations of the variables x, y with mean value \bar{x} and \bar{y} respectively and r is the correlation coefficient between the two variables.

In Euclidean geometry, the locus of the points bearing the same distance to a center is a circumference. These results to be a particular case of Mahalanobis distance when both variables have the same standard deviations and are not correlated between them (Fig. 1).

The locus of points in which Mahalanobis distance to a fixed point has the same value is an ellipse. In Fig. 2 some families of this ellipses are shown as plots of $\cos(kD)$ with k a scale constant.

2.1. Use of Mahalanobis distance in the Holodiagram

To be able to show a graphical description as is the HD the number of variables has to be two. If more than two variables are involved we will only be able to plot cuts of the surfaces that will be generated by imposing that the sum or the difference of the distances be the same value.

We define as the MHD to the family of curves that is obtained when the parameter D in the following expression is continuously varied.

$$n_1 D_1 \pm n_2 D_2 = D$$

where D_1 is the distance from a generic point P in the plane of the variables to a focus F_1 , D_2 is the distance of the same point to the other focus F_2 and n_1 and n_2 are coefficients.

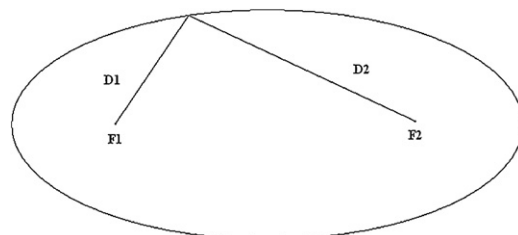


Fig. 1. An ellipse and the Euclidean distances defining it.

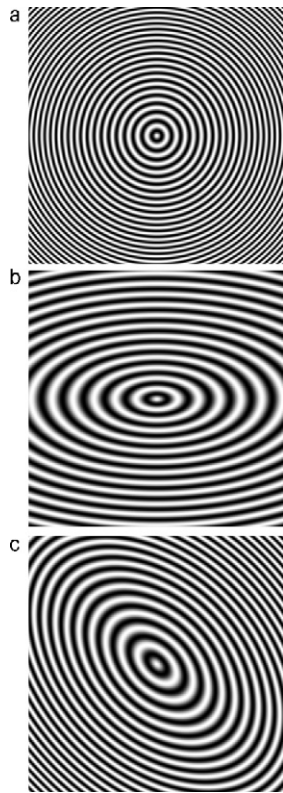


Fig. 2. Loci of the points with equal Mahalanobis distance to a center: (a) variables with the same standard deviation and uncorrelated variables (Euclidean distance), (b) different standard deviations, uncorrelated variables, (c) different standard deviations, partially correlated variables.

2.2. The sum MHD

The sum MHD can be shown as $\cos(kD)$ with k a scale constant. Some examples are shown in Fig. 3.

3. The MHD and variational principles

If we have some constraints on the space of parameters, given for example by a subset of this space, or by a level set $f(\vec{x}) = C$ of a function on this space, or for any other constraint limiting the possible values of the parameters, then we can look for the maximum and minimum of $d(x)$ over this set. In Fig. 4 we show the HD and an example of constraint given by a function (white curve) relating a two-dimensional space of parameters. In the case of the first example this function could link, say for example, the price of a good with its size (a cost function). Note that the points where the curve is tangent to the HD identify the extreme (stationary) values of the function D (maxima and minima) that satisfy the cost function as light does in mirrors for the optical path.

If the variances of the variables are interpreted as speeds, Mahalanobis distances correspond to times and the points of stationarity satisfy a (generalized) Fermat's Principle.

The expression $d(x) = p_A d_A(x, \vec{x}^A) + p_B d_B(x, \vec{x}^B)$ combines two different Mahalanobis distances and then it could be interpreted as the total optical path for a refraction of light, where light would travel first in a medium with refractive index $p_A/\sqrt{s_A}$ and immediately in another with refractive index $p_B/\sqrt{s_B}$. The points P where $d(x)$ is stationary correspond then to points where light coming from a source A refracts towards B for an arbitrarily shaped curve.

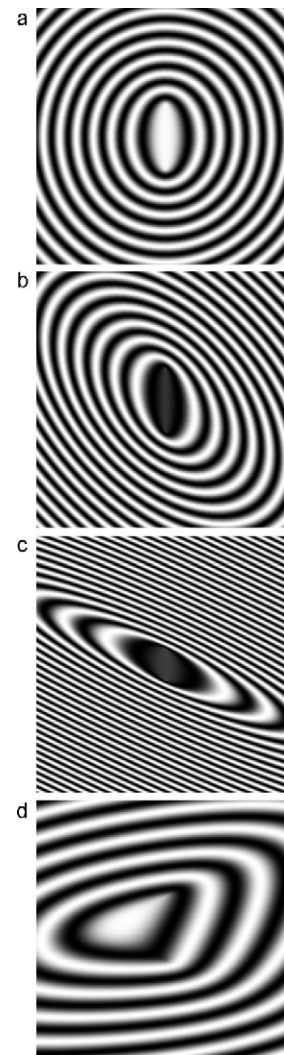


Fig. 3. (a) Classical Abramson sum holodiagram, (b–d) examples of MHD.

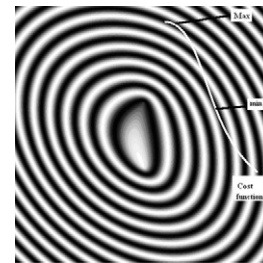


Fig. 4. Sum Mahalanobis holodiagram with a constrain curve.

By choosing the value of $p_B/\sqrt{s_B}$ negative, the effect of a metamaterial, it is, a material with negative refractive index, is simulated. The situation is similar to image forming when either the source or the image is virtual, but not both.

4. Sensitivity vector

In full analogy with the case of holographic interferometry, when a point moves in the space of the parameters a certain displacement vector \mathbf{d} , then the change in the total path L of the ellipses

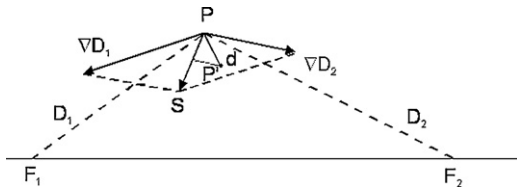


Fig. 5. Geometry for the calculation of sensitivity S . The sensitivity vector in the sum HD is defined as the sum of the gradient vectors with respect to the corresponding M distances.

changes in $\mathbf{S} \cdot \mathbf{d}$ (the point indicates dot product of the vectors \mathbf{S} and \mathbf{d}). Due to the way we chose to show the results as $\cos(kS)$, if the number of fringes crossed in the displacement is N , the component of vector \mathbf{d} in the direction of the sensitivity vector is then the change in L from the beginning to the end of the displacement and is measured in units of $\mathbf{S} \cdot \mathbf{d} = N2\pi/k$.

For a given displacement, this change is bigger when more fringes are crossed. So that visual inspection of the HD looking for places where the fringes are more tightly packed indicates loci of high sensitivity and conversely. Moving along a fringe does not change the total path and moving in the direction of the gradient of S produces the higher changes in its value. We are going to look then for that gradient using the geometry shown in Fig. 5. We first calculate the derivatives of $d(x, y)$ with respect to x and y (Figs. 6–11).

$$d(x, y) = \sqrt{\frac{1}{1-r^2} \left(\left(\frac{x-x_0}{\sigma_1} \right)^2 + \left(\frac{y-y_0}{\sigma_2} \right)^2 - 2r \left(\frac{x-x_0}{\sigma_1} \right) \left(\frac{y-y_0}{\sigma_2} \right) \right)}$$

$$\frac{\partial}{\partial x} d(x, y) = \frac{1}{2d(x, y)} \left[\frac{1}{1-r^2} \left[\frac{2(x-x_0)}{\sigma_1^2} - 2r \frac{1}{\sigma_1} \left(\frac{y-y_0}{\sigma_2} \right) \right] \right]$$

$$\frac{\partial}{\partial y} d(x, y) = \frac{1}{2d(x, y)} \left[\frac{1}{1-r^2} \left[\frac{2(y-y_0)}{\sigma_2^2} - \frac{2r}{\sigma_2} \left(\frac{x-x_0}{\sigma_1} \right) \right] \right]$$

Now we look for the gradient

$$\nabla d(x, y) = \frac{\partial}{\partial x} d(x, y) \hat{i} + \frac{\partial}{\partial y} d(x, y) \hat{j}$$

And its modulus is

$$|\nabla d(x, y)| = \sqrt{\left(\frac{\partial d(x, y)}{\partial x} \right)^2 + \left(\frac{\partial d(x, y)}{\partial y} \right)^2}$$

For the gradient of the sum or difference:

$$\nabla d(x, y) = \frac{\partial}{\partial x} d(x, y) \hat{i} + \frac{\partial}{\partial y} d(x, y) \hat{j} = p_A \nabla d_A(x, y) \pm p_B \nabla d_B(x, y)$$

where

$$d_A(x, y) = \sqrt{\frac{1}{1-r_A^2} \left(\left(\frac{x-x_{A0}}{\sigma_{A1}} \right)^2 + \left(\frac{y-y_{A0}}{\sigma_{A2}} \right)^2 - 2r_A \left(\frac{x-x_{A0}}{\sigma_{A1}} \right) \left(\frac{y-y_{A0}}{\sigma_{A2}} \right) \right)}$$

$$d_B(x, y) = \sqrt{\frac{1}{1-r_B^2} \left(\left(\frac{x-x_{B0}}{\sigma_{B1}} \right)^2 + \left(\frac{y-y_{B0}}{\sigma_{B2}} \right)^2 - 2r_B \left(\frac{x-x_{B0}}{\sigma_{B1}} \right) \left(\frac{y-y_{B0}}{\sigma_{B2}} \right) \right)}$$

5. Examples

If the variables are uncorrelated and have the same standard deviation, the classical elliptical Abramson sum HD is obtained and the locus of points with equal modulus of the sensitivity vector (named k curves in the literature) is composed by circumferences containing the points A and B .

For other more general situations the sensitivity vector distribution is deformed as shown in Fig. 7.

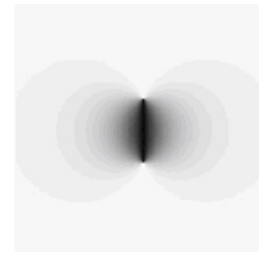


Fig. 6. The modulus of vector S shown as gray levels: sensitivity for the classical Abramson HD. Notice the low sensitivity to displacements in the region between the foci and the high sensitivity in the opposite regions away of the foci.

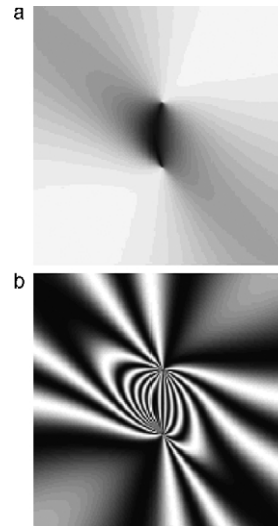


Fig. 7. The modulus of vector S for the MHD shown as gray levels and as fringes $\cos(kS)$. When compared with the classic case shown in Fig. 6, it can be perceived the non symmetric deformation in the sensitivity introduced by the correlation between the variables.

5.1. The difference MHD

In this type of MHD, the classical optical situation (uncorrelated variables with the same variances) corresponds to the Young’s fringes experiment. Fringes show the loci of equal optical path difference. It also corresponds to the possibility of real image formation at F_2 of a real source in F_1 in metamaterials. It is, the shape of the fringe indicates the shape of the interface between a material and a metamaterial that conjugates one point into the other.

In the classical case there is a straight fringe, that corresponds to equal optical paths and is called the zero interference order, that is also a symmetry axis.

It can be seen in the figures that in our case of Mahalanobis distance, the zero order fringe departs from a straight line, the fringe tilts in one or other direction and symmetry is broken. This fringe indicates the locus of points where Mahalanobis distance to both points has the same value. So, if in a statistical situation we are classifying a set of samples by minimum distance (nearest neighbor) this fringe shows the decision frontier.

If a point is at one side of this frontier, it should be classified as nearest neighbor of the corresponding focus

Besides, for any point P , the fringe that contains it defines the direction where variations in the parameters do not improve or worsen the classification decision. Traveling along a fringe does not change the class in definition. Conversely, if point P moves perpendicular to the fringes it changes the D value in the fastest way.

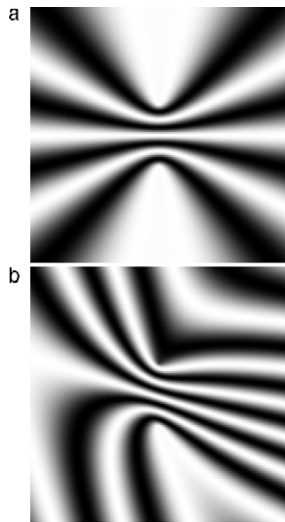


Fig. 8. The difference MHD shown as fringes $\cos(k(D_1 - D_2))$. (a) Classical Young's fringes. (b) Correlated variables and unequal standard deviations.

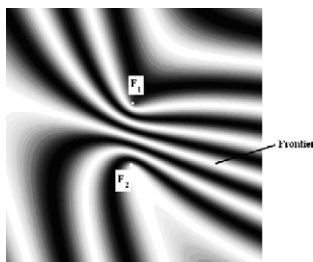


Fig. 9. The difference MHD showing the frontier for nearest neighbor.

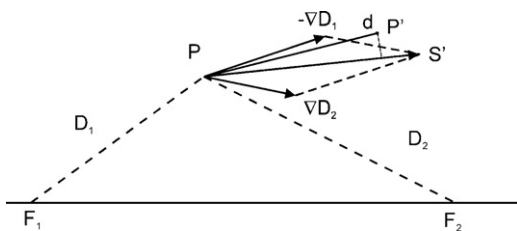


Fig. 10. Geometry for the calculation of sensitivity S' . In this case, the sensitivity vector in the difference HD is defined as the difference in the gradient vectors with respect to the corresponding M distances.

It is, the maximum sensitivity to changes in the parameters occurs in the direction perpendicular to the fringes, and the magnitude of that change is given by how tightly packed are the fringes in that point as mentioned before.

The wide white region at left is a region where M distance does not decide for a classification purpose. Its points are at (approximately) the same M distance of both foci F_1 and F_2 .

6. Refraction

If the correlation coefficients r are both zero and, if both variances are equal in the first point and also equal in the second (but eventually a different value), then the MHD are Cartesian ovals of the egg and apple types and correspond to the surfaces that conjugate one point into the other by refraction between two media [3,4] and rays from one source obey Snell's Law in each point of the HD.

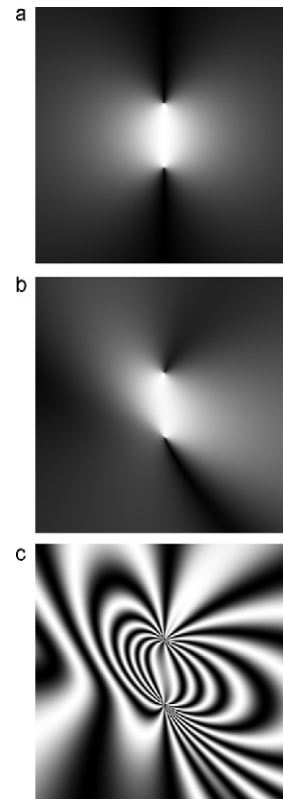


Fig. 11. (a) Sensitivity S' shown here as gray levels for the classical Young's fringes HD. Notice how the regions of high and low sensitivity are interchanged when compared with the sum HD. (b) Sensitivity when the variables are correlated. (c) S' is here shown as fringes $\cos(kS')$.

In the case of the MHD then the relative refractive index can be obtained from the values of the corresponding variances s .

$$D_1^2 = \left(\left(\frac{x - \bar{x}}{s_1} \right)^2 + \left(\frac{y - \bar{y}}{s_1} \right)^2 \right) = \frac{1}{s_1^2} ((x - \bar{x})^2 + (y - \bar{y})^2) = n_1^2 r_1^2$$

$$D_2^2 = \left(\left(\frac{x - \bar{x}}{s_2} \right)^2 + \left(\frac{y - \bar{y}}{s_2} \right)^2 \right) = n_2^2 r_2^2$$

where r_1 and r_2 are Euclidean distances and we have called:

$$n_1 \equiv \frac{1}{s_1}$$

$$n_2 \equiv \frac{1}{s_2}$$

As the refractive index $n = c/v$, with c and v the speeds of light in vacuum and in a medium, variances can be thought as proportional to that speeds and the ratios inside Mahalanobis distance between geometrical distances and standard variations s as times of flight.

The result is the exact expression for Cartesian Ovals

$$n_1 r_1 + n_2 r_2 = A$$

and Snell's Law is fulfilled in every point.

7. Comparison between MHD and RHD for birefringent materials for the extraordinary ray

We are going to see now that Holodiagrams in birefringent media are special cases of MHDs.

To show it we are going to compare the families of curves that give origin to each of them.

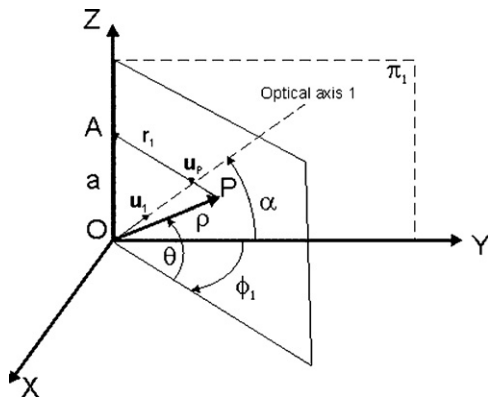


Fig. 12. Definition of geometrical parameters for the birefringent crystal.

If we find that both families are equivalent, as the HD is obtained by adding or subtracting the families, then the equivalence will be demonstrated.

We have seen that for the 2D case, Mahalanobis distance is defined as

$$D^2 = \frac{1}{1-r^2} \left(\left(\frac{x-\bar{x}}{s_1} \right)^2 + \left(\frac{y-\bar{y}}{s_2} \right)^2 - 2r \left(\frac{x-\bar{x}}{s_1} \right) \left(\frac{y-\bar{y}}{s_2} \right) \right)$$

without loose of generality we can choose:

$$\bar{x} = \bar{y} = 0$$

The family of curves is then

$$\left(\frac{x}{s_1} \right)^2 + \left(\frac{y}{s_2} \right)^2 - 2r \left(\frac{x}{s_1} \right) \left(\frac{y}{s_2} \right) = C'$$

Besides, the families of curves for the birefringent materials for the extraordinary ray and arbitrary orientation of the optical axis can be obtained⁵ as follows.

The optical axis in the medium, the coordinates origin O and a generic point P determine a plane π_1 (see Fig. 12).

The plane where the family of curves will be calculated and π_1 form an angle ϕ_1 .

We are going to use the expression for the extraordinary refractive index [5–7] in any direction

$$(n'')^2 = n_e^2 + (n_o^2 - n_e^2)(\tilde{u}_p \tilde{u}_1)^2$$

To calculate each family, $\cos \varphi$ must be found for any direction of the axis, where φ the angle between PA and the optical axis.

To that end we look for a unit vector u_p in the direction joining P with A and a unit vector u_1 in the direction of the optical axis 1 (see Fig. 12).

$$\vec{a} = (0, 0, a)$$

$$\vec{P} = (\rho \cos \theta \sin \phi_1, \rho \cos \theta \cos \phi_1, \rho \sin \theta)$$

then:

$$PA = \sqrt{\rho^2 \cos^2 \theta \sin^2 \phi_1 + \rho^2 \cos^2 \theta \cos^2 \phi_1 + (a - \rho \sin \theta)^2}$$

$$\cos \varphi = \tilde{u}_p \tilde{u}_1 = \frac{-\rho}{PA} \cos \theta \cos \phi_1 \cos \alpha + \frac{(a - \rho \sin \theta)}{PA} \sin \alpha$$

For each family, ϕ_1 and α are constants. Without loss of generality we can choose $a=0y$, and use $OA=0$

$$r_1^2 n''^2 = L^2 = C$$

The family of curves is going to be the plot of

$$I = \cos(kn''r_1)$$

We are going to find now the relationship between $\cos \varphi$ with r_1, s_1 and s_2 .

$$n''^2 r_1^2 = n_e^2 r_1^2 + (n_o^2 - n_e^2) r_1^2 \cos^2 \varphi = C$$

$$n_e^2 r_1^2 \sin^2 \varphi + n_o^2 r_1^2 \cos^2 \varphi = C$$

By using $r_1^2 = \rho^2$ and calculating

$$\cos^2 \varphi = \cos^2 \theta \cos^2 \phi_1 \cos^2 \alpha + \sin^2 \theta \sin^2 \alpha + 2 \cos \theta \cos \phi_1 \cos \alpha \sin \theta \sin \alpha$$

$$r_1^2 \cos^2 \varphi = x^2 \cos^2 \phi_1 \cos^2 \alpha + y^2 \sin^2 \alpha + 2xy \cos \phi_1 \sin \alpha$$

$$r_1^2 \sin^2 \varphi = x^2 + y^2 - (x^2 \cos^2 \phi_1 \cos^2 \alpha + y^2 \sin^2 \alpha + 2xy \cos \phi_1 \sin \alpha)$$

$$= x^2(1 - \cos^2 \phi_1 \cos^2 \alpha) + y^2(1 - \sin^2 \alpha) - 2xy \cos \phi_1 \sin \alpha$$

These results, when replaced in the last equation give

$$n_e^2(x^2(1 - \cos^2 \phi_1 \cos^2 \alpha) + y^2(1 - \sin^2 \alpha) - 2xy \cos \phi_1 \sin \alpha) + n_o^2(x^2 \cos^2 \phi_1 \cos^2 \alpha + y^2 \sin^2 \alpha + 2xy \cos \phi_1 \sin \alpha) = C$$

This result is the equation of an ellipse. We now compare it with Mahalanobis ellipse. It is, we look now for the relationship between r, s_1 and s_2 with the parameters of the birefringent HD.

After come calculations we obtain

$$s_1^2 = ((1 - \cos^2 \phi_1 \cos^2 \alpha)n_e^2 + (\cos^2 \phi_1 \cos^2 \alpha)n_o^2)^{-1}$$

$$s_2^2 = ((1 - \sin^2 \alpha)n_e^2 + (\sin^2 \alpha)n_o^2)^{-1}$$

$$\frac{r}{s_1 s_2} = \cos \phi_1 \sin \alpha (n_e^2 - n_o^2)$$

It means that by manipulating the parameters n_e, n_o, α and ϕ_1 we can modify r, s_1, s_2 .

It can also be seen that all the previously known cases are obtained for particular values.

If $n_e = n_o, r$ results to be zero and $s_1 = s_2 = 1$, it is the families are circumferences (isotropic case).

If $\alpha = 0^\circ$ or if $\phi_1 = 90^\circ$ canonical ellipses are obtained for any value of the refractive indices.

8. Conclusions

We have applied the Mahalanobis distance concept to generalize the classical Abramson Holodiagram. It was found that reflection and refraction in both isotropic and birefringent materials are obtained as particular cases. Mathematically, if abstraction is done of its statistical origin, Mahalanobis distance corresponds to a linear transformation of Euclidean distance, that is to a Euclidean distance expressed in a different non orthonormal vector basis. This is expressed in the fact that the variances s do not depend of position of the point in space. If it would not be so, then it would correspond to a space variable refractive index, or, what is the same, to a Riemannian metrics, in which light moves along the corresponding geodesics. All the cases developed in this work are then particular cases of this more general one.

It was found that two not straightforwardly connected fields can be linked between them as a consequence of their similar geometry involved concepts.

The Holodiagram idea can then be extended by including different concepts of distance to graphically describe other phenomena.

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