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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, however, frequently made on an *ad hoc* basis. We rigorously demonstrate that optimization strategies in Stokes polarimetry based on three common metrics, namely the Frobenius condition number of the instrument matrix, the determinant of the associated Gram matrix, or the equally weighted variance, are frequently formally equivalent. In particular, using each metric, we derive the same set of constraints on the measurement states, correcting a previously reported proof, and show that these can be satisfied using spherical 2 designs. Discussion of scenarios in which equivalence between the metrics breaks down is also given. Our conclusions are equally applicable to optimization of the illumination states in Mueller matrix polarimetry. © *2019 Society of Photo-Optical Instrumentation Engineers (SPIE)* [DOI: 10.1117/1.OE.58.8.082410]

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

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1 Introduction

Quantitative analysis of the state of polarization of light provides a powerful tool in modern science. Applications vary from microscopy, biomedical diagnosis, and astrophysics[1–3] to crystallographic, material, and single-molecule studies.[4,5] While the polarization state of light itself can be used to transmit information, hence presenting new opportunities in optical data storage and communications,[6–9] changes in polarization induced by a material can alternatively be used for object detection[10] 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 $\mathbf{S}$, comprise of N (≥ 4) distinct measurements that can be multiplexed in time,[14] frequency,[15] 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 vector $\mathbf{W}_j$, i.e., $I_j = \mathbf{W}_j^{\mathrm{T}}\mathbf{S}$. Central to the description and design of Stokes polarimeters is hence the so-called instrument or measurement matrix $\mathbb{W} = (\mathbf{W}_1, \mathbf{W}_2, \ldots,)^{\mathrm{T}}$ 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 (EWV),[24,25] and condition number.[21–23,25–29]

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

Recently, the equivalence of a number of optimization metrics, namely the EWV, the condition number of $\mathbb{W}$, and the determinant of the associated Gram matrix, was discussed by Foreman et al.[35] Additionally, Foreman et al. proved that a Stokes polarimeter is optimal (as characterized by these metrics) when the set of analysis states defines a spherical 2 design[36] on the unit Poincaré sphere. A re-examination of the equivalence between these metrics is, however, necessary due to an error in the proof presented in Ref. 35. The goal of this paper is, therefore, to provide a rigorous proof that the conclusions of Ref. 35 hold. Our derivations also elicit greater insight into the optimization of nonideal Stokes polarimeters, which is hence discussed. We additionally note that our results are equally applicable to optimization of the probing states used in Mueller matrix polarimetry due to the similar matrix structure of the problem.[31,37]

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:

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

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where $\mathbf{r}$ 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 while blackboard bold font denotes matrices. 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. Generalization of our results to arbitrary instrument matrices will be discussed in Sec. 4.

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

$$\mathbf{I} = \mathbb{W}\mathbf{S} + \boldsymbol{\Delta}, \tag{2}$$

where $\boldsymbol{\Delta}$ 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 $\mathbf{S}$ is obtained by

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

where

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

denotes the pseudoinverse matrix. The estimate $\hat{\mathbf{S}}$ is a random vector of mean $\mathbf{S}$ (i.e., the estimator is unbiased) and of covariance matrix[17,23,24]

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

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 $\mathbb{W}$ that minimizes the sum of these variances, i.e., the trace of $\mathbb{K}_{\mathbf{S}}$. The corresponding performance metric is called the EWV, i.e.,

$$\mathrm{EWV} = \mathrm{tr}(\mathbb{K}_{\mathbf{S}}) = \sigma^2 \mathrm{tr}(\mathbb{G}^{-1}), \tag{6}$$

where

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

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

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

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

The inverse of the Gram matrix can then be expressed in the form[38]

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

where the matrix

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

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

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

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

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

where $\mathbf{q} = \mathbb{Q}^{\mathrm{T}}\mathbf{r}$ is an N-dimensional vector. Upon using the identity[38]

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

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

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

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

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

where we have also used the cyclic property of the trace operation and the identity $\mathrm{tr}(\mathbb{X}\mathbf{q}^{\mathrm{T}}\mathbf{q}) = \mathbf{q}^{\mathrm{T}}\mathbb{X}\mathbf{q}$ for arbitrary $\mathbb{X}$.[38]

Noting that $N > 0$ and that $\mathbb{Q}^{\mathrm{T}}\mathbb{Q}$ is positive definite, it follows immediately that the first two terms in Eq. (15) are positive. We show in Sec. 6 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, i.e., when $\mathbf{q} = \mathbb{Q}^{\mathrm{T}}\mathbf{r} = \mathbf{0}$ or equivalently

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

Importantly, Eq. (16) expresses a polynomial constraint that must be satisfied by an optimal measurement matrix and is equivalent to that given in Eq. (4) of Ref. 35. When Eq. (16) holds, minimizing $\mathrm{tr}(\mathbb{G}^{-1})$ is equivalent to minimizing $\mathrm{tr}[(\mathbb{Q}^{\mathrm{T}}\mathbb{Q})^{-1}]$. This optimization has to be done under the constraint that the trace of the matrix $\mathbb{Q}^{\mathrm{T}}\mathbb{Q}$ 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

$$\mathrm{tr}(\mathbb{Q}^{\mathrm{T}}\mathbb{Q}) = \mathrm{tr}(\mathbb{Q}\mathbb{Q}^{\mathrm{T}}) = N. \tag{17}$$

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

$$\Psi(\mathbb{Q}) = \mathrm{tr}[(\mathbb{Q}^{\mathrm{T}}\mathbb{Q})^{-1}] - \mu[\mathrm{tr}(\mathbb{Q}^{\mathrm{T}}\mathbb{Q}) - N], \tag{18}$$

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

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

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 $\boldsymbol{\beta}$ 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

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

Equation (20) is the second set of polynomial constraints derived from Ref. 35. The form of the Gram matrix $\mathbb{G}$ that hence minimizes the EWV of the instrument matrix is thus

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

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

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

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

Finally, the conditions expressed by Eqs. (16) and (20) are satisfied when the set of measurement states on the normalized Poincaré sphere, defined by $\{\mathbf{w}_j\}$, $j \in [1, N]$, constitute a spherical 2 design (see Sec. 7 for a proof) 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 well-known examples of spherical 2 designs. A geometric scheme to construct optimal polarimeters for any even N, any factorable odd value of N, and for prime $N > 5$ has also been described in Ref. 35. Further examples of spherical designs and construction strategies can be found in Refs. 39–41. Critically, spherical 2 designs are known to exist for any $N \geq 4$, with the important exception of $N = 5$.[39,41] In the context of optimal polarimetry, this implies that for $N = 5$ the constraints described by Eqs. (16) and (20) cannot be fully satisfied. Recalling Eq. (15), this arises because the second and third terms cannot be simultaneously minimized. Although the resulting measurement states do not form a spherical 2 design, the sum of these two terms, and hence the EWV, can nevertheless be minimized yielding a value of $8.119\sigma^2$. The corresponding analysis states define a square pyramid inscribed by the unit Poincaré sphere.

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.

3.1 *Condition Number*

The condition number κ of the instrument matrix is defined by $\kappa = \|\mathbb{W}\|\|\mathbb{W}^+\|$, where $\mathbb{W}^+$ is the pseudoinverse matrix and $\| \cdots \|$ denotes the matrix norm. In principle, any choice of matrix norm can be made, however, within the context of polarimetry, the most common choices are those of either the 2-norm,[42,43] defined as the maximum singular value of $\mathbb{W}$, or the Frobenius norm,[27,35,43] given by[38]

$$\|\mathbb{P}\|_F = [\mathrm{tr}(\mathbb{P}^T\mathbb{P})]^{1/2} = [\mathrm{tr}(\mathbb{P}\mathbb{P}^T)]^{1/2}. \tag{23}$$

In general, the 2-norm and Frobenius norms for a matrix $\mathbb{W}$ satisfy the inequality: $\|\mathbb{W}\|_2 \leq \|\mathbb{W}\|_F \leq \sqrt{r}\|\mathbb{W}\|_2$, where r denotes the rank of $\mathbb{W}$. Equality is only achieved for a rank one matrix, which is insufficient in Stokes polarimetry since a rank four matrix is required to ensure that the polarization reconstruction problem is not underdetermined. Accordingly, it is important to note that the choice of matrix norm can affect the result of optimization as has also previously been reported.[43] In this paper, we exclusively consider the Frobenius norm (and henceforth drop the subscript F). This selection is motivated by the resulting equivalence between the condition number and EWV. To prove this equivalence [for polarimeters with instrument matrix of the form of Eq. (1)], we first note that our choice of normalization of the measurement states $\mathbf{W}_j = [1, \mathbf{w}_j]^T/2$ implies that

$$\|\mathbb{W}\|^2 = \mathrm{tr}(\mathbb{W}^T\mathbb{W}) = \frac{N}{2}. \tag{24}$$

Moreover, using the definition of the pseudoinverse and EWV given by Eqs. (4) and (6) respectively, it is easily shown that

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

Consequently, one can write

$$\kappa = \sqrt{\frac{N}{2\sigma^2}\mathrm{EWV}}. \tag{26}$$

For any polarimeter with a measurement matrix of the form of Eq. (1), the condition number is thus simply proportional to the square root of the EWV (regardless of whether Eqs. (16) and (20) hold or not). It is thus evident that minimizing the condition number, defined in terms of the Frobenius norm, is equivalent to minimizing the EWV. Accordingly, the minimum condition number is $\kappa = \sqrt{20} \approx 4.472$ except for the $N = 5$ case where the minimum condition number is found to be ≈ 4.505.

3.2 *Determinant of the Gram Matrix*

The first works on Stokes polarimeter optimization considered devices with a minimal number ($N = 4$) of measurement vectors.[26] Optimization of such systems used the determinant of the matrix $\mathbb{W}$ (which for this value of N is square and nonsingular) as a performance metric. In this case, the optimal structure found dictated that the measurement vectors defined a regular tetrahedron on the Poincaré sphere, a result that we also found above by optimizing the EWV. We show in this section that this result comes from the strict equivalence of these two optimization metrics. This equivalence can be generalized to any value of N if one considers the optimization of the determinant of the Gram matrix $\mathbb{G}$ since for $N > 4$ the matrix $\mathbb{W}$ itself is rectangular and its determinant is thus not defined. Notice that this equivalence was mentioned in Ref. 35, but there was an erroneous step in the logic presented in that work (see Sec. 8 for more details).

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]

$$|\mathbb{G}| = |A - \mathbf{B}^{\mathrm{T}}\mathbb{D}^{-1}\mathbf{C}||\mathbb{D}| = \frac{1}{256}[N - \mathbf{r}^{\mathrm{T}}\mathbb{Q}(\mathbb{Q}^{\mathrm{T}}\mathbb{Q})^{-1}\mathbb{Q}^{\mathrm{T}}\mathbf{r}]|\mathbb{Q}^{\mathrm{T}}\mathbb{Q}|. \tag{27}$$

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

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

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

Following the standard optimization procedure we find, similarly to Sec. 2, that $\beta_j = 1/\mu = N/3$ for all $j \in [1,2,3]$. As shown in Sec. 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 Frobenius 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.

4 Discussion

The main conclusion from the analysis presented in the Secs. 2 and 3 is that among all measurement matrices of the form described by Eq. (1), those that maximize the condition number, the EWV and the determinant are exactly the same. Our result can thus be said to unify many previous works on polarimeter optimization, e.g., the early work of Azzam et al.[26] (which optimized based on the instrument matrix determinant), Ambirajan and Look[22] (based on the condition number and determinant), Sabatke et al.[24] (based on the EWV and determinant), and Tyo[44] (based on condition number), among many others.

Modeling of $\mathbb{W}$ based on Eq. (1) implies that the transmittance of each polarization analyzer and the degree of polarization of the transmitted light are both equal to one. This assumption is frequently made in polarimetry, however, it is interesting to consider the case where it is not fulfilled. In the general case, each analyzer, as described by each row of the measurement matrix, may have a different transmission t_i, $i \in [1, N]$, and a different resulting degree of polarization P_i, $i \in [1, N]$, such that the measurement matrix can be expressed in the form:

$$\mathbb{W} = \frac{1}{2}\begin{bmatrix} t_1 & t_1P_1\mathbf{w}_1^{\mathrm{T}} \\ t_2 & t_2P_2\mathbf{w}_2^{\mathrm{T}} \\ \vdots & \vdots \\ t_N & t_NP_N\mathbf{w}_N^{\mathrm{T}} \end{bmatrix} \triangleq \frac{1}{2}(\mathbb{T}\mathbf{r} \quad \mathbb{T}\mathbb{P}\mathbb{Q}), \tag{29}$$

where $\mathbb{T} = \mathrm{diag}(t_1, \ldots, t_N)$ and $\mathbb{P} = \mathrm{diag}(P_1, \ldots, P_n)$ are diagonal matrices. It is easy to demonstrate that this general form yields

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

Consequently, one can generalize Eq. (26) to

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

Notably, Eq. (31) allows us to generalize the result obtained in Sec. 3. Specifically, when the transmission and degree of polarization of each analysis vector is fixed (albeit arbitrary), optimization of the positions of the analysis state vectors on the normalized Poincaré sphere (i.e., of $\mathbf{w}_n$) yields the same result regardless of whether the condition number or the EWV is used as the performance metric. The EWV, however, also depends on the transmission and polarization factors (t_i and P_i), such that this equivalence breaks down when P_i and t_i are not fixed for each individual measurement. Letting $\mathbf{t} = \mathbb{T}\mathbf{r}$, $\mathbb{Y} = \mathbb{T}\mathbb{P}\mathbb{Q}$, and $\mathbf{y} = \mathbb{Y}\mathbf{t}$, by following a similar logic to Sec. 2 it can be shown [in analogy to Eq. (15)] that

$$\mathrm{EWV} = 4\sigma^2\left\{\frac{1}{T} + \mathrm{tr}[(\mathbb{Y}^\mathrm{T}\mathbb{Y})^{-1}] + \frac{\mathbf{y}^\mathrm{T}[T(\mathbb{Y}^\mathrm{T}\mathbb{Y})^{-2} + (\mathbb{Y}^\mathrm{T}\mathbb{Y})^{-1}]\mathbf{y}}{T[T - \mathbf{y}^\mathrm{T}(\mathbb{Y}^\mathrm{T}\mathbb{Y})^{-1}\mathbf{y}]}\right\}, \tag{32}$$

where $T = \mathbf{t}^\mathrm{T}\mathbf{t} = \sum_{i=1}^{N} t_i^2$. When the transmittances and degrees of polarization are identical (and fixed) for all N measurements (i.e., $t_i = \tau$ and $P_i = \rho$ for all i), it follows that

$$\mathrm{EWV} = \frac{4\sigma^2}{\tau^2}\left\{\frac{1}{N} + \frac{1}{\rho^2}\mathrm{tr}[(\mathbb{Q}^\mathrm{T}\mathbb{Q})^{-1}] + \frac{\mathbf{q}^\mathrm{T}[(N/\rho^2)(\mathbb{Q}^\mathrm{T}\mathbb{Q})^{-2} + (\mathbb{Q}^\mathrm{T}\mathbb{Q})^{-1}]\mathbf{q}}{N[N - \mathbf{q}^\mathrm{T}(\mathbb{Q}^\mathrm{T}\mathbb{Q})^{-1}\mathbf{q}]}\right\}, \tag{33}$$

and the resulting optimal structures found upon minimization of Eq. (33) are once again spherical 2 designs. The minimum EWV in this case is $4\sigma^2(1 + 9\rho^{-2})/(\tau^2 N)$, corresponding to a condition number of $\kappa = \sqrt{(1 + \rho^2)(1 + 9\rho^{-2})}$. Determining the optimal structures for the more general case (which are not spherical designs) is, however, an interesting question that remains as future work.

Another important practical question is which of the three considered metrics is the most appropriate for evaluating the performance of a polarimeter under more general conditions. Indeed, from this point of view, the metrics are not necessarily equivalent, particularly in complex noise regimes or when nonideal polarization state analyzers are used. This is most easily seen by noting that the three metrics can be expressed in the form:

$$|\mathbb{G}| = \prod_{i=1}^{4}\nu_i, \tag{34}$$

$$\kappa = \left(\sum_{i=1}^{4}\nu_i\right)^{1/2}\left(\sum_{i=1}^{4}\frac{1}{\nu_i}\right)^{1/2}, \tag{35}$$

$$\mathrm{EWV} = \sum_{i=1}^{4}\gamma_i, \tag{36}$$

where ν_i, $i \in [1,4]$ denote the eigenvalues of $\mathbb{G}$ and γ_i are the eigenvalues of the covariance matrix $\mathbb{K}_\mathbf{S}$. While in the presence of additive white noise $\mathbb{K}_\mathbf{S}$ takes the form given by Eq. (5) such that $\gamma_i = \sigma^2/\nu_i$, for more general noise regimes the form of the covariance matrix is more complex viz.

$$\mathbb{K}_\mathbf{S} = \mathbb{G}^{-1}\mathbb{W}^\mathrm{T}\mathbb{K}_\mathbf{I}\mathbb{W}\mathbb{G}^{-\mathrm{T}}, \tag{37}$$

where $\mathbb{K}_\mathbf{I}$ is the covariance matrix of the measured intensities. Although the form of each metric is similar, there are nevertheless important differences. In particular, two different sets of eigenvalues $\{\nu_i\}$ may lead to the same value of κ, but different values of $|\mathbb{G}|$ and EWV, and vice versa. This is most obvious when the noise variances on each detector are unequal, however, it can also result in the case of depolarizing or partially transmitting polarization analyzers due to the different parametric dependencies of Eqs. (34)–(36). The question of how to choose the best metric is, therefore, somewhat arbitrary; however, we argue that there is a strong objective advantage to use of the EWV. Indeed, the EWV corresponds to an estimation variance, which has a clear and useful statistical meaning. For example, it enables easy comparison of two different polarimeter structures: saying that polarimeter A has an EWV double that of polarimeter B signifies that the variance of the estimated Stokes vector is twice as large. In sharp contrast, a ratio of matrix determinants or condition numbers is more difficult to interpret in terms of estimation errors.

Another strong advantage of the EWV is that it can be used for polarimeter optimization in the presence of nonadditive noises sources. The EWV has been used to determine the optimal measurement frames in the presence of Poisson shot noise.[45,46] In this case, the covariance matrix of the Stokes estimate takes a different form to that of Eq. (5). Consequently, the EWV is no longer given by Eq. (6), and thus not proportional to the square of the condition number. Furthermore, when measurements are simultaneously affected by several types of statistically independent noise sources, the total EWV is simply the sum of the individual EWVs for each noise source. This additive property has been recently employed to characterize the actual performance of microgrid-based polarimetric cameras in the presence of both additive detection noise and Poisson shot noise.[47]

In conclusion, the key finding of the present work is that when optimizing the estimation performance of a polarimeter in the presence of additive Gaussian noise, the Frobenius condition number of the instrument matrix, the Gram determinant, and EWV are three strictly equivalent metrics. When evaluating and comparing the performance of different polarimeters however, or when optimizing polarimeters in the presence of nonadditive, non-Gaussian noise sources, the EWV has strong advantages compared with the other two metrics.

5 Conclusions

We have shown that optimization of the EWV, of the Frobenius 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 consequence, in contrast to the two other metrics, the EWV can be used for polarimeter optimization in the presence of noise sources with nonadditive, non-Gaussian, or mixed statistics. As discussed above, this problem has already been addressed by optimizing the EWV obtained after application of the pseudoinverse estimator.[45,46] Although this procedure gives satisfying results in practice,[48] it is not strictly optimal. Indeed, in the presence of nonadditive and non-Gaussian noise, by virtue of the Cramér-Rao lower bound, the appropriate criterion is the trace of the inverse Fisher information matrix.[17,18] The value of this metric corresponds to the EWV of an efficient estimator (where "efficient" is meant here in the precise sense used in estimation theory[49]), whereas in general the pseudoinverse estimator is not efficient. The interesting problem of analyzing the differences between the optimal measurement structures found using a Fisher information-based metric and the spherical 2 designs remains as future work.

6 Appendix A: Positivity of the Third Term of Eq. (15)

We demonstrate in this section that the third term of the expression of $\mathrm{tr}(\mathbb{G}^{-1})$ 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 analyze 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

$$\mathbb{Q}(\mathbb{Q}^T\mathbb{Q})^{-1}\mathbb{Q}^T = \mathbb{U}\mathbb{F}\mathbb{U}^T, \tag{38}$$

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

$$\mathbf{q}^T(\mathbb{Q}^T\mathbb{Q})^{-1}\mathbf{q} = \mathbf{v}^T\mathbb{F}\mathbf{v} = \sum_{i=1}^{3} v_i^2, \tag{39}$$

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

$$\sum_{i=1}^{3} v_i^2 \le \sum_{i=1}^{N} v_i^2 = \|\mathbf{v}\|^2 = \|\mathbf{r}\|^2 = N, \tag{40}$$

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

$$\mathbf{q}^T(\mathbb{Q}^T\mathbb{Q})^{-1}\mathbf{q} \le N, \tag{41}$$

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

7 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:

$$\sum_{j=1}^{N} f(\mathbf{w}_j) = N \int f(\mathbf{w}) \mathrm{d}\sigma_{\mathbf{w}}, \tag{42}$$

where $\mathrm{d}\sigma_{\mathbf{w}}$ 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. (42). Considering first the case $f(\mathbf{w}) = w_s$ ($s \in [1,3]$), substitution into Eq. (42) yields:

$$\sum_{j=1}^{N} w_{sj} = N \int w_s \mathrm{d}\sigma_{\mathbf{w}}, \tag{43}$$

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 $4\pi\mathrm{d}\sigma_{\mathbf{w}} = \sin\theta \mathrm{d}\theta\,\mathrm{d}\phi$. It is then simple to show that $\int w_s \mathrm{d}\sigma_{\mathbf{w}} = 0$ for $s \in [1,3]$ such that Eq. (43) reduces to Eq. (16). Similarly, using the polynomial function $f(\mathbf{w}) = w_s w_t$ for $\{s,t\} = \{1,2,3\}$, Eq. (42) becomes:

$$\sum_{j=1}^{N} w_{sj}w_{tj} = N \int w_s w_t \mathrm{d}\sigma_{\mathbf{w}}. \tag{44}$$

Evaluating the integral on the right-hand side yields $\delta_{st}/3$, such that Eq. (44) 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 $t-1$ design.

8 Appendix C: Previous Derivation

The constraints derived in Sec. 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 form:[35]

$$\kappa^2 = \frac{N}{2}\mathrm{tr}[(\mathbb{W}^T\mathbb{W})^{-1}] = \frac{N}{2}\sum_{i=1}^{4}\frac{\partial \ln|\mathbb{G}|}{\partial G_{ii}}, \tag{45}$$

where G_{ii} are the diagonal elements of $\mathbb{G}$. Based on Eq. (45), Foreman et al. claim that the equivalence of optimization metrics follows from the differential relation $2\mathrm{d}\ln\kappa = -\mathrm{d}\ln|\mathbb{G}|$. Regrettably, this relation does not follow from Eq. (45), nor in fact does it hold in general, as can be seen by expressing both $\ln[\mathrm{tr}(\mathbb{G}^{-1})] = 2\ln\kappa + \mathrm{const.}$ and $\ln|\mathbb{G}|$ in terms of the eigenvalues of $\mathbb{G}$.

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