Integrating bias and gain invariance with the generalized Anscombe transform for wavefront sensing

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ABSTRACT

In image-based wavefront sensing by phase retrieval, the sum-squared difference (SSD) of simulated and measured PSF intensities, i.e., the intensity error metric (IEM), suffers from noise model mismatch. The IEM assumes additive Gaussian noise, but the true noise model is mixed Poisson-Gaussian (PG). The generalized Anscombe transform (GAT) addresses this issue by transforming the noise model from mixed PG to approximately additive Gaussian. We developed a method that uses the bias and gain terms derived for the bias-and-gain-invariant (BGI) IEM to create a BGI GAT error metric (GEM) and a BGI SSD of field amplitudes, i.e., amplitude error metric (AEM). We performed simulations comparing the retrieval accuracy of the three BGI metrics for various amounts of mixed PG noise. We found that the BGI GEM performs comparable or better than the BGI IEM and AEM for all amounts of mixed PG noise. Therefore, the BGI GEM is a good general-use error metric that works well for any mixed PG noise.

Keywords: phase retrieval, wavefront sensing, bias and gain invariant, generalized Anscombe transform

1. INTRODUCTION

When performing image-based wavefront sensing using phase retrieval by nonlinear optimization, a simulated point-spread function (PSF), $I$, is calculated from an exit pupil wavefront estimate and compared to a measured data PSF, $D$, using an error metric, and the calculated error is used to refine the pupil wavefront estimate via nonlinear optimization. The error metric used is important because it can affect the accuracy and convergence rate of the retrieved wavefront. A highly desired property for an error metric is bias and gain invariance, i.e., the error metric is invariant to bias and gain errors between the simulated and data PSF.\textsuperscript{1} Bias and gain invariance allows for faster testing, as it removes the need for calibration steps needed to account for these factors and gives a more accurate estimate when the calibration is imperfect.

To emphasize the importance of bias and gain invariance, we can look at the history of error metrics used for phase retrieval by nonlinear optimization. Two error metrics that are most common that we will focus on are 1) the sum-squared difference in image field amplitude (i.e., magnitude, the square root of the PSF intensities),\textsuperscript{2} and 2) the sum-squared difference in PSF intensities.\textsuperscript{3,4} We will call the first error metric the amplitude error metric (AEM), and the second the intensity error metric (IEM). Initially, the AEM was preferred over the IEM for many reasons,\textsuperscript{3} but for now it will suffice to say that it is because the AEM would perform better than the IEM in some cases (which we will explain later). We will give the intuitive reason here first, but we will give a mathematical explanation later in this section. Intuitively, as the intensity increases, the variance of the Poisson noise also increases, and thus even though higher intensity pixels have higher signal-to-noise ratio (SNR), they also have more Poisson noise. Therefore, if in an error metric the intensity at each pixel is inversely weighted by the variance of the noise at that pixel, which is reasonable, then higher intensity pixels should be weighted less than lower intensity pixels. This is why the AEM may perform better than the IEM, because in effect the square root enforces this sort of relative weighting on the pixels. Connected with that, the AEM was known to give an approximately maximum likelihood estimate for a Poisson noise model and the IEM was known to give the maximum likelihood estimate for additive Gaussian noise, as described in Ref. 4. Then, in 2009, Thurman developed a bias-and-gain-invariant (BGI) form of the IEM.\textsuperscript{1} The BGI IEM had the significant advantages that 1) it was much more convenient to not have to consider bias and gain errors, which are common with existing cameras, while still maintaining good retrieval performance, and 2) as will be discussed later, there was no

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equivalent for the AEM, since the derivation for the bias and gain invariance for the IEM does not work for the AEM due to a square root. Thus, even though the AEM should have better performance than the IEM when Poisson noise dominates, we more often use the BGI IEM. Later in this paper, however, we will discuss a way to have a BGI form of the AEM, but it is more of a stepping stone to an even better error metric.

An issue of the IEM, however, is noise model mismatch. As mentioned previously, it has been shown that the IEM is the maximum likelihood estimate for an additive Gaussian noise model. Paxman et al. also derive an error metric for a pure Poisson noise case. However, in reality, the noise model is most accurately represented as a combination of signal-independent additive Gaussian noise and signal-dependent Poisson noise, which we will call mixed Poisson-Gaussian (PG) noise. Thus, because the IEM is maximum likelihood for additive Gaussian noise, but the true noise model is mixed PG noise, there is a noise model mismatch between the IEM and the noise in the data PSF. In previous work, we discussed how the generalized Anscombe transform (GAT) (shown in Eq. (4) later in this paper) can help with this noise model mismatch. This is because the GAT is a variance-stabilizing transform (VST) for mixed PG noise, which in short means that the variance for each pixel after the GAT is approximately the same, i.e., the variance is “stabilized.” In other words, the GAT transforms a mixed PG noise model to an approximately additive Gaussian noise model. Therefore, there should be a better noise model match between using the sum-squared error after performing the GAT on the simulated and data PSFs as the error metric compared to the IEM. We call this error metric of the sum-squared error between GAT-transformed simulated and data PSFs the GAT error metric (GEM). It also turns out that the square root function is a very simple VST that works well for Poisson noise at high intensity levels. This explains why the AEM may perform better than the IEM in some cases as mentioned before: when the noise model is more Poisson-like (i.e., high intensities), the AEM will out-perform the IEM, but when the noise model is more additive Gaussian-like (i.e., more dominated by read noise), then the IEM will out-perform the AEM. Note for the pure Poisson noise case, the GAT simplifies to the classical Anscombe transform, which has better variance-stabilization for pure Poisson noise than the simple square root function, so the AEM could have been further improved by replacing the square root with the classical Anscombe transform for the pure Poisson noise model case, and it should have similar performance to using the Poisson error metric. However, once there is some additive Gaussian noise, we would expect the GEM to perform the best.

Since the GEM also has a square root function within it inside the GAT, the GEM has the same issue as the AEM in that the derivation of the bias and gain invariance that works for the IEM does not work for the GEM. However, in this paper, we developed a method that allows us to use the bias and gain terms derived for the BGI IEM case in service to the GEM and AEM, in effect creating BGI forms of the GEM and AEM. We then performed simulations to verify the validity of this method, and we demonstrate that the benefits of the GEM over the IEM and AEM as shown previously are maintained for the BGI GEM.

2. INTENSITY, AMPLITUDE, AND GAT ERROR METRICS

2.1 Intensity Error Metric

The intensity error metric (IEM), $E_{\text{Int}}$, is the normalized sum-squared error between the simulated and data PSFs, i.e.,

$$E_{\text{Int}} = \frac{\sum_{x,y} w \circ (I - D)^2}{\sum_{x,y} w \circ D^2},$$

where $\circ$ denotes a Hadamard product, $w$ is a weighting function (such as a bad pixel mask), $I$ is the simulated PSF, and $D$ is the data PSF. This is a common error metric that is used in phase retrieval. The sum-squared difference in the IEM comes from its derivation of giving the maximum likelihood estimate for additive Gaussian noise model. While the true noise model is mixed Poisson-Gaussian, since the GAT (and the amplitude transform as well, though to a lesser extent) transforms the mixed PG noise model to an approximately additive Gaussian noise model, the GAT and amplitude error metrics will also contain a sum-squared difference but in the transformed space. Thus, the IEM, AEM, and GEM are similar to each other because they all contain a sum-squared difference.
2.2 Amplitude and GAT Error Metric

The amplitude error metric (AEM), $E_{\text{Amp}}$, and GAT error metric (GEM), $E_{\text{GAT}}$, can be thought of as performing a transform on both the simulated and data PSFs before taking the normalized sum-squared error. The amplitude transform is defined as

$$A(X) = \begin{cases} \sqrt{X} & \text{for } X > 0 \\ 0 & \text{otherwise} \end{cases},$$

and accordingly the amplitude error metric is then

$$E_{\text{Amp}} = \frac{\sum_{x,y} w \circ [A(I) - A(D)]^2}{\sum_{x,y} w \circ [A(D)]^2},$$

Similarly, the GAT error metric uses the generalized Anscombe transform (GAT), which is defined as

$$G(X) = \begin{cases} \sqrt{X + 3/8 + \sigma_g^2} & \text{for } X + 3/8 + \sigma_g^2 > 0 \\ 0 & \text{otherwise} \end{cases},$$

and accordingly the GAT error metric is then

$$E_{\text{GAT}} = \frac{\sum_{x,y} w \circ [G(I) - G(D)]^2}{\sum_{x,y} w \circ [G(D)]^2}.$$
for the intensity, amplitude, and GAT error metrics, respectively. We have considered three methods to deal with
the bias and gain terms: 1) calibration is done to determine reasonable guesses for the bias and gain, and then have α and β be fixed, 2) have α and β be unknown parameters, which are then solved for during optimization, or 3) find analytic expressions that are functions of the simulated PSF that find reasonable estimates for α and β, i.e., α and β become α(I) and β(I). These methods can be combined, such as doing a calibration in order to have initial values when optimizing for α and β. Methods 2 and 3 have the advantage of not needing any calibration, but between Method 2 and 3, it is not known whether Method 2 or Method 3 is guaranteed to be better. For the work in this paper, we employ Method 3.

The analytic expressions used for α and β in Method 3 were initially done by Thurman and are explicitly written in the appendix of Moore’s paper.

\[ \alpha = \frac{\langle 1 \rangle \langle D, I \rangle - \langle I \rangle \langle D \rangle}{\langle 1 \rangle \langle I, I \rangle - \langle I \rangle^2} \]  \hspace{1cm} \text{(9)}

\[ \beta = \frac{\langle I, I \rangle \langle D \rangle - \langle I \rangle \langle D, I \rangle}{\langle 1 \rangle \langle I, I \rangle - \langle I \rangle^2} \]  \hspace{1cm} \text{(10)}

where

\[ \langle X, Y \rangle = \sum_{x,y} w \circ X \circ Y \]  \hspace{1cm} \text{(11)}

\[ \langle X \rangle = \sum_{x,y} w \circ X \]  \hspace{1cm} \text{(12)}

\[ \langle 1 \rangle = \sum_{x,y} w \]  \hspace{1cm} \text{(13)}

These analytic expressions were derived for the IEM, where these values of α and β are such that \( \partial E/\partial \alpha = \partial E/\partial \beta = 0 \). Using reverse-mode algorithmic differentiation (RMAD) to compute the gradient as proposed by Jurling, following his notation where \( \bar{\alpha} = \bar{\beta} = 0 \), the gradient calculation when using the IEM is made simpler because there are no additional terms to the gradient calculation. For the AEM and GEM cases, using the expressions in Eqs. (9) and (10), so one may ask why not use them for AEM and GEM since they still provide reasonable estimates for α and β.

4. SIMULATIONS

To generate a simulated PSF, \( I \), we had a circular exit pupil with a diameter of 128 pixels, and a wavefront was generated over the exit pupil that was the linear superposition of Zernike polynomials up to 6th radial order, ignoring piston (27 total polynomials). The Zernike coefficients were weighted such that the higher Zernike terms had lower magnitudes than lower Zernike terms, and then the wavefront was scaled to have an RMS wavefront error of 0.1 waves. The simulated PSFs were computed to be at 4 waves of defocus, so a quadratic phase corresponding to 4 waves of defocus was added to the wavefront. The wavefront was zero-padded to have an FFT size of 512 pixels before calculated the PSF as the squared magnitude of the Fourier transform of the exit pupil. Then the center 256 pixel square of the PSF was used as the simulated PSF to reduce the effect of
aliasing. In terms of pupil and image sampling ratios, \( Q_P \) and \( Q_I \), respectively, as defined by Jurling,\(^{11} \) \( Q_P = 4 \) and \( Q_I = 2 \).

To generate a noisy data PSF, \( D \), with mixed PG noise, the simulated PSF was scaled to some amount of peak photons, \( \sigma_{p,\text{peak}}^2 \) before adding Poisson noise, and then Gaussian noise with standard deviation \( \sigma_g \) was added. Then \( \sigma_{p,\text{peak}}^2 \) and \( \sigma_g \) were changed to vary the amounts of Poisson and Gaussian noise. To have a slightly better measure of the amount of Poisson noise in the data PSF, the mean intensity of the simulated PSF after scaling for peak photons but before adding Poisson noise was calculated. The mean intensity corresponds to \( \sigma_{p,\text{mean}}^2 \), and the average amount of Poisson noise in the data PSF is equal to \( \sigma_{p,\text{mean}} \).

To test the accuracy of an error metric for a specific amount of mixed PG noise, 10 wavefronts were generated, and for each wavefront, 100 noise realizations in \( D \) were generated. Then for each \( D \), phase retrieval was performed with that error metric starting from the true Zernike coefficients (ignoring piston), and then accuracy was measured by the RMS difference between the true and retrieved wavefronts, also known as the residual RMS wavefront error (WFE). We start from the true solution because we are testing accuracy, so this method allows us to evaluate how much the retrieved wavefront deviates from the true solution for each error metric without having to worry about issues of stagnation in local minima. The average and standard deviation of the accuracy was found across all wavefronts and noise realizations, and the average \( \sigma_{p,\text{mean}} \) was found across the different wavefronts. This was done for all three BGI error metrics, with the wavefronts and noise realizations being the same across all error metrics.

To test the accuracy across various amounts of Poisson and Gaussian noise, \( \sigma_g \) would be fixed, and peak photons \( \sigma_{p,\text{peak}}^2 \) varied from 1 to 70 million photons. This was done for \( \sigma_g = 0, 1, 5 \) and 20 photo-electrons. The accuracy of each error metric was found for each combination of Poisson and Gaussian noise.

5. RESULTS

Figure 1 shows the residual RMS WFE as a function of different amounts of Poisson-Gaussian noise for each of the three BGI error metrics. Lower residual RMS WFE is better and indicates higher retrieval accuracy. Subplots (a), (b), (c), and (d) correspond to \( \sigma_g = 0, 1, 5 \), and 20 photo-electrons, respectively. The bottom horizontal axis corresponds to mean photons of the true PSF, \( \sigma_{p,\text{mean}}^2 \), and the top horizontal axis corresponds to peak photons of the true PSF, \( \sigma_{p,\text{peak}}^2 \), and these axes are also equal to the variances of the average and peak amount of Poisson noise, respectively, in the data PSF. Note that \( \sigma_g = 0 \) is equivalent to pure Poisson noise. Moving from left to right within a plot, the noise model moves from more Gaussian-like to more Poisson-like (except for \( \sigma_g = 0 \)). In subplot (d), the two large error bars for the BGI Amp error metric at low mean intensity indicate that the retrieval accuracy was very inconsistent, and thus it should be interpreted that BGI Amp performs much more poorly at those points than the mean accuracy might indicate.

6. DISCUSSION

In general, as the mean intensity increases, the residual RMS WFE decreases, regardless of error metric. This is expected because as mean intensity increases, the signal-to-noise ratio increases, improving retrieval accuracy.

We expected that the IEM would perform better when the noise model is more Gaussian, the AEM to perform better when the noise model is more Poisson. Since the noise model goes from more Gaussian to more Poisson as mean intensity increases, we expected the IEM to perform better at lower intensities, and for AEM to perform better at higher intensities, which we see in Figure 1. Thus, there is a cross-over point in each of the plots from which IEM performs better to AEM performs better. In practice, it is difficult to know this point ahead of time, as it is a function of the ratio between the amount of Poisson noise and Gaussian noise, the specific wavefront under test, and system parameters (e.g., \( Q_P \), \( Q_I \), amount of defocus).

Because the GAT simplifies to the classical Anscombe transform when \( \sigma_g = 0 \), which has better variance-stabilization for pure Poisson noise than the simple square root of the amplitude transform, we expected the GEM to perform better than the AEM even for the pure Poisson noise case, which we seen for the lower levels of mean photons in Fig. 1(a). At the higher levels of mean photons, the added term \( 3/8 \) in Eq. (4) is too small to make a difference.
Figure 1. Residual RMS WFE vs various amounts of mixed Poisson-Gaussian noise for the different BGI error metrics. Subplots (a), (b), (c), and (d) correspond to $\sigma_g = 0, 1, 5,$ and $20$ photo-electrons, respectively. The bottom horizontal axis corresponds to the mean photons, $\sigma_{p,\text{mean}}^2,$ and the top horizontal axis corresponds to the peak photons, $\sigma_{p,\text{peak}}^2,$ for two different estimates of the amount of Poisson noise in the data PSF. Lower residual RMS WFE is better and indicates higher retrieval accuracy.

We expected the GEM to perform well for various mixed PG noise models, and Figure 1 shows this. In general, the GEM performs comparable to or better than the IEM and AEM for all values of mixed PG noise. Therefore, while for certain cases the IEM or AEM may perform slightly better than the GEM, the GEM is a good general-use error metric that has comparable or better performance over all mixed PG noise cases.

Figures 1(a) and 1(b) do show that the IEM may perform better than the GEM for very low amounts of Poisson noise when the Gaussian noise is low as well. This is likely due to the fact that the GAT has poor variance-stabilization at very low intensities. However, interestingly, as the amount of Gaussian noise increases, the variance stabilization of the GAT improves for low Poisson noise, which is why the GEM starts to perform better than the IEM as seen in Fig. 1(c), and this improvement is more apparent in Fig. 1(d).

Future work involves comparing these results to Method 2 mentioned in Section 3, where $\alpha$ and $\beta$ are...
optimization parameters; including analysis for a BGI form of an error metric that assumes pure Poisson noise; comparing convergence speed and convergence success rate of the different error metrics; and exploring whether going between the different metrics is advantageous.

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APPENDIX A. GRADIENT CONTRIBUTIONS FROM BIAS AND GAIN

The gradient contributions to $I$ from gain, $\alpha$, and bias, $\beta$, denoted as $I_\alpha$ and $I_\beta$, respectively, were determined through RMAD as described in Ref. 10. Starting from Eqs. (9) and (10), using quotient rule for derivatives, and then simplifying, we obtain

$$I_\alpha = \frac{-\langle 1 \rangle w \circ \left( |\alpha I + \beta - D| + \alpha |I - \mu(I, 1)| \right)}{\langle 1 \rangle \langle I, I \rangle - \langle I \rangle^2} \overline{\alpha}, \quad (A.1)$$

$$I_\beta = \frac{\langle I \rangle w \circ \left( 2 |\alpha I + \beta - D| + |D - \mu(D, I)| \right)}{\langle 1 \rangle \langle I, I \rangle - \langle I \rangle^2} \overline{\beta}, \quad (A.2)$$

where $\mu(X, Y) = \langle X, Y \rangle / \langle Y \rangle$, which may be interpreted as the weighted average of $X$ with weighting $Y$.

Note that the expressions for $I_\alpha$ and $I_\beta$ are the same for all three error metrics, but $\overline{\alpha}$ and $\overline{\beta}$ will be different across error metrics, as seen by Eqs. (B.4), (B.9), and (B.14) for $\overline{\alpha}$ and Eqs. (B.5), (B.10), and (B.15) for $\overline{\beta}$ in the next section.

APPENDIX B. GRADIENTS FOR BGI IEM, AEM, AND GEM

The gradient expressions using RMAD for BGI IEM, AEM, and GEM only differ up to $I$, beyond which the gradient expressions are the same and can be found in Ref. 9. It should also be noted that for AEM and GEM, these gradients expressions are for pixels that are not clipped by the transform as discussed in Section 2.2. For pixels that are clipped by the transform, the gradient for that pixel is zero. For the following gradient expressions, $N_c$ is the normalization constant for the error metric, $\alpha$ and $\beta$ are calculated according to Eqs. (9) and (10), respectively, $I_E$ is the gradient contribution to $I$ from the error metric, and $I_\alpha$ and $I_\beta$ are found according to Eqs. (A.1) and (A.2), respectively.

B.1 Gradient for BGI Intensity Error Metric

Starting with Eq. (6):

$$N_c = \sum_{x,y} w \circ D^2 \quad (B.1)$$

$$E_{BGI_{int}} = \frac{1}{N_c} \sum_{x,y} w \circ (\alpha I + \beta - D)^2 \quad (B.2)$$

$$\overline{E} = 1$$

$$I_E = \frac{2}{N_c} \left( \alpha w \circ (\alpha I + \beta - D) \right) \overline{E} \quad (B.3)$$

$$\overline{\alpha} = \frac{2}{N_c} \left( \sum_{x,y} w \circ (\alpha I + \beta - D) \circ I \right) \overline{E} = 0 \quad (B.4)$$

$$\overline{\beta} = \frac{2}{N_c} \left( \sum_{x,y} w \circ (\alpha I + \beta - D) \right) \overline{E} = 0 \quad (B.5)$$
\[ T = T_E + T_\alpha + T_\beta = T_E. \]

Note that for the IEM, \( \alpha \) and \( \beta \) are such that \( \alpha = \beta = 0 \), which causes \( T_\alpha = T_\beta = 0 \). This is not the case for the BGI AEM and GEM.

**B.2 Gradient for BGI Amplitude Error Metric**

Starting with Eq. (7):

\[ N_c = \sum_{x,y} w \circ [A(D)]^2 \quad (B.6) \]
\[ E_{BGIAmp} = \frac{1}{N_c} \sum_{x,y} w \circ [A(\alpha I + \beta) - A(D)]^2 \quad (B.7) \]
\[ T = T_E + T_\alpha + T_\beta, \]

where \( A(X) \) is defined by Eq. (2). Note that the gradient expressions for BGI GAT look exactly the same as for BGI Amp, only replacing the amplitude transform with the GAT.

\[ N_c = \sum_{x,y} w \circ [G(D)]^2 \quad (B.11) \]
\[ E_{BGIGAT} = \frac{1}{N_c} \sum_{x,y} w \circ [G(\alpha I + \beta) - G(D)]^2 \quad (B.12) \]
\[ T = T_E + T_\alpha + T_\beta, \]

where \( G(X) \) is defined by Eq. (4).
REFERENCES