Permitted experimental errors for optimized variable-retarder Mueller-matrix polarimeters

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Abstract: An optimized Mueller-matrix polarimeter is simulated. The polarimeter is optimized by finding the configurations of the polarization state generator and polarization state analyzer that give the minimum condition number. Noise is included in the measurement of the polarimeter intensities, and the eigenvalue calibration procedure is used to reduce the errors in the final Mueller matrix. Controlled errors are introduced to the polarimeter configuration, and the error in the final measured Mueller matrix is calculated as a function of these configuration errors. It is found that the alignment of the retarder axes in the polarimeter is much more important than the use of the ideal, optimized retardance values. In particular, the misalignment of the retarders farthest from the sample is the error source with the highest impact in the precision of the polarimeter.

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1. Introduction

The complete polarization characterization of a sample is its Mueller matrix $M$, defined by the relationship between a Stokes vector incident on the sample, $S^{\text{inc}}$, and the corresponding Stokes vector leaving the sample, $S^{\text{det}}$; $S^{\text{det}} = MS^{\text{inc}}$ [1]. A typical Mueller matrix polarimeter, and in particular a variable-retardance Mueller-matrix polarimeter, which is the polarimeter type studied in this paper, and is shown schematically in Fig. 1, measures the Mueller matrix of the sample by constructing a minimum of 16 different and independent combinations of incident and detected Stokes vectors and detecting the intensity in the first element of $S^{\text{det}}$ [2–14]. This is performed by constructing a polarization state generator (PSG) to create the polarization states $S^{\text{inc}}$ of the light before the sample, and a polarization state analyzer (PSA) to project the desired polarization states $S^{\text{det}}$ to the detected intensity.

For the general case of $N$ incident polarization states and $N$ detected polarization states, the characteristic matrices of the polarimeter can be constructed [2]:

$$P^{\text{inc}} = \begin{pmatrix} S^{\text{inc}1} & S^{\text{inc}2} & \ldots & S^{\text{inc}N} \end{pmatrix}$$

$$P^{\text{det}} = \begin{pmatrix} S^{\text{det}1} & S^{\text{det}2} & \ldots & S^{\text{det}N} \end{pmatrix}$$

Tyo [11] showed that the propagation of the experimental errors from the measured intensity values for each of the PSG and PSA combinations is determined by the condition numbers, $\kappa^{\text{inc}}$, of $P^{\text{inc}}$, and $\kappa^{\text{det}}$, of $P^{\text{det}}$, where the condition number is defined as the ratio of the largest singular value of the characteristic matrix divided by the smallest singular value of the characteristic matrix. For a measurement configuration to be optimized, both $\kappa^{\text{inc}}$ and $\kappa^{\text{det}}$ must be as small as possible, and Tyo showed that, for $N = 4$, the minimum condition number is $\kappa = \sqrt{3} = 1.7321$.

To measure a Mueller matrix, at least 16 intensities must be measured, the Mueller matrix must be reconstructed, and finally a calibration step [12] should be performed to remove errors and polarization effects of other optical components in the polarimeter (for example, lenses or beam splitters). The errors in the final Mueller matrix can be caused by noise in the intensity measurements or by errors in the experimental setup for the polarimeter, which could be, for example, errors in the angular positions of the axes of the retarders or polarizers or errors in the retardances. We assumed no azimuth-angle errors in the polarization components, as they are simpler to detect from the direction of the reflected beam.

Fig. 1. Experimental setup for a Mueller-matrix polarimeter. The angles associated with each component refer to the relative angle of the optical axis of that component with respect to the horizontal plane.

Variable-retardance liquid-crystal polarimeters have some advantages over other options: cost, size and weight, and very low voltage requirements, and we have been studying them for...
applications in scatterometry [9]. For this reason we study this type of polarimeter in this paper.

In this paper, numerical simulations are performed to estimate the errors in the measured Mueller matrix, including different levels of noise in the intensity measurements and errors in the experimental implementation of the polarimeter, with the aim of finding the acceptable limits in the experimental polarimeter errors for given levels of noise in the intensity measurements and the limits of applicability of the full data-extraction process. Although it is possible to use other metrics, particularly based on singular value decomposition in polarimeters with error sources [15], we used the condition number as it has proved to be very stable and is one of the most used in the literature. In section 2 the steps in the simulation are described, and results are presented in section 3. Finally section 4 includes the discussion and conclusions of this work.

2. Simulation

The polarimeter was assumed to be of the form shown in Fig. 1. For a given sample, the intensity detected for any configuration of the polarimeter can be calculated using the Mueller matrices of the components:

\[ S_{\text{out}} = M^{\text{PSA}} M^S M^{\text{PSG}} S_{\text{in}}, \]  

(3)

where \( M^S \) is the Mueller matrix of the sample, \( S_{\text{in}} \) is the Stokes vector of the incident laser light, and \( M^{\text{PSA}} \) and \( M^{\text{PSG}} \) are the Mueller matrices of the PSA and PSG, respectively, and are given by

\[ M^{\text{PSG}} = M^{R2} M^{R1} M^{P1}, \]  

(4)

\[ M^{\text{PSA}} = M^{R2} M^{R4} M^{R3}, \]  

(5)

where \( M^{P_i} \) is the Mueller matrix for the \( i \)th polarizer. It is assumed that the polarizers are perfect linear polarizers, so that the Mueller matrices for these elements only depend on the angles of the transmission axes with the horizontal. In the simulation, the transmission axes are taken to be exactly horizontal for all cases (i.e. no errors of the alignment of the polarizers is taken into account). The \( M^{R_j} \) are the Mueller matrices of the retarders, and they depend on the retardance values of the retarders and the angles of the fast axes with respect to the horizontal. The simulation includes errors in the two retardance values and the two fast-axis positions used (see below).

The polarimeter was optimized following the procedure discussed by DeMartino, Smith and Tyo, and associates [6,7,11]. This process involves numerically sampling the polarimeter parameters, retardance values and retarder fast-axes positions, over the full range of their possible values, and calculating the condition number for each configuration. The cases with the minimum value of condition number are stored, to be used as the base values in the error-analysis simulation. The values of the optimized polarimeter for the retarder fast-axes positions were chosen to be [6]

\[ \theta_1 = \theta_4 = 27.4^\circ, \]  

(6)

\[ \theta_2 = \theta_3 = 72.4^\circ, \]  

(7)

where the subindex indicates which retarder the axis position refers to, and the retardance values used in the PSG and the PSA are given by the sequence
with $\Delta_1 = 135^\circ$ and $\Delta_2 = 315^\circ$. This setup gives an optimized polarimeter. The errors introduced in the polarimeter were the same in the PSG and the PSA, i.e. there was one error associated with $\theta_1$ and $\theta_4$, one error associated with $\theta_2$ and $\theta_3$, and an error in each of $\Delta_1$ and $\Delta_2$. It is important to note that we assume only these systematic errors in the polarimeter parameters, there is no random error contribution. In this sense the simulations presented here are limited, but we believe they give a very good indication of the limitations in the whole data-extraction process, including the eigenvalue calibration.

Once the intensities are measured in the polarimeter, the sample Mueller matrix must be reconstructed [2]. This is valid for the calibration Mueller matrices, which we calculate here as a measure of the quality of the polarimeter, or for an unknown sample. The matrix calculated here is the raw, uncalibrated sample Mueller matrix. From Eq. (3), assuming unpolarized light incident, the first element of $S_{\text{out}}$, which corresponds to the total detected intensity, can be written

$$S_{\text{out}} = \sum_{i=1}^{4} \sum_{j=1}^{4} M_{ij}^{\text{PSA}} M_{ji}^{\text{PSG}} M_{ij}^S,$$  

(9)

where the subindices indicate the element of the Stokes vector or Mueller matrix.

Changing the Mueller matrix $M_{ij}$ into a 16x1 column vector

$$M^T = \begin{pmatrix} M_{11}^S & M_{12}^S & M_{13}^S & M_{14}^S & M_{21}^S & \cdots & M_{44}^S \end{pmatrix},$$

(10)

and defining a row vector

$$W^I = \begin{pmatrix} M_{11}^{\text{PSA}} M_{11}^{\text{PSG}} & M_{12}^{\text{PSA}} M_{12}^{\text{PSG}} & M_{13}^{\text{PSA}} M_{13}^{\text{PSG}} & M_{14}^{\text{PSA}} M_{14}^{\text{PSG}} & M_{21}^{\text{PSA}} M_{21}^{\text{PSG}} & \cdots & M_{44}^{\text{PSA}} M_{44}^{\text{PSG}} \end{pmatrix},$$

(11)

where the superindex $I$ indicates the first combination of retardances in the polarimeter, Eq. (9) can be written

$$S_{\text{out}}^{\text{raw}} = W^I M^T.$$

(12)

Now, an equation of the form of Eq. (12) can be written for every one of the 16 combinations of retardances in the polarimeter described by Eq. (8):
and this equation can be written in the form

\[ I = W M^{s} \],

with

\[
\begin{pmatrix}
S_{1}^{\text{out}1} \\
\vdots \\
S_{1}^{\text{out}16}
\end{pmatrix}
= \begin{pmatrix}
W^{1} \\
\vdots \\
W^{16}
\end{pmatrix}
\]

(13)

\[ W = \begin{pmatrix}
W^{1} \\
\vdots \\
W^{16}
\end{pmatrix} \]

(16)

Then, the matrix \( M^{s} \) can be found from

\[ M^{s} = W^{-1} I. \]

(17)

The column vector \( M^{s} \) can be reordered to give the reconstructed 4x4 Mueller matrix \( M_{z} \).

To simulate noise in the measurements, we added a random value to each element of the signal vector \( I \) taken from a Gaussian random distribution with a standard deviation given by a fixed percentage of each signal value. The percentage value of the standard deviation was in the range 0.5% to 5%.

The measured Mueller matrix must be corrected for errors by using a calibration procedure. The calibration scheme used in this paper is that of Compain [12–14], which is a very robust, general calibration procedure. This method requires four known samples to be measured. The samples used were [12]: no sample (transmission in air), a horizontal linear polarizer, a vertical linear polarizer and a quarter-wave plate with its fast axis at 30° to the horizontal.

The simulation follows the procedure described here:

1. The matrix \( W \) is calculated using Eqs. (11) and (13) assuming an ideal system with the parameters given by Eqs. (6)-(8).

2. The experimental errors in the polarimeter are simulated by introducing errors in the parameters of the retarder axes positions and the retardances used in the polarimeter. One combination of the error values are systematically chosen from an evenly-spaced distribution of values in a predefined range. The condition number for the polarimeter with this combination of errors is calculated.
3. The detected intensities for the simulated polarimeter, including the errors in the parameters, are calculated for the calibration samples (no sample, a horizontal linear polarizer, a vertical linear polarizer and a quarter-wave plate with its fast axis at 30° to the horizontal), for the 16 combinations of PSG and PSA retardances. Although the selection of the calibration samples can also be optimized [16], this was not performed here.

4. A noise term is added to the 16 calculated signals as described above.

5. The Mueller matrices for the four calibration samples are reconstructed using Eq. (17) and the ideal polarimeter parameters.

6. The reconstructed calibration sample Mueller matrices are used in the Compain calibration method to correct these same calibration sample Mueller matrices.

7. The rms differences between the expected and calculated Mueller matrices are calculated for the reconstructed Mueller matrices before and after the calibration process, and the total rms error is calculated using the formula

\[
\text{rms} = \frac{1}{64} \sqrt{\sum_{N} \sum_{i=1}^{4} \sum_{j=1}^{4} (M_{ij}^{N} - M_{ij}^{\text{theory}})^2},
\]

where the subindex \( N \) indicates the matrices for each of the four calibration samples, and \( M_{ij}^{\text{theory}} \) is the theoretically expected Mueller matrix for the known sample. Note that in the absence of intensity measurement noise the Compain calibration recovers the simple Mueller matrix exactly, independently of the systematic polarimeter errors. However, including noise in the intensity measurements, which will always be the case in experiments, the systematic errors in the polarimeter configuration are coupled to the intensity noise, thus affecting the noise in the final Mueller matrix, Eq. (18), and meaning that the eigenvalue calibration process does not recover the sample Mueller matrix exactly. So, the results are obtained as rms differences (errors) in the calculated (step 5. above) and calibrated (step 6. above) Mueller matrices as a function of the condition number of the polarimeter with errors.

8. Return to point 2 with different values of the polarimeter parameters, and repeat to cover the desired range of parameter values.

In the results presented in this paper we used a range of \( \pm 20° \) in each of the parameters of the polarimeter (two axes angles and two retardance values), with a step of \( 2° \), giving a total of \( 21^4 = 194481 \) sample points for each case studied. This error range was found to be adequate for the possible systematic axes errors found in the characterization of our liquid-crystal variable retarders [17] and in the retardance errors due to temperature and voltage variations. They also allowed us to have accurate fits to Gaussian functions to obtain estimations of the overall error limits for each parameter. The equations were programmed in MatLab and took approximately 2 hours per case on a computer working at 3.4GHz. We also checked that the simulation gave perfect results for the case of perfect (no noise) intensity measurements for any value of the system parameters, after the eigenvalue calibration procedure.

3. Results

First of all, in Fig. 2, we present results of the rms error in the reconstructed Mueller matrices after the calibration process as a function of the condition number of the system with errors, for different noise levels in the measured intensity data. Each point in the graphs corresponds to the simulation result for a particular configuration of the polarimeter parameters.
The graphs in Fig. 2 correspond to measurement error levels of 0.5%, 1.5% and 5%, from top to bottom, respectively. For each value of condition number, there are various values of the total rms error, corresponding to different combinations of the polarimeter parameters which give the same condition number. It can be seen that for values of the condition number close to the optimum value of $\kappa = 1.7321$ the total rms values are tightly grouped around a very small value, whereas, when the condition number is larger the total rms values cover a much wider range of values, indicating that for these cases the final result of the polarimeter data-extraction process depends on the particular configuration of the polarimeter. It can also be seen that for higher error levels in the intensity measurements, the total rms error in the final results increases faster with an increase in the condition number of the polarimeter with errors. To quantify this increase, we estimated the condition numbers that guarantee that the total rms error was lower than given values. This data was obtained from the total rms error as a function of condition number, ordering the data in ascending total rms error, and analysing the condition number data for values of the total rms error from 0 up to the given maximum value. In Fig. 2 these limits are shown in gray lines. The horizontal grey lines show the values of the total rms error of 0.02, 0.05 and 0.10 (as examples chosen from a previous study of the errors, showing that an rms error of 0.02 gives a maximum percentage error of less than 1%, and an rms error of 0.1 gives a maximum percentage error of more than 50% in the final Mueller matrix), and the vertical gray lines indicate the maximum value of condition number which guarantees a total rms error equal to or below the desired total rms value. That is, above the condition number indicated the total rms value may be above or below the desired value, depending on the specific polarimeter configuration, whereas below this condition number the total rms value is always on or below the desired value.

In Fig. 3 we show the limiting condition numbers for total rms errors of 0.02, 0.05 and 0.10. These curves show that, as the intensity measurement error increases the range of acceptable condition numbers for the polarimeter, for a fixed acceptable final rms error, decreases. The next step is to relate the limiting condition numbers to the experimental configuration errors in the polarimeter.

The data shown in Fig. 2 relate the particular values of the polarimeter parameters to the value of the condition number for that configuration. Thus, taking all the polarimeter configurations giving a condition number less than a given limiting value, all the values of the polarimeter parameters can be analyzed to find the range of each of the parameters which is permitted for that limiting condition number. Here, we calculated the frequency distribution of the values of the two retarder values $\delta_{1,4}$ and $\delta_{2,3}$, and the two retarder axes positions $\theta_{1,4}$ and $\theta_{2,3}$ for two values of condition number.

Figure 4 shows the frequency values (frequency of occurrence of the given parameter values in the data limited by condition number). In this figure, the points are the frequency values calculated from the simulation results, and the lines are fits of Gaussian functions to these frequency values, to calculate the width of the distributions, which is given by the separation from the centre of the Gaussian at which the curve falls to $1/e$ of the maximum. Figure 5 shows the $1/e$ width of the Gaussian fits shown in Fig. 4, as a function of the condition number of the polarimeter with errors.

The $R^2$ parameter of the fits was above 0.97 for all cases for $\delta_{1,4}$, $\delta_{2,3}$ and $\theta_{2,3}$, and was between 0.91 and 0.98 for the case of $\theta_{1,4}$, because of the slightly non-Gaussian shape of the distribution of this parameter which can be seen in Fig. 4. As expected, a larger condition number shows a wider range of permitted error values for the polarimeter parameters.
Fig. 2. Values of the total rms error after the data-extraction and calibration process for polarimeters with errors and noise, for noise levels of 0.5% (top graph), 1.5% (middle graph) and 5% (bottom graph). Each point on a graph represents the simulation results for a particular configuration of the polarimeter with errors. The gray lines show the limiting values of condition number for given values of the total rms error.
Fig. 3. Graph of the estimated limiting condition number for different values of the error level in the measured intensity data, and for different levels of the desired limiting total rms level in the final Mueller matrix.

Fig. 4. The distribution of values of each of the four polarimeter parameters from the simulation for two values of the limiting condition number: \( \delta_{1,4}, \) filled squares; \( \delta_{2,3}, \) open circles; \( \theta_{1,4}, \) filled upward triangles, and \( \theta_{2,3}, \) open downward triangles. The points are the frequency values calculated from the simulation results, and the lines are fits of Gaussian functions to these frequency values.
From Fig. 5, it can be seen that the retarder axes positions have a smaller range of permitted values than the retardance values for all the condition numbers studied. In fact, the two retardance values have almost the same permitted range of values over the whole interval of condition numbers studied, the acceptable ranges for the axes of the retarders $R_2$ and $R_3$, which are the retarders closest to the sample, are a factor of between 2 and 3 smaller than the range for the retardances, and the axes of the retarders $R_1$ and $R_4$, have the smallest permitted range of a factor of between 5 and 9 times smaller than the range for the retardances, i.e. any value of the condition number of the experimental system with errors, the correct alignment of the retarder axes, particularly for $R_1$ and $R_4$, has a tighter tolerance than the use of the correct retardance values. It is interesting that Tyo [18] found that the axis position errors are also critical in a rotating-retarder Stokes polarimeter. As an example, for a condition number of 7, the retardance values have a permitted range of $\pm 90^\circ$ around the optimized values, whereas the retarder axes angles for $R_2$ and $R_3$ have to be within a range of $\pm 30^\circ$, and the axes angles of $R_1$ and $R_4$ have to be in the much smaller range of $\pm 10^\circ$ around the designed angles.

Finally, Fig. 6 shows the combination of Figs. 3 and 5, which gives the permitted experimental error ranges for each of the polarimeter parameters, for a given noise level in the intensity measurements and a given value of total rms error in the final calculated Mueller matrix after the calibration procedure has been performed.

![Fig. 5. The 1/e width of the frequency distributions of the acceptable polarimeter parameter errors as a function of condition number from a Gaussian fit to the simulation data for each limiting condition number](image-url)
Fig. 6. Permitted polarimeter parameter errors, in each of the four polarimeter parameters, as a function of the percentage errors in the intensity measurements for given required total rms errors in the final, calibrated Mueller matrix

4. Conclusions

We have shown results of simulations of a Mueller-matrix polarimeter including noise in the measurement of the intensity and errors in the experimental setup. The eigenvalue calibration procedure was also included in the simulation to give a realistic measurement result. The ideal polarimeter was optimized so that the PSA and PSG had the minimum condition number of $\sqrt{3}$. This optimized polarimeter has four parameters: two retardance values and two angular positions of retarder axes. Analyzing the simulation results, it was found that the permitted error in the retardance values, for a given noise level in the intensity measurements and a fixed rms error in the final Mueller matrix, is much larger than the permitted error in the retarder axes positions. In fact, the retardance error can be about 3 times the error in the axes positions for the retarders closest to the sample ($R_2$ and $R_3$ in Fig. 1), and 9 times the error in the axes positions for the retarders furthest from the sample ($R_1$ and $R_4$ in Fig. 1). This means that for any optimized polarimeter it is more important to concentrate in reducing the errors in all the retarder axes positions, but particularly the axes positions of $R_1$ and $R_4$, to reduce the error in the final Mueller matrix. Although the analysis performed in this work was limited to the four calibration Mueller matrices, the results are representative of the polarimeter performance, and cover all of the reconstructed Mueller matrix elements. Analyses such as that made in Fig. 6 give the limits of the polarimeter parameter errors for given experimental conditions.
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