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1 On the equivalence of optimization metrics in Stokes polarimetry

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Abstract. Optimization of polarimeters has historically been achieved using an assortment of performance metrics. Selection of an optimization parameter is frequently made, however, on an ad hoc basis. In this article we rigorously demonstrate that optimization strategies in Stokes polarimetry based on three common metrics; namely the condition number of the instrument matrix, the determinant of the associated Gram matrix, or the equally weighted variance, are formally equivalent. In particular, using each metric we derive the same set of constraints on the measurement states, and show that these can be satisfied using spherical 2 designs. Our conclusions are equally applicable to optimization of the illumination states in Mueller matrix polarimetry.

14 Keywords: polarimetry, optimization, spherical design, instrument matrix, equally weighted variance.

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16 **1 Introduction**

17 Quantitative analysis of the state of polarization of light provides a powerful tool in modern sci-

¹⁸ ence. Applications vary from microscopy, biomedical diagnosis and astrophysics^{1–3} to crystallo-

¹⁹ graphic, material and single molecule studies.^{4,5} Whilst the polarization state of light itself, can be

²⁰ used to transmit information, hence presenting new opportunities in optical data storage and com-

²¹ munications,^{6–9} changes in polarization induced by a material can alternatively be used for object

²² detection¹⁰ or to characterize sample properties, such as chirality or molecular orientation.^{11–13}

Stokes polarimeters, which allow a complete characterization of the polarization state of input light as described by the associated 4×1 Stokes vector **S**, comprise of $N \geq 4$ distinct measurements that can be multiplexed in, for example, time,¹⁴ frequency¹⁵ or space.¹⁶ Fundamentally, each constituent measurement outputs an intensity I_j ($j \in [1, N]$) which is proportional to the projection of the incident Stokes vector onto an analysis state \mathbf{W}_j , i.e., $I_j = \mathbf{W}_j^T \mathbf{S}$. Central to the description and design of Stokes polarimeters is hence the so-called instrument or measurement matrix $\mathbb{W} = [\mathbf{W}_1, \mathbf{W}_2, \ldots]^T$ formed from stacking the set of analysis vectors. In order to obtain an estimate of the Stokes vector from the set of projections I_j , the measurement matrix must be inverted. So as to limit noise propagation through this inversion process, optimization of the measurement matrix is hence frequently performed. Optimization in this vein has been performed using different metrics including the associated information content,^{17–19} matrix determinant,^{20–22} signal to noise ratio,²³ equally weighted variance^{24,25} and condition number.^{21–23,25–29}

³⁵ Mueller matrix polarimeters, on the other hand, combine a Stokes polarimeter with use of ³⁶ multiple incident polarized states so as to measure the full Mueller matrix of an object. Variation ³⁷ of the probing polarization states (as can be described using an analogous illumination matrix) ³⁸ therefore introduces additional degrees of freedom, hence admitting further optimization.^{17, 28–32} ³⁹ Application specific optimization of polarimeters has also been reported, for example, in detection ⁴⁰ and imaging problems the polarization contrast is a more suitable metric.^{33, 34}

Recently, the equivalence of a number of optimization metrics, namely the equally weighted 41 variance, the condition number of W and the determinant of the associated Gram matrix, was 42 discussed by Foreman et al.³⁵ Additionally, Foreman et al. proved that a Stokes polarimeter is 43 optimal (as characterized by these metrics) when the set of analysis states defines a spherical 2 44 design³⁶ on the unit Poincaré sphere. A re-examination of the equivalence between these metrics 45 is, however, necessary due to an error in the proof presented in Ref. 35. The goal of this article is 46 therefore to provide a rigorous proof that the conclusions of Ref. 35 hold. Our derivations also elicit 47 greater insight into the optimization of Stokes polarimeters. We additionally note that our results 48 are equally applicable to optimization of the probing states used in Mueller matrix polarimetry due 49 to the similar matrix structure of the problem. 31,37 50

51 2 Optimal polarimetry with spherical 2-designs

The instrument matrix, \mathbb{W} , of a polarimeter is an $N \times 4$ matrix, the rows of which are the Stokes vectors of the N polarization states being analyzed, normalized such that the polarimeter is passive. Accordingly the instrument matrix has the parametric form

$$\mathbb{W} = \frac{1}{2} \begin{bmatrix} 1 & \mathbf{w}_1^T \\ 1 & \mathbf{w}_2^T \\ \vdots & \vdots \\ 1 & \mathbf{w}_N^T \end{bmatrix} \triangleq \frac{1}{2} \begin{bmatrix} \mathbf{r} & \mathbb{Q} \end{bmatrix}, \qquad (1)$$

where **r** is an $N \times 1$ vector of ones and \mathbb{Q} is the matrix formed from the 3×1 vectors \mathbf{w}_j ($j \in [1, N]$) of unit norm. Note that throughout this work bold notation is used to signify column vectors whilst blackboard font denotes matrices. Please also note that we have assumed an "ideal" instrument matrix, in the sense that the transmittance and degree of polarization of all the rows are equal to one. The generalization of the obtained results to arbitrary instrumentation matrices will be discussed in Section 4.

In Stokes polarimetry, one performs N intensity measurements $I_j, j \in [1, N]$ by projecting the input Stokes vector S onto each of the N analyzers described by the N rows of the matrix W. If these measurements are stacked in an N-dimensional vector $\mathbf{I} = [I_1, I_2, \dots, I_N]^T$, and if we assume that the measurements are perturbed by white additive noise, we obtain

$$\mathbf{I} = \mathbf{W}\mathbf{S} + \mathbf{B},\tag{2}$$

where **B** is an $N \times 1$ random vector with covariance matrix $\sigma^2 \mathbb{I}_N$ and \mathbb{I}_n denotes the $n \times n$ identity

matrix. The maximum-likelihood estimate of S is obtained by

$$\widehat{\mathbf{S}} = \mathbb{W}^+ \mathbf{I} \tag{3}$$

where

$$\mathbb{W}^{+} = (\mathbb{W}^{T}\mathbb{W})^{-1}\mathbb{W}^{T} \tag{4}$$

denotes the pseudo-inverse matrix. The estimate \widehat{S} is a random vector of mean S (i.e., the estimator is unbiased), and of covariance matrix^{17,23,24}

$$\mathbb{K}_{\mathbf{S}} = \sigma^2 (\mathbb{W}^T \mathbb{W})^{-1}.$$
 (5)

The estimation variances of each element of the Stokes vector estimate are the diagonal elements of this matrix. A natural goal of polarimeter optimization is to find the measurement matrix W that minimizes the sum of these variances, that is, the trace of \mathbb{K}_{S} . The corresponding performance metric is called the equally weighted variance (EWV), i.e.,

$$\mathbf{EWV} = \sigma^2 \mathbf{tr}[\mathbb{G}^{-1}] \tag{6}$$

where

$$\mathbb{G} = \mathbb{W}^T \mathbb{W} \tag{7}$$

 $_{58}$ denotes the Gram matrix associated with $\mathbb W.$

To optimize the EWV, we first express the Gram matrix \mathbb{G} in block format, viz.

$$\mathbb{G} = \frac{1}{4} \begin{bmatrix} N & \mathbf{r}^T \mathbb{Q} \\ \mathbb{Q}^T \mathbf{r} & \mathbb{Q}^T \mathbb{Q} \end{bmatrix} \triangleq \begin{bmatrix} A & \mathbf{B}^T \\ \mathbf{C} & \mathbb{D} \end{bmatrix}.$$
 (8)

The inverse of the Gram matrix can then be expressed in the form³⁸

$$\mathbb{G}^{-1} = \begin{bmatrix} A^{-1} + A^{-1} \mathbf{B}^T \mathbb{M}^{-1} \mathbf{C} A^{-1} & -A^{-1} \mathbf{B}^T \mathbb{M}^{-1} \\ -\mathbb{M}^{-1} \mathbf{C} A^{-1} & \mathbb{M}^{-1} \end{bmatrix},$$
(9)

where the matrix

$$\mathbb{M} = (\mathbb{D} - \mathbf{C}A^{-1}\mathbf{B}^T) \tag{10}$$

is the Schur complement of the upper left block of \mathbb{G} . This implies that the trace we seek can be written as

$$tr[\mathbb{G}^{-1}] = A^{-1} + A^{-1}\mathbf{B}^T \mathbb{M}^{-1} \mathbf{C} A^{-1} + tr[\mathbb{M}^{-1}].$$
(11)

Substituting Eq. (8) into Eq. (10), the Schur complement takes the form:

$$\mathbb{M} = \frac{1}{4} \left(\mathbb{Q}^T \mathbb{Q} - \frac{\mathbf{q} \mathbf{q}^T}{N} \right) \tag{12}$$

where $\mathbf{q} = \mathbb{Q}^T \mathbf{r}$ is an *N*-dimensional vector. Upon using the identity³⁸

$$(\mathbb{Z} + \mathbf{x}\mathbf{y}^T)^{-1} = \mathbb{Z}^{-1} - \frac{\mathbb{Z}^{-1}\mathbf{x}\mathbf{y}^T\mathbb{Z}^{-1}}{1 + \mathbf{y}^T\mathbb{Z}^{-1}\mathbf{x}}$$
(13)

with $\mathbf{x} = -\mathbf{y} = \mathbf{q}/\sqrt{N}$ and $\mathbb{Z} = \mathbb{Q}^T \mathbb{Q}$, we find

$$\mathbb{M}^{-1} = 4 \left(\mathbb{Q}^T \mathbb{Q} \right)^{-1} + 4 \frac{(\mathbb{Q}^T \mathbb{Q})^{-1} \mathbf{q} \mathbf{q}^T (\mathbb{Q}^T \mathbb{Q})^{-1}}{N - \mathbf{q}^T (\mathbb{Q}^T \mathbb{Q})^{-1} \mathbf{q}}.$$
 (14)

Direct substitution from Eqs. (8) and (14) into Eq. (11) yields

$$\operatorname{tr}[\mathbb{G}^{-1}] = 4 \left\{ \frac{1}{N} + \operatorname{tr}\left[(\mathbb{Q}^T \mathbb{Q})^{-1} \right] + \frac{\mathbf{q}^T [N(\mathbb{Q}^T \mathbb{Q})^{-2} + (\mathbb{Q}^T \mathbb{Q})^{-1}] \mathbf{q}}{N[N - \mathbf{q}^T (\mathbb{Q}^T \mathbb{Q})^{-1} \mathbf{q}]} \right\},$$
(15)

⁵⁹ where we have also used the cyclic property of the trace operation and the identity $tr[Xq^Tq] =$ ⁶⁰ $q^T Xq$ for arbitrary X.³⁸

Noting that N > 0 and that $\mathbb{Q}^T \mathbb{Q}$ is positive definite, it follows immediately that the first two terms in Eq. (15) are positive. We show in Appendix A that the third term is also positive. Consequently, the trace in Eq. (15) is minimal when its three terms are minimal. The first term is constant, and the third is minimal when it is null, that is, when $\mathbf{q} = \mathbb{Q}^T \mathbf{r} = \mathbf{0}$ or equivalently

$$\sum_{n=1}^{N} \mathbf{w}_n = \mathbf{0}.$$
 (16)

⁶¹ Importantly, Eq. (16) expresses a polynomial constraint that must be satisfied by an optimal mea-⁶² surement matrix, and is equivalent to that given in Eq. (4) of Ref. 35. When Eq. (16) holds, minimizing tr[\mathbb{G}^{-1}] is equivalent to minimizing tr [($\mathbb{Q}^T \mathbb{Q}$)⁻¹]. This optimization has to be done under the constraint that the trace of the matrix $\mathbb{Q}^T \mathbb{Q}$ is constant as follows from the normalization of \mathbf{w}_j . Indeed, since each row of the matrix \mathbb{Q} is a unit-norm vector, we have

$$\operatorname{tr}[\mathbb{Q}^T \mathbb{Q}] = \operatorname{tr}[\mathbb{Q}\mathbb{Q}^T] = N.$$
(17)

We thus have to solve the following constrained optimization problem, set in Lagrange form

$$\Psi(\mathbb{Q}) = \operatorname{tr}[(\mathbb{Q}^T \mathbb{Q})^{-1}] - \mu \left(\operatorname{tr}[\mathbb{Q}^T \mathbb{Q}] - N\right)$$
(18)

where μ is a Lagrange multiplier. The Lagrange function can also be expressed as

$$\Psi(\boldsymbol{\beta}) = \sum_{j=1}^{3} \frac{1}{\beta_j} + \mu\left(\sum_{j=1}^{3} \beta_j - N\right)$$
(19)

where β_j , $j \in [1,3]$, are the positive eigenvalues of the matrix $\mathbb{Q}^T \mathbb{Q}$. Equating the gradient of Eq. (19) with respect to β to zero and enforcing the constraint $(\partial \Psi / \partial \mu = 0)$ yields $\beta_j = 1/\sqrt{\mu} = N/3$ for all $j \in [1,3]$, such that

$$\mathbb{Q}^T \mathbb{Q} = \sum_{j=1}^m \mathbf{w}_j \mathbf{w}_j^T = \frac{N}{3} \mathbb{I}_3.$$
 (20)

Eq. (20) is the second set of polynomial constraints derived in Ref. 35. The form of the Gram

matrix G which hence minimizes the EWV of the instrument matrix is thus

$$\mathbb{G} = \mathbb{W}^T \mathbb{W} = \frac{N}{12} \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$
 (21)

According to Eq. (5), the corresponding covariance of the Stokes vector estimate is hence:

$$\mathbb{K}_{\mathbf{S}} = \frac{4}{N} \sigma^2 \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 3 \end{bmatrix}.$$
 (22)

This result is important since it specifies, in a very simple closed-from, the fundamental limit 63 of the estimation variance that can be reached by a Stokes polarimeter with a given number of 64 measurement vectors in the presence of additive noise. For example, we note that the minimum 65 achievable variance on an estimate of the intensity (i.e. the first element of the Stokes vector) is 66 three times better than that on the other Stokes parameters. Moreover, the covariance matrix is 67 diagonal, which means that the fluctuations of each element of the Stokes vector estimator are 68 statistically independent. This property is important when performing theoretical computations 69 involving Stokes vector estimators. Incidently, we note that the minimum value of the equally 70 weighted variance is EWV = $40\sigma^2/N$. 71

Finally, we can show that the conditions expressed by Eqs. (16) and (20) are satisfied when

the set of measurement states on the Poincaré sphere, defined by $\{\mathbf{w}_j\}$, $j \in [1, N]$, constitute a spherical 2 design (see Appendix B) as reported in Ref. 35. A spherical *t*-design is defined as a collection of N points $\{\mathbf{w}_j\}$ on the surface of the unit sphere (in our case in \mathcal{R}^3) for which the normalized integral of any polynomial function, $f(\mathbf{w})$, of degree *t* or less is equal to the average taken over the N points. The Platonic solids, i.e., the regular tetrahedron (N = 4), the octahedron (N = 6), the cube (N = 8), the icosahedron (N = 12), and the dodecahedron (N = 20), are spherical 2 designs, as well as many other measurement frames illustrated in.³⁵

80 3 Equivalence of optimization metrics

We will now demonstrate that the optimization of two other popular metrics, namely the condition number and the determinant of the Gram matrix, lead to exactly the same measurement frames as the EWV, so that these three criteria are strictly equivalent.

84 3.1 Condition number

The condition number κ of the instrument matrix is defined by $\kappa = ||W|| ||W^+||$ where W^+ is the pseudo-inverse matrix and the Hilbert-Schmidt matrix norm³⁸ of any matrix \mathbb{P} is defined as:

$$\|\mathbb{P}\| = (\operatorname{tr}[\mathbb{P}^T \mathbb{P}])^{1/2} = (\operatorname{tr}[\mathbb{P} \mathbb{P}^T])^{1/2}$$
(23)

Our choice of normalization of the measurement states $\mathbf{W}_j = [1, \mathbf{w}_j]^T / 2$ implies that

$$\|\mathbb{W}\|^2 = \operatorname{tr}[\mathbb{W}^T \mathbb{W}] = \frac{N}{2}.$$
(24)

Moreover, using the expression of the pseudo-inverse in Eq. (4), it is easily shown that

$$\|\mathbb{W}^{+}\|^{2} = \operatorname{tr}[(\mathbb{W}^{+})^{T}\mathbb{W}^{+}] = \operatorname{tr}[(\mathbb{W}^{T}\mathbb{W})^{-1}] = \frac{\operatorname{EWV}}{\sigma^{2}}.$$
(25)

Consequently, one can write

$$\kappa = \frac{\sqrt{N}}{\sqrt{2}\sigma} \sqrt{\text{EWV}}.$$
(26)

For any measurement matrix verifying Eq. (1), the condition number is thus simply proportional to the square root of the EWV. It is thus obvious that minimizing the condition number is equivalent to minimizing the EWV.

88 3.2 Determinant of the Gram matrix

The first works on Stokes polarimeter optimization considered devices with a minimal number 89 (N = 4) of measurement vectors.²⁶ Optimization of such systems used the determinant of the 90 matrix \mathbb{W} (which for this value of N is square and non singular) as a performance metric. In this 91 case the optimal structure found dictated that the measurement vectors defined a regular tetrahe-92 dron on the Poincaré sphere, a result that we also found above by optimizing the EWV. We show 93 in this section that this result comes from the strict equivalence of these two optimization metrics. 94 This equivalence can be generalized to any value of N if one considers the optimization of the 95 determinant of the Gram matrix \mathbb{G} , since for N > 4 the matrix \mathbb{W} itself is rectangular and its 96 determinant is thus not defined. Notice that this equivalence was mentioned in Ref. 35, but there 97 was an erroneous step in the logic presented in that work (see appendix C for more detail). 98

We intend here to show that maximization of the determinant $|\mathbb{G}|$ yields the same polynomial

constraints embodied in Eqs. (16) and (20). Considering the block form of the Gram matrix in Eq. (8), its determinant can be written as^{38}

$$|\mathbb{G}| = |A - \mathbf{B}^T \mathbb{D}^{-1} \mathbf{C}||\mathbb{D}|$$

= $\frac{1}{256} \left[N - \mathbf{r}^T \mathbb{Q} (\mathbb{Q}^T \mathbb{Q})^{-1} \mathbb{Q}^T \mathbf{r} \right] |\mathbb{Q}^T \mathbb{Q}|.$ (27)

¹⁰² Maximizing this expression means maximizing the two factors appearing in the product. The first ¹⁰³ factor is maximized if the positive subtractive term is zero, that is to say when the vector $\mathbb{Q}^T \mathbf{r} = \mathbf{0}$, ¹⁰⁴ corresponding to the first polynomial constraint expressed in Eq. (16).

For the second factor, we note that $|\mathbb{Q}^T \mathbb{Q}| = \prod_{j=1}^3 \beta_j$ where β_j , $j \in [1,3]$, are the eigenvalues of the matrix $\mathbb{Q}^T \mathbb{Q}$ which are positive since $\mathbb{Q}^T \mathbb{Q}$ is positive definite. Moreover, according to Eq. (17), the matrix $\mathbb{Q}^T \mathbb{Q}$ has constant trace. Maximization of $|\mathbb{Q}^T \mathbb{Q}|$ is thus once again a constrained optimization problem which can be solved using the method of Lagrange multipliers. We will consider maximization of $\ln |\mathbb{Q}^T \mathbb{Q}|$ since the logarithmic function is monotonically increasing. The Lagrange function then becomes

$$\Psi(\boldsymbol{\beta}) = \sum_{j=1}^{3} \ln \beta_j - \mu \left(\sum_{j=1}^{3} \beta_j - N \right).$$
(28)

Following the standard optimization procedure we find, similarly to Section 2, that $\beta_j = 1/\mu = N/3$ for all $j \in [1, 2, 3]$. As shown in Section 2, the second polynomial constraint expressed in Eq. (20) then follows. Therefore, we have ultimately shown that minimization of the EWV (and thus also of the condition number of the instrument matrix) of a polarimeter yields the same set of optimality constraints as maximizing the determinant of the associated Gram matrix.

110 4 Discussion

The main conclusion of the previous sections is the following: among all the measurement matrices verifying Eq. (1), the ones that maximize the condition number, the EWV and the determinant are exactly the same. It can be said that this results unifies many previous works on polarimeter optimization: for example, the early work of Azzam²⁶ (based on determinant), Ambirajan and Look²² (based on condition number and determinant), Sabatke et al.²⁴ (based on EWV and determinant), and Tyo⁴³ (based on condition number), among many others.

Modeling of \mathbb{W} with Eq. (1) implies that the transmittance and the degree of polarization of all rows of \mathbb{W} are equal to one. This hypothesis is frequently done in polarimetry, but it is interesting to consider the case where it is not fulfilled. In the general case, each row of the measurement matrix may have a different transmission $t_i, i \in [1, N]$, and a different degree of polarization $P_i, i \in [1, N]$. In this case, the measurement matrix can be expressed in the following form:

$$W = \frac{1}{2} \begin{bmatrix} t_1 & t_1 P_1 \mathbf{w}_1^T \\ t_2 & t_2 P_2 \mathbf{w}_2^T \\ \vdots & \vdots \\ t_N & t_N P_N \mathbf{w}_N^T \end{bmatrix} \triangleq \frac{1}{2} \begin{bmatrix} \mathbb{T} \mathbf{r} & \mathbb{TPQ} \end{bmatrix},$$
(29)

where $\mathbb{T} = \text{diag}(t_1, \ldots, t_N)$ and $\mathbb{P} = \text{diag}(P_1, \ldots, P_n)$. In this general form, it is easy to demon-

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118 strate that

$$\|\mathbb{W}\|^2 = \frac{1}{4} \sum_{i=1}^{N} (1 + P_i^2) t_i^2$$
(30)

¹¹⁹ Consequently, one can generalize Eq. (26) to:

$$\kappa = \frac{\sqrt{\sum_{i=1}^{N} (1 + P_i^2) t_i^2}}{2\sigma} \sqrt{\text{EWV}}$$
(31)

This entails a generalization of the result obtained in Section 3: for arbitrary, but fixed values 120 of transmissions and degree of polarization of the analysis vectors, optimization of the vectors' 121 positions on the normalized Poincaré sphere (i.e., of the vectors \mathbf{w}_n) yields the same result if the 122 condition number or the EWV are used as criteria. If, in addition, the transmissions and degree of 123 polarizations are identical for all the N measurements, it is easy to show that the resulting optimal 124 structures are spherical 2 designs. If they are not identical, the optimal structures are no longer the 125 spherical designs. Determining the optimal structures in this case is an interesting perspective to 126 the present work. 127

Another important practical question is which one of the three considered metrics is the most appropriate for evaluating the performance of any polarimeter, be it optimal or not. Indeed, on this point of view, the metrics are not equivalent. This is most easily seen by noticing that the three metrics only depend on the measurement matrix through the eigenvalues of \mathbb{G} , denoted $\mu_i, i \in$ [1, 4], and have the following form:

$$|\mathbb{G}| = \prod_{i=1}^{4} \mu_i \tag{32}$$

$$\kappa = \left(\sum_{i=1}^{4} \mu_i\right)^{1/2} \left(\sum_{i=1}^{4} \frac{1}{\mu_i}\right)^{1/2}$$
(33)

$$\text{EWV} = \sum_{i=1}^{4} \frac{1}{\mu_i} \tag{34}$$

It is seen that although they look similar, they are different. In particular, two different sets of 128 eigenvalues may lead to the same value of κ , but different values of $|\mathbb{G}|$ and EWV, and vice versa. 129 The question of how to choose the best metric could seem arbitrary, but we think there is a strong 130 objective argument in favor of EWV. Indeed, the EWV corresponds to an estimation variance, 131 which has a clear and useful statistical meaning. For example, it makes it handier to compare 132 two different polarimeter structures: saying that polarimeter A has a EWV twice than polarimeter 133 B just means that the variance of the estimated Stokes vector is twice. In sharp contrast, a ratio 134 between two determinants or two condition numbers is much less easy to interpret in terms of 135 estimation error. 136

Another strong advantage of the EWV is that it can be used for polarimeter optimization in the 137 presence of non-additive noises sources. The EWV has for example been used to derive the optimal 138 measurement frames in the presence of Poisson shot noise.^{39,40} In this case, the expression of the 139 covariance matrix of the Stokes estimate was different from Eq.(5). Consequently, the EWV was 140 different from Eq. (6), and was thus no longer proportional of the square of the condition number, 141 which had no statistical meaning. Furthermore, when measurements are simultaneously affected 142 by several types of statistically independent noise sources, the value of the EWV is simply the sum 143 of the EWVs corresponding to each noise source. This property has for example been recently 144 employed to characterize the actual performance of micro-grid based polarimetric cameras in the 145 presence of both additive detection noise and Poisson shot noise.⁴¹ 146

In conclusion, the message of the present work could be summarized as follows. When optimizing the estimation performance of a polarimeter in the presence of additive Gaussian noise, condition number, determinant, and EWV are three strictly equivalent metrics. When evaluating and comparing the performance of different polarimeters, or when optimizing polarimeters in the presence of non-additive, non-Gaussian noise sources, the EWV has strong advantages compared
with the two other metrics.

153 5 Conclusions

We have shown that optimization of the EWV, of the condition number, or of the determinant of the Gram matrix of a Stokes polarimeter leads to the same optimal measurement structures, namely, spherical 2 designs. These structures yield a very simple closed-form expression for the covariance matrix of the Stokes vector estimator, and thus of the variances of each element of the Stokes vector. These expressions constitute the fundamental limit of the estimation variance that can be reached by a Stokes polarimeter in the presence of additive noise.

As a conclusion, we would like to stress that although the three considered metrics are equivalent for polarimeter optimization in the presence of additive noise, the EWV has the simplest physical interpretation since it corresponds to an estimation variance, which has a clear and useful statistical meaning. As a consquence, in contrast to the two other metrics, the EWV can be used for polarimeter optimization in the presence of noise sources with non-additive, non-Gaussian, or mixed statistics.

¹⁶⁶ A very interesting perspective is the determination of the optimal measurement matrices in the ¹⁶⁷ presence of non-additive noise sources. As said above, this problem has already been addressed ¹⁶⁸ by optimizing the EWV obtained after application of the pseudo-inverse estimator.^{39,40} Although ¹⁶⁹ this procedure give satisfying results in practice,⁴² it is not strictly optimal. Indeed, in the presence ¹⁷⁰ of non additive and non Gaussian noise, by virtue of the Cramér-Rao lower bound, the appropriate ¹⁷¹ criterion is the trace of the inverse Fisher information matrix.^{17,18} The value of this criterion ¹⁷² corresponds to the EWV of an efficient estimator, which the pseudo-inverse estimator is not in general. An exciting perspective is to work at determining the measurement matrices optimizing
this Fisher criterion, and at analyzing the differences between the obtained optimal structures and
the spherical 2 designs.

176 Appendix A: Positivity of the third term of Eq. (15)

We demonstrate in this appendix that the third term of the expression of tr[\mathbb{G}^{-1}] in Eq. (15) is positive definite. Since the matrix $\mathbb{Q}^T \mathbb{Q}$ is by definition a positive matrix, the numerator of this term is also positive. We therefore need only analyse the denominator. Considering then the singular value decomposition $\mathbb{Q} = \mathbb{U}\mathbb{F}\mathbb{V}^T$, where \mathbb{U} and \mathbb{V} are unitary matrices and \mathbb{F} is diagonal, it is easily seen that

$$\mathbb{Q}(\mathbb{Q}^T \mathbb{Q})^{-1} \mathbb{Q}^T = \mathbb{U} \mathbb{F} \mathbb{U}^T$$
(35)

where $\mathbb{F} = \mathbb{D}(\mathbb{D}^T \mathbb{D})^{-1} \mathbb{D}^T$ is a diagonal $N \times N$ matrix. The first three diagonal elements of \mathbb{F} are unity, whereas the other elements are zero. We thus have

$$\mathbf{q}^{T}(\mathbb{Q}^{T}\mathbb{Q})^{-1}\mathbf{q} = \mathbf{v}^{T}\mathbb{F}\mathbf{v} = \sum_{i=1}^{3} v_{i}^{2}$$
(36)

where $\mathbf{v} = \mathbb{U}^T \mathbf{r}$ is an *N*-dimensional vector. Moreover

$$\sum_{i=1}^{3} v_i^2 \le \sum_{i=1}^{N} v_i^2 = \|\mathbf{v}\|^2 = \|\mathbf{r}\|^2 = N$$
(37)

since \mathbb{U} is a unitary matrix. Hence

$$\mathbf{q}^T(\mathbb{Q}^T\mathbb{Q})^{-1}\mathbf{q} \le N,\tag{38}$$

which means that the third term of Eq. (15) is positive.

Appendix B: Satisfying Eqs. (16) and (20) with spherical t designs

Consider a finite set of points $\{\mathbf{w}_j\}$ $(j \in [1, N])$, which lie on the surface of the three dimensional unit sphere. The set of points $\{\mathbf{w}_j\}$ are said to constitute a spherical *t* design if for *any* polynomial function $f(\mathbf{w})$ of order *t* or lower

$$\sum_{j=1}^{N} f(\mathbf{w}_j) = N \int f(\mathbf{w}) d\sigma_{\mathbf{w}},$$
(39)

where $d\sigma_{\mathbf{w}}$ is the normalized surface area element of the unit sphere.

Proof that Eqs. (16) and (20) can be satisfied using spherical 2 designs follows by showing that we can generate the constraints through appropriate choice of polynomial functions $f(\mathbf{w})$ of second order degree or less in Eq. (39). Considering first the case $f(\mathbf{w}) = w_s$ ($s \in [1,3]$), substitution into Eq. (39) yields

$$\sum_{j=1}^{N} w_{sj} = N \int w_s d\sigma_{\mathbf{w}}$$
(40)

where w_{sj} is the value of the *s*th element of \mathbf{w}_j . We can express \mathbf{w} in terms of the usual spherical polar coordinates, i.e., $\mathbf{w} = [\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta]^T$ such that $4\pi d\sigma_{\mathbf{w}} = \sin\theta d\theta d\phi$. It is then simple to show that $\int w_s d\sigma_{\mathbf{w}} = 0$ for $s \in [1,3]$ such that Eq. (40) reduces to Eq. (16). Similarly, using the polynomial function $f(\mathbf{w}) = w_s w_t$ for $\{s, t\} = \{1, 2, 3\}$ Eq. (39) becomes

$$\sum_{j=1}^{m} w_{sj} w_{tj} = N \int w_s w_t d\sigma_{\mathbf{w}}.$$
(41)

Evaluating the integral on the right hand side yields $\delta_{st}/3$, such that Eq. (41) reduces to Eq. (20), therefore completing our proof. Although we have proven that Eqs. (16) and (20) can be satisfied by a spherical 2 design, it is worthwhile to note that it automatically follows that they can also be satisfied by a spherical design of higher order, $t \ge 2$, because a spherical t design is also a t - 1design.

Appendix C: Previous derivation

The constraints derived in Section 2 through direct minimization of the EWV were first derived by Foreman et. al exploiting a claimed equivalence between minimizing the trace of \mathbb{G}^{-1} and maximizing the determinant of \mathbb{G} . Specifically, using the definition of the matrix inverse and Jacobi's formula it was first shown that the condition number can be expressed in the form³⁵

$$\kappa^{2} = \frac{N}{2} \operatorname{tr}[(\mathbb{W}^{T} \mathbb{W})^{-1}] = \frac{N}{2} \sum_{i=1}^{4} \frac{\partial \ln |\mathbb{G}|}{\partial G_{ii}}$$
(42)

where G_{ii} are the diagonal elements of \mathbb{G} . Based on Eq. (42) Foreman et al. claim that the equivalence of optimization metrics follows from the differential relation $2d \ln \kappa = -d \ln |\mathbb{G}|$. Regrettably this relation does not follow from Eq. (42), nor in fact does it hold in general, as can be seen by expressing both $\ln[tr[\mathbb{G}^{-1}]] = 2 \ln \kappa + \text{const.}$ and $\ln |\mathbb{G}|$ in terms of the eigenvalues of \mathbb{G} .

191	Discl	osures

¹⁹² The authors declare they have no conflicts of interest.

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