

COHERENT MODEL-BASED OPTICAL RESOLUTION AND SNR

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ABSTRACT

In this paper a new parameter estimation based criterion for two-point resolution is proposed. Unlike the classical resolution criteria, the new criterion takes account of noise and systematic errors. A resolution limit in terms of the observations is derived. This limit depends on the point spread function used and the degree of coherence supposed. For statistical observations the probability of resolution as a function of the SNR is derived. This probability can be used as a performance measure in the assessment of optical instruments.

1. INTRODUCTION

Resolution as a performance criterion of imaging systems has achieved a unique position in the technical world. It is used as a universal quality factor of any imaging systems regardless of their configuration and specific purpose. Widely used as a resolution measure is the so-called *two-point resolution*, which is defined as the ability of an imaging system to resolve two object points of equal intensity. The model of an object in the form of two points was related to astronomical problems, occupying an honourable place in science for a long time. In general, as a result of the electromagnetic nature of light and the finite dimensions of the imaging aperture, the light from a point source is spread out in a diffraction pattern, of which the distribution is called the *point spread function (PSF)*. Classical criteria for two-point resolution, like Rayleigh's [1] and Sparrow's [2], consider resolution *as observed by the eye* and provide resolution limits which are defined in terms of the system's PSF only. In the frequency domain the resolution limit is usually represented by the cut-off frequency of the system's *transfer function* [3]. Since the PSF and the transfer function are each others Fourier transforms, both representations of the resolution limit are directly related. The classical theory assumes that resolution is only limited by diffraction. It disregards the dependence of resolution on noise, aberrations and other characteristics of the system including source and/or detector. In essence, the classical theory concerns so-called *calculated images* [4], i.e., images that are by their very nature noise free and exactly describable by a known mathematical two-component model. However, if calculated images would

exist and visual inspection is replaced by intensity measurement, one could numerically fit the two-component model to the observations with respect to the component amplitudes and locations, the resulting fit would be perfect and there would be no limit to resolution. In practice, however, only *detected* images are encountered [4]. For these, fitting a two-component model will never result in a perfect fit. This is due to noise (non-systematic errors) and differences between the model fitted and the one underlying the observations (systematic errors). It is this lack of fit and *not* diffraction that prevents unlimited resolution. This insight has given rise to alternate resolution definitions and criteria, provided from several different points of view. Several of them are based on statistical parameter estimation theory [5-8], resulting in so-called Cramér-Rao Lower Bounds (CRLBs) on the variance of estimators of object parameters like the locations and intensities of point sources. The CRLBs are a measure of the attainable precision and, therefore, of resolution. However, the theory assumes that (i) the model is properly specified, that is, the PSF is exactly known and only random errors are present, (ii) the joint probability density function of the errors or, equivalently, that of the observations is known and (iii) a very large number of observations is available. These assumptions are often not realistic in practice. They are not made in an alternative parameter estimation based definition of two-point resolution proposed in this paper. The presented work is related to earlier work on parametric model-based optical resolution [9-14]. The results have been extended to include two-dimensional (partially) coherent sources of unknown intensity. A further generalization is that the two-component model underlying the observations and that chosen by the experimenter need not to be the same.

2. THE PARAMETRIC MODEL AND THE CRITERION OF GOODNESS OF FIT

Suppose that a set of observations w_1, \dots, w_N on a two-dimensional composite intensity distribution in the image of two point sources is available and that the following two-point image model [15]

$$g_n(\mathbf{a}, \ell, \mathbf{b}) = a[\ell^2 f^2(x_n - b_{x1}, y_n - b_{y1}) + (1 - \ell)^2 f^2(x_n - b_{x2}, y_n - b_{y2}) + 2\gamma \ell(1 - \ell) f(x_n - b_{x1}, y_n - b_{y1})f(x_n - b_{x2}, y_n - b_{y2})] \quad (1)$$

is fitted to the observations with respect to the parameters \mathbf{a} , ℓ and $\mathbf{b} = (b_{x1}, b_{x2}, b_{y1}, b_{y2})^T$, where the superscript T denotes transposition. In (1) $f(x, y)$ is the amplitude PSF, $a\ell^2$ and $a(1-\ell)^2$ are the peak intensities of the individual point images, (b_{x1}, b_{y1}) and (b_{x2}, b_{y2}) are the locations and γ is the real part of the complex degree of coherence, with $|\gamma| \leq 1$ [15]. The parameter ℓ determines the peak intensity ratio. The variables (x_n, y_n) are the measurement points, which are assumed to be known. The model is fitted in least squares (LS) sense. This means that the LS criterion

$$J_2(\mathbf{a}, \ell, \mathbf{b}) = \sum_n d_n^2(\mathbf{a}, \ell, \mathbf{b}), \quad n = 1, \dots, N, \quad (2)$$

is minimized with respect to $(\mathbf{a}, \ell, \mathbf{b})$, where $d_n(\mathbf{a}, \ell, \mathbf{b}) = w_n - g_n(\mathbf{a}, \ell, \mathbf{b})$. Furthermore, in (2) the subscript 2 refers to the fact that a *two*-component model such as the model (1) is fitted. To simplify the procedure, the minimization with respect to $(\mathbf{a}, \ell, \mathbf{b})$ is replaced by minimization with respect to (\mathbf{a}, \mathbf{b}) for all allowable values of ℓ . These are usually all values on a subinterval of the interval (0,1). The best fit is taken as a solution. If a priori knowledge about the *peak-to-peak ratio* $\ell^2 / (1-\ell)^2$ is available, this can be used directly by determining the value of ℓ . By definition, two-point resolution concerns two point sources of *equal* intensity. Accordingly, one should impose a constraint on ℓ , since an estimate that shows only a weak companion cannot be claimed as a successful restoration of an object known to comprise two equal components [16]. Let this criterion be $\ell_a \leq \ell \leq (1-\ell_a)$, where ℓ_a is the smallest allowable value of ℓ . Setting $\ell_a = 0.5$ forces the two estimated peak intensities to be exactly the same [12]. However, this constraint might be too strict, since when an estimate showing two components with slightly different peak intensities is found, the two components may be considered resolved. Adopting the peak-to-peak ratio constraint $2/3 \leq \ell^2 / (1-\ell)^2 \leq 3/2$ yields $\ell_a \approx 0.45$ [13,16].

Next, suppose that the one-component model

$$a f^2(x - b_x, y - b_y) \quad (3)$$

is fitted to the same observations and that the minimum of the corresponding LS criterion

$$J_1(\mathbf{a}, b_x, b_y) = \sum_n d_n^2(\mathbf{a}, b_x, b_y), \quad (4)$$

with $d_n(\mathbf{a}, b_x, b_y) = w_n - a f^2(x_n - b_x, y_n - b_y)$, is given by $(\hat{a}, \hat{b}_x, \hat{b}_y)$. Then, in the parameterization of $J_2(\mathbf{a}, \ell, \mathbf{b})$, the point $(\hat{a}, \hat{b}_x, \hat{b}_y)$ is represented by the points:

$$(\bar{a}, \ell, \hat{b}_x, \hat{b}_x, \hat{b}_y, \hat{b}_y) \quad (5)$$

for all \hat{a} and \bar{a} satisfying $\hat{a} = \bar{a} / (\ell^2 + (1-\ell)^2 + 2\gamma \ell(1-\ell))$, for any ℓ . Like in [10-11], it can be shown that the

points (5) are stationary points of $J_2(\mathbf{a}, \ell, \mathbf{b})$. Notice that at (5) the location parameters are equal in pairs. Depending on the particular set of observations used, the so-called *one-component stationary points* (5) are either saddle points or minima [10-11]. If the points are saddle points, the LS solutions for the locations $(\hat{b}_{x1}, \hat{b}_{y1})$ and $(\hat{b}_{x2}, \hat{b}_{y2})$ are distinct and the point sources are resolved. If the points (5) are minima, the solutions coincide exactly and resolution is impossible. This remarkable coincidence phenomenon is a consequence of a change in the number and nature of the stationary points of the LS criterion under influence of the observations. A precise mathematical description of such a structural change, which is called a *singularity*, can be given on basis of singularity and catastrophe theory [17], but this is outside the scope of this paper. It can easily be shown, that at the points (5) the value of $J_2(\mathbf{a}, \ell, \mathbf{b})$ is for all ℓ equal to $J_1(\hat{a}, \hat{b}_x, \hat{b}_y)$. Hence, if there is any ℓ for which the model fitting solution $(\hat{a}, \ell, \hat{b}_{x1}, \hat{b}_{x2}, \hat{b}_{y1}, \hat{b}_{y2})$ is different from (5), i.e., for which (5) is a saddle point, the value of $J_2(\mathbf{a}, \ell, \mathbf{b})$ at $(\hat{a}, \ell, \hat{b}_{x1}, \hat{b}_{x2}, \hat{b}_{y1}, \hat{b}_{y2})$ must be smaller than $J_1(\hat{a}, \hat{b}_x, \hat{b}_y)$. Since the best fit is taken as the solution, this means that resolution is always possible unless the point (5) is a minimum for all ℓ .

3. THE RESOLUTION DISCRIMINANT

The nature of the stationary points (5) is determined by the signs of the eigenvalues of the Hessian matrix \mathbf{H}_2 , i.e., the matrix of second order derivatives, of the criterion (2) with respect to the parameter vector $(\mathbf{a}, b_{x1}, b_{x2}, b_{y1}, b_{y2})$, evaluated at (5). After a linear coordinate transform, the Hessian matrix of the criterion in the new coordinates is found to be equal to the block diagonal matrix [10-11]

$$\text{diag}(\mathbf{H}_1 \quad \mathbf{P}_1). \quad (6)$$

In this expression the 3×3 matrix \mathbf{H}_1 is the Hessian matrix of the criterion (4) for fitting the one-component model (3) evaluated at the minimum $(\hat{a}, \hat{b}_x, \hat{b}_y)$. Therefore, \mathbf{H}_1 is always positive definite. The 2×2 matrix \mathbf{P}_1 is defined by its (k, m) -th element [11]

$$P_{km}(\ell) = \frac{4\ell(1-\ell)\hat{a}}{(\ell^2 + (1-\ell)^2 + 2\gamma\ell(1-\ell))^2} \times \{c_1(\ell)\chi_{km} - c_2(\ell)\psi_{km}\}, \quad (7)$$

where $c_1(\ell) = \ell(1-\ell)(\gamma^2 - 1)$, $c_2(\ell) = ((1-\ell) + \gamma\ell) \times (\ell + \gamma(1-\ell))$, and

$$\chi_{km} = \sum_n d_n \frac{\partial f_n}{\partial b_k} \frac{\partial f_n}{\partial b_m}, \quad \psi_{km} = \sum_n d_n \frac{\partial^2 f_n}{\partial b_k \partial b_m} f_n, \quad (8)$$

with $b_1 = b_x$, $b_2 = b_y$, $f_n = f(x_n - b_x, y_n - b_y)$ and $d_n = w_n - a f_n^2$. The quantities d_n , f_n and the derivatives of f_n are evaluated at $(\hat{a}, \hat{b}_x, \hat{b}_y)$. The smallest eigenvalue of \mathbf{P}_1 is given by

$$\eta_1 = \frac{1}{2} \left\{ (P_{11} + P_{22}) - \sqrt{(P_{11} + P_{22})^2 - 4(P_{11}P_{22} - P_{12}^2)} \right\}. \quad (9)$$

If η_ℓ is negative, the point (5) is a saddle point. If η_ℓ is positive, the point (5) is a minimum. Consequently, resolution is impossible if η_ℓ is positive for all allowable values of ℓ . Then the one-component stationary point is the (absolute) minimum of $J_2(\mathbf{a}, \ell, \mathbf{b})$ and the model fitting solutions for the locations exactly coincide. Since the sign of η_ℓ thus determines whether the two point sources can be resolved or not, η_ℓ is called the *resolution discriminant*. To decide whether or not two point sources can be resolved from a given set of observations, firstly the one-component model (3) must be fitted. Secondly, the one-component solution must be substituted in (9) and the sign of the resolution discriminant must be assessed for all allowable values of ℓ . Since the first term in (7) is always positive, it will from now on be omitted in the analysis of η_ℓ .

For a Gaussian PSF it can be shown that $\chi_{km} = \psi_{km}$, taking into account that $(\hat{a}, \hat{b}_x, \hat{b}_y)$ is a stationary point of $J_1(\mathbf{a}, b_x, b_y)$. Then (9) can be written as:

$$\eta_\ell = c_\ell \times X, \quad (10)$$

with $c_\ell = 1/2 (c_1(\ell) - c_2(\ell))$ and

$$X = (\chi_{11} + \chi_{22}) - \sqrt{(\chi_{11} + \chi_{22})^2 - 4(\chi_{11}\chi_{22} - \chi_{12}^2)}. \quad (11)$$

It can be shown that c_ℓ is a parabola which is concave and has its minimum at $\ell = 0.5$, at which $c_{0.5} \leq 0$. For $\ell_a = 0.45$, the roots of c_ℓ are located on the allowable interval (0.45, 0.55) only if $\gamma < -0.98$. Therefore, c_ℓ is negative for all allowable ℓ if $\gamma > -0.98$. Then it follows from (10) that $\eta_\ell > 0$ for all ℓ , if and only if (i) $\gamma > -0.98$, and (ii) $X < 0$. Resolution is impossible if both these conditions are satisfied. Notice that condition (i) is rarely if ever violated.

4. THE RESOLUTION LIMIT

Suppose that a set of observations w_1, \dots, w_N is available. Furthermore, suppose that these observations are the coordinates of an N-dimensional Euclidean space. Then every point of this space represents a particular set of observations. Like in [10-12], it can be shown that in this space of the observations a hypersurface can be computed that divides the space in two complementary subspaces. From sets of observations in the one subspace the components can be resolved since $\eta_\ell < 0$ for at least one value of ℓ and the model fitting solutions for the component locations are thus distinct. For observations in the other subspace $\eta_\ell > 0$ for all ℓ , the solutions *exactly* coincide and resolution is impossible. The hypersurface thus represents the *resolution limit* in terms of the observations, and will be addressed as such from now on. The resolution limit depends on the type of PSF *fitted* and the degree of coherence supposed. It can be computed for any number of observations and does not depend on statistical assumptions. However, if the observations *are* statistical, the probability of resolving the components from noisy observations can be computed as a function of the Signal-to-Noise Ratio (SNR). This will be shown in the next section.

5. PROBABILITY OF RESOLUTION

In this section the probability of resolution as a function of the SNR is derived, given a set of N independent observations w_1, \dots, w_N with expectations $E[w_n]$ and variances σ_n^2 , respectively. For this purpose the statistical properties of the resolution discriminant (9) must be determined. The resolution discriminant is a function of the one-component solution $(\hat{a}, \hat{b}_x, \hat{b}_y)$. Since the peak intensity parameter a occurs linearly in the one-component model (3), a closed form expression can be derived for the solution \hat{a} as a function of the solutions \hat{b}_x and \hat{b}_y [12]. The parameter a can thus be eliminated from the minimization procedure. The expectation and variance of \hat{a} are given by

$$E[\hat{a}] = \frac{\sum_n E[w_n] f_n^2}{\sum_n f_n^4} \quad \text{and} \quad \text{Var}\{\hat{a}\} = \frac{\sum_n f_n^4 \sigma_n^2}{\left(\sum_n f_n^4\right)^2}, \quad (12)$$

respectively. The location parameters b_x and b_y occur nonlinearly in model (3). Therefore, their solutions must be determined iteratively by numerical nonlinear minimization of (4). However, the SNR, of which the standard definition, expressed in dB, is given by

$$\text{SNR} = 10^{10} \log \left(\frac{\sum_n E[w_n]^2}{\sum_n \sigma_n^2} \right), \quad (13)$$

is supposed to be sufficiently large to assume that the solutions \hat{b}_x and \hat{b}_y will hardly vary under the influence of the noise. Furthermore, due to the functional shape of most conventional PSFs, the terms χ_{km} and ψ_{km} in (7) will hardly vary with slight changes in \hat{b}_x and \hat{b}_y . Therefore, \hat{b}_x and \hat{b}_y may be taken as constants in the following analysis. Their values are set equal to the LS estimates obtained from fitting the model (3) to the $E[w_n]$. Simulation results have shown that this simplification is justified. If the number of observations is sufficiently large for the central limit theorem to hold, it follows that the terms χ_{km} and ψ_{km} , and therefore the matrix elements p_{km} , are all normally distributed. It follows from (7-9) that η_ℓ as a function of ℓ has a maximum or minimum at $\ell = 0.5$ and is symmetrical around this point. Furthermore, it follows from simulation results that for $\ell_a = 0.45$, η_ℓ is monotonously decreasing or increasing on the interval (0.45, 0.5). Consequently, η_ℓ is positive for all allowable values of ℓ , if both $\eta_{0.45}$ and $\eta_{0.5}$ are positive, that is, if

$$\text{Tr}(\mathbf{P}_{0.45}) > 0 \wedge |\mathbf{P}_{0.45}| > 0 \wedge \text{Tr}(\mathbf{P}_{0.5}) > 0 \wedge |\mathbf{P}_{0.5}| > 0. \quad (14)$$

In (14) $\text{Tr}(\cdot)$ and $|\cdot|$ are the Trace and Determinant operators, respectively. Now, let $\mathbf{p} = (p_{11}(0.45), p_{12}(0.45), p_{22}(0.45), p_{11}(0.5), p_{12}(0.5), p_{22}(0.5))^T$. Then \mathbf{p} has a *multivariate normal distribution* f given by [18]

$$f(\mathbf{p}) = \frac{1}{(2\pi)^3 |\mathbf{\Psi}|^{1/2}} \exp(-1/2 (\mathbf{p} - \mathbf{E}[\mathbf{p}])^T \mathbf{\Psi}^{-1} (\mathbf{p} - \mathbf{E}[\mathbf{p}])), \quad (15)$$

where Ψ is the 6×6 covariance matrix of \mathbf{p} . Using the knowledge of the statistics of the observations, the expectation of \mathbf{p} follows directly from (8) and (12) and the elements of Ψ are given by

$$\begin{aligned} \text{Cov}(p_{ij}(\ell_1), p_{km}(\ell_2)) &= \sum_{r=1}^N \left(\text{Var}\{\hat{a}\} - \frac{\sigma_r^2}{\sum_{q=1}^N f_q^4} \right) \times \\ &\left(c_1(\ell_2) f_r^3 \frac{\partial^2 f_r}{\partial b_k \partial b_m} + c_2(\ell_2) f_r^2 \frac{\partial f_r}{\partial b_k} \frac{\partial f_r}{\partial b_m} \right) \times \\ &\sum_{n=1}^N \left(c_1(\ell_1) f_n^3 \frac{\partial^2 f_n}{\partial b_i \partial b_j} + c_2(\ell_1) f_n^2 \frac{\partial f_n}{\partial b_i} \frac{\partial f_n}{\partial b_j} \right) + \\ &\sum_{n=1}^N \sigma_n^2 \left(c_1(\ell_1) f_n \frac{\partial^2 f_n}{\partial b_i \partial b_j} + c_2(\ell_1) \frac{\partial f_n}{\partial b_i} \frac{\partial f_n}{\partial b_j} \right) \times \\ &\left\{ c_1(\ell_2) f_n \frac{\partial^2 f_n}{\partial b_k \partial b_m} + c_2(\ell_2) \frac{\partial f_n}{\partial b_k} \frac{\partial f_n}{\partial b_m} \right. \\ &\left. - \frac{f_n^2}{\sum_{q=1}^N f_q^4} \sum_{r=1}^N \left(c_1(\ell_2) f_r^3 \frac{\partial^2 f_r}{\partial b_k \partial b_m} + c_2(\ell_2) f_r^2 \frac{\partial f_r}{\partial b_k} \frac{\partial f_r}{\partial b_m} \right) \right\}, \end{aligned} \quad (16)$$

with $\ell_1, \ell_2 \in \{0.45, 0.5\}$. Then it follows from (14-15) that the probability of resolution is given by

$$1 - \int_0^{\infty} \int_{-\sqrt{p_{11}(0.45)} \ p_{22}(0.45)}^{\sqrt{p_{11}(0.45)} \ p_{22}(0.45)} \int_0^{\infty} \int_{-\sqrt{p_{11}(0.5)} \ p_{22}(0.5)}^{\sqrt{p_{11}(0.5)} \ p_{22}(0.5)} \int_0^{\infty} f(\mathbf{p}) \ d\mathbf{p} \quad (17)$$

For a Gaussian PSF, the analysis is drastically simplified. Then, as discussed in Section 3, the solutions for the locations coincide if (i) $\gamma > -0.98$ and (ii) $X < 0$. Provided that condition (i) is fulfilled, and taking into account that the elements χ_{km} are normally distributed, the probability of resolution is now given by

$$\int_0^{\infty} \int_{-\sqrt{\chi_{11}} \ \chi_{22}}^{\sqrt{\chi_{11}} \ \chi_{22}} \int_0^{\infty} \frac{\exp(-1/2(\boldsymbol{\chi} - \mathbf{E}[\boldsymbol{\chi}])^T \boldsymbol{\Omega}^{-1} (\boldsymbol{\chi} - \mathbf{E}[\boldsymbol{\chi}]))}{(2\pi)^{3/2} |\boldsymbol{\Omega}|^{1/2}} \ d\boldsymbol{\chi} \quad (18)$$

where $\boldsymbol{\chi} = (\chi_{11}, \chi_{12}, \chi_{22})^T$, $\boldsymbol{\Omega}$ is the 3×3 covariance matrix of $\boldsymbol{\chi}$. The value of $\mathbf{E}[\boldsymbol{\chi}]$ follows directly from (8) and (12). The computation of $\boldsymbol{\Omega}$ is straightforward and to a certain extent analogous to that of Ψ . It will therefore not be presented here.

6. CONCLUSIONS

In this paper a new definition for two-point resolution has been presented. It has been shown that two distinct types of sets of observations can be distinguished. For the one type, the model fitting solutions for the component locations are distinct. Then the components are resolved. For the other type, the solutions exactly coincide and the components are

not resolved. Which type occurs depends on the particular set of observations. It has been shown how these types can be determined for any two-component model. Furthermore, if a priori knowledge about the statistics of the observations is available, the probability of resolution can be computed as a function of the SNR for any PSF fitted and any degree of coherence supposed. This probability can be used to compare the performance of different imaging systems.

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