Least Squares Arrival Time Estimators for Single and Piled Up Scintillation Pulses

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ABSTRACT

The ability to accurately determine the detection time of gamma rays has important applications in nuclear science. For gamma ray imaging systems, improvements in detector timing resolution can substantially reduce the signal to noise ratio of the images. This paper will develop a new arrival time estimator for the detection of gamma rays using scintillation detectors. The estimator structure reduces to a weighted least squares (WLS) estimate of the arrival time and has been found to be the optimal estimator for scintillation pulses. This WLS estimator was applied to scintillation type pulses with fast rise times and exponential decays. The timing resolution was calculated and compared to the resolution of leading edge and constant fraction triggers for a Burle 8850 photomultiplier tube, and to the Cramér-Rao lower bound on estimator performance. The WLS estimator has out performed these conventional arrival time estimators and has the added ability of simultaneously estimating the arrival times of multiple overlapping pulses. This allows for piled up pulses to be effectively separated permitting their individual energies to be estimated.

I. INTRODUCTION

Typical arrival time estimators employed with scintillation detectors, such as leading edge [1] and constant fraction [2] timers do not take into account any of the statistical correlation, covariance and higher order moments, of the scintillation counter's output waveform. The approach taken in this work is to improve timing estimation by incorporating both first and second order statistics into an arrival time estimator structure. This is accomplished by applying a WLS technique. Petrick *et al.* [3] developed a general WLS estimator that was applied to the output signal of a Burle 8850 photomultiplier (PM) tube stimulated by either a single photon or a pair of photons. The approach taken in this work directly applies the general WLS estimators developed in [3] to scintillator type optical pulses having a fast rise and a longer exponential decay. Each stimulating pulse produces between 100 and 1500 photo-electrons in the PM tube's photocathode which is a range consistent with the optical signals produced by common scintillation crystals such as BGO and NaI(Tl) when stimulated by 511 KeV gamma rays. As the photo-electron intensity increases, the output can be approximated by a Gaussian random process and the WLS estimator becomes identical to the maximum likelihood arrival time estimator developed by Tomitani [4] and Hero *et al.* [5].

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II. SINGLE PULSE WEIGHTED LEAST SQUARES TIMING ESTIMATOR

A. Estimator Structure

The general form for the single pulse WLS timing estimator is derived in [3] and takes on the form:

$$\tau^{*}_{wls} = \arg\min_{\tau}(\mathbf{X} - \hat{\mu}(\tau))^T \hat{\mathbf{K}}^{-1}(\tau)(\mathbf{X} - \hat{\mu}(\tau)), \quad (1)$$

where:

$$\hat{\mu}(\tau) = E\{\mathbf{X}(\tau)\} \quad (2)$$
$$\hat{\mathbf{K}}(\tau) = E\{(\mathbf{X}(\tau) - \hat{\mu})(\mathbf{X}(\tau) - \hat{\mu})^T\}, \quad (3)$$

denote the estimated mean and covariance functions, respectively, of the vector $\mathbf{X}$ of digitized time samples for a particular gamma ray photon arrival time, τ.

B. Digitization of the PM Tubes Response

The single pulse WLS estimator was applied to the digitized output signals produced by a Burle 8850 PM tube in response to a single optical pulse. The experimental apparatus for digitizing the Burle 8850 PM tube's response to single optical pulses is depicted in Figure 1. The optical pulses were exponentially shaped having a 20 nsec rise time and a 50 nsec decay time. The rise and fall times are measured as the time between 10% and 90% of the mean signal peak. The optical intensity along with a typical photo-electron distribution is shown in Figure 2 for an optical pulse impinging on the PM tube at time τ.

Four different sets of complete Burle 8850 PM tube detector responses were digitized and stored with a Tektronix RTD720 real time digitizer using a 0.5 nsec sampling interval. The different sets correspond to different magnitudes

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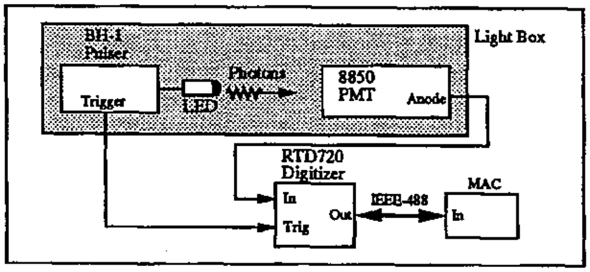

Figure 1: The experimental apparatus used to digitize the Burle 8850 PM tube's response to single optical pulse stimulation.

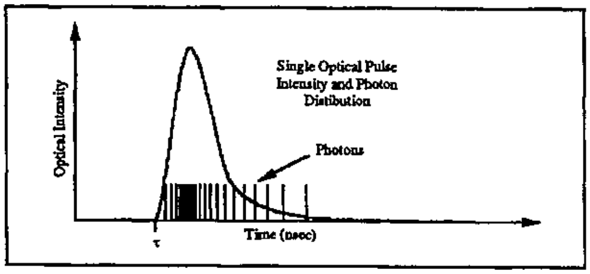

Figure 2: The exponentially shaped optical intensity and photo-electron distribution used to stimulate the Burle 8850 PM tube. The intensity has 20 nsec rise and 50 nsec decay components.

of the optical intensity shown in Figure 2. Mean magnitudes of 100, 500, 1000 and 1500 photo-electron per optical pulses were used in this experiment. Note that the exponential shape (*i.e.* the rise and fall times) of the stimulating pulses shown in Figure 2 changes only slightly as the magnitude increases.

C. Cramér-Rao Lower Bound on Timing Error

In order to compare the WLS estimator's timing performance with an optimal minimum mean squared error estimator, the Cramér-Rao (CR) lower bound over a range of large photo-electron intensities is formulated. The general form of the unbiased CR lower bound has been derived in many texts [6],[7] and states if $\hat{\tau} = \hat{\tau}(\mathbf{X})$ is any unbiased estimator of τ (*i.e.* $E(\hat{\tau}) = \tau$) then:

$$E\left\{(\tau - \hat{\tau}(\mathbf{X}))^2\right\} \geq J^{-1} \tag{4}$$

where J^{-1} is the Fisher information associated with the p.d.f. $p(\mathbf{X}|\tau)$ given by either of the following equivalent definitions:

$$J := E\left\{\left[\frac{d}{d\tau}\ln p(\mathbf{X}|\tau)\right]^2\right\} \tag{5}$$

$$J := -E\left\{\frac{d^2}{d\tau^2}\ln p(\mathbf{X}|\tau)\right\}. \tag{6}$$

Using the assumption that the detector response becomes Gaussian as the number of photo-electrons increases, it is possible to to develop an expression for the CR lower bound based solely on the mean and covariance of the detector response. This CR lower bound for single pulses is given as:

$$\text{CR Bound} = \left[\frac{d\mu(\tau)^T}{d\tau}\,\mathbf{K}^{-1}(\tau)\,\frac{d\mu(\tau))}{d\tau} - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{d^2[\mathbf{K}^{-1}(\tau)]_{i,j}}{d\tau^2}[\mathbf{K}(\tau)]_{i,j}\right]^{-1}, \tag{7}$$

where $\mu(\tau)$ and $\mathbf{K}(\tau)$ correspond to the mean and covariance of the detector response.

D. Comparison of Timing Estimators

Using the sets of digital PM tube responses, the mean and covariance for the different magnitude optical intensities were estimated based on 2092 responses. Figures 3 and 4 depict the mean response and covariance of the Burle 8850 PM tube when stimulated by exponential pulses containing an average of 500 photo-electrons. Once the means and covariances were found, the single pulse WLS estimator of Equation (1) was applied to four sets of 523 PM tube responses. The standard deviation (SD), $\sqrt{E\{(\hat{\tau} - \mu(\hat{\tau}))^2\}}$, of the WLS estimates was then calculated and compared to the SD of both leading edge and true constant fraction timing. Unlike the WLS arrival time estimator with a bias of less than 0.5 nsecs, both the leading edge and constant fraction timers are severely biased necessitating the use of the standard deviations for comparison. The resulting timing resolutions for single optical pulse detection obtained using the WLS, leading edge and constant fraction estimators are summarized in Table 1 along with the single pulse CR lower bound on timing error.

III. WEIGHTED LEAST SQUARES TIMING ESTIMATOR FOR PILED UP PULSES

A. Estimator Structure

A WLS estimator for the detection of a pair of optical pulses which have piled up detector responses was also investigated. This situation corresponds to a pair of gamma rays being detected at nearly the same time and their arrival times, τ_1 and τ_2, must be estimated. The double pulse WLS estimator was also derived in [3] and is approximated by:

$$\tau_{wls}^d = \arg\min_{\tau_1,\tau_2}[(\mathbf{X} - \hat{\mu}(\tau_1) - \hat{\mu}(\tau_2))^T \cdot (\hat{\mathbf{K}}(\tau_1) + \hat{\mathbf{K}}(\tau_2))^{-1} \cdot (\mathbf{X} - \hat{\mu}(\tau_1) - \hat{\mu}(\tau_2))], \tag{8}$$

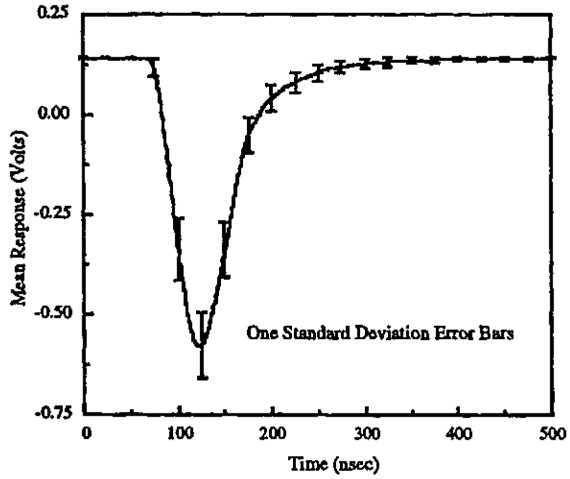

Figure 3: The estimated mean response of the Burle 8850 PM tube to an exponential optical intensity with a magnitude of 500 photo-electrons.

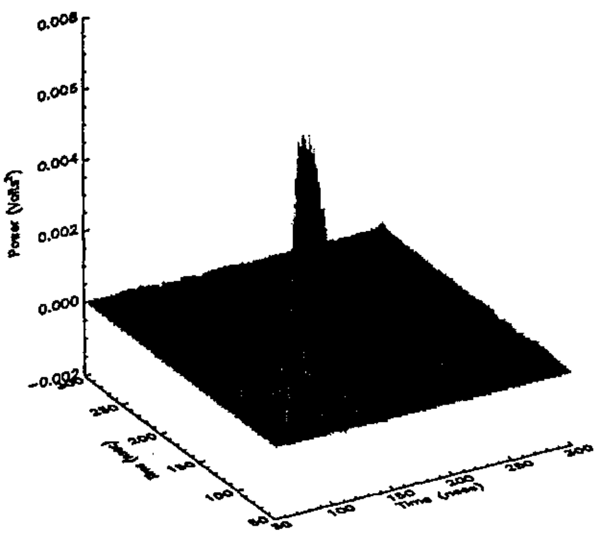

Figure 4: The estimated covariance of the Burle 8850 PM tube output in response to an exponential optical intensity with a magnitude of 500 photo-electrons.

Photons per Pulse	LE Error (nsec)	CF Error (nsec)	WLS Error (nsec)	CR Lower Bound (nsec)
100	3.03	2.96	1.99	0.117
500	1.98	1.92	1.40	0.109
1000	1.67	1.68	0.36	0.089
1500	1.53	1.51	0.19	0.083

Table 1: The performance of the leading edge, constant fraction and WLS arrival time estimators in the detection of single optical pulses having 20 nsec rises and 50 nsec decays along with the Cramér-Rao lower bound.

where $\hat{\mu}(\tau_i)$ and $\hat{\mathbf{K}}(\tau_i)$ correspond to the estimated single pulse mean and covariance described in Section II shifted by τ_i. Note, Equation (4) is valid when:

$$|\tau_1 - \tau_2| >> \frac{1}{f_{SER}}, \quad (9)$$

where f_{SER} is the bandwidth of the Burle 8850 PM tube's single electron response.

B. Cramér-Rao Lower Bound on Timing Error

For double pulses, there are two unknown primary photon arrival times, τ_1 and τ_2. The Cramér-Rao lower bound on the 2×2 covariance matrix of unbiased estimator errors $\hat{\underline{\tau}} - \underline{\tau} := [\hat{\tau}_1(\mathbf{X}) - \tau_1, \hat{\tau}_2(\mathbf{X}) - \tau_2]^T$ is given by:

$$E\left\{(\hat{\underline{\tau}} - \tau)(\hat{\underline{\tau}} - \tau)^T\right\} \geq \mathbf{J}^{-1}, \quad (10)$$

where $\mathbf{J}$ is the 2×2 Fisher information matrix [6]. The elements of $\mathbf{J}$ can be written as:

$$[\mathbf{J}]_{i,j} = -E\left\{\frac{\partial^2 \ln p(\mathbf{X}|\tau_1, \tau_2)}{\partial\tau_i \partial\tau_j}\right\} \quad (11)$$

and the CR bound on the variance of unbiased estimators for one of the arrival times, τ_i say, is:

$$E\left\{(\tau_i - \hat{\tau}_i(\mathbf{X}))^2\right\} \geq [\mathbf{J}^{-1}]_{i,i} \ , \quad (12)$$

where $[\mathbf{J}^{-1}]_{i,i}$ is the i, i^{th} element of the Fisher information matrix $\mathbf{J}$ [6].

Again using the assumption that the detector response becomes Gaussian as the number of photo-electrons increases, it is possible to to develop an expression for the high intensity CR lower bound based solely on the mean and covariance of the detector response. This double pulse CR bound reduces to the form:

$$\text{CR Bound} = \sqrt{[\mathbf{J}^{-1}]_{1,1} + [\mathbf{J}^{-1}]_{2,2}}\ , \quad (13)$$

where:

$$[\mathbf{J}]_{i,j} = \frac{1}{2}\frac{\partial \mu^T}{\partial \tau_i}\mathbf{K}^{-1}\frac{\partial \mu}{\partial \tau_j} + \frac{1}{2}\frac{\partial \mu^T}{\partial \tau_j}\mathbf{K}^{-1}\frac{\partial \mu}{\partial \tau_i} - \frac{1}{2}\sum_{l=1}^{n}\sum_{m=1}^{n}\frac{\partial^2[\mathbf{K}^{-1}]_{l,m}}{\partial\tau_i\partial\tau_j}[\mathbf{K}]_{l,m}\ . \quad (14)$$

The parameters μ and $\mathbf{K}$ in Equation (14) corresponds to the double pulse mean and covariance function, and were approximated using:

$$\mu(\tau_1, \tau_2) = \hat{\mu}(\tau_1) + \hat{\mu}(\tau_1) \quad (15)$$

$$\mathbf{K}(\tau_1, \tau_2) = \hat{\mathbf{K}}(\tau_1) + \hat{\mathbf{K}}(\tau_2). \quad (16)$$

B. Timing Error for the Piled Up Responses

The piled up Burle 8850 PM tube responses were constructed by adding pairs of shifted single pulse responses of

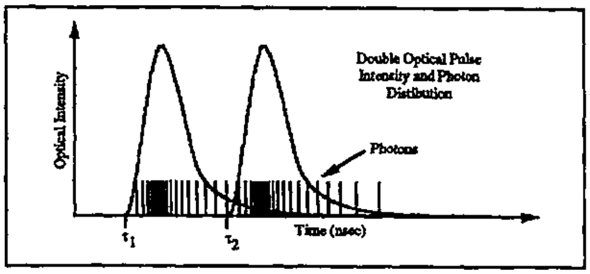

Figure 5: The exponentially shaped optical intensity and photo-electron distribution for a pair of overlapping optical pulses. Each of the single pulse intensities has a 20 nsec rise and a 50 nsec decay component.

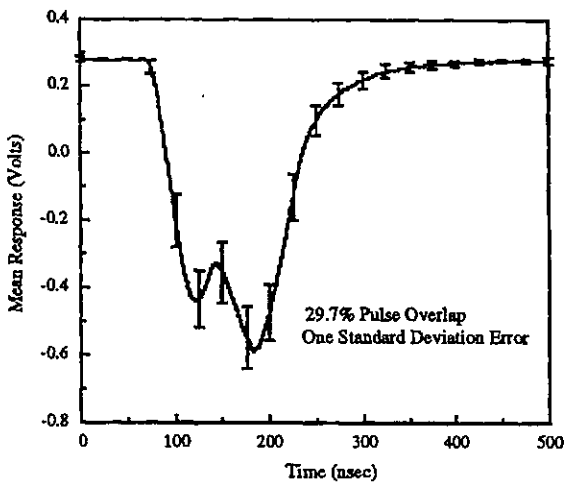

Figure 6: The estimated mean response of the Burle 8850 PM tube to a pair of exponential optical pulses with a magnitude of 500 photo-electrons and overlap of 29.7%.

Photons per Pulse	Overlap	WLS SD Error	CR Lower Bound
100	48.9%	5.71 nsec	0.297 nsec
500	50.9%	3.61 nsec	0.269 nsec
1000	50.7%	1.44 nsec	0.228 nsec
1500	50.4%	2.47 nsec	0.209 nsec

Table 2: The performance of the WLS arrival time estimator and the Cramér-Rao lower bound for the detection of 50% piled up optical pulse having 20 nsec rises and 50 nsec decays.

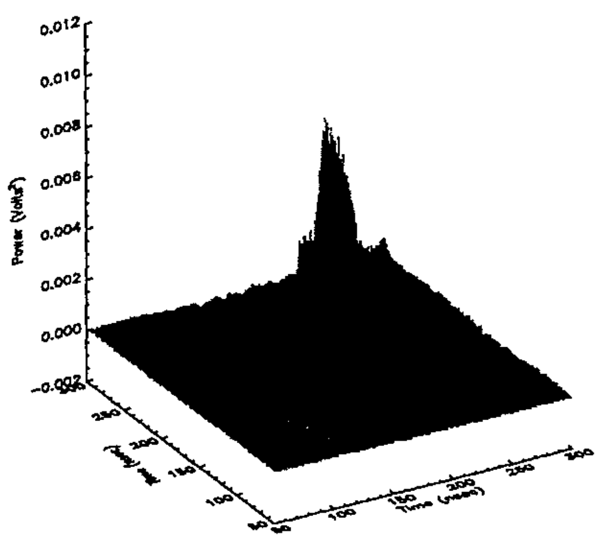

Figure 7: The estimated covariance of the Burle 8850 PM tube output in response to a pair of exponential optical pulses with a magnitude of 500 photo-electrons and overlap of 29.7%.

the same intensity magnitude together. The offset between the two pulses was selected so that the overlapping area would be approximately 50%. Using this technique, four complete sets of piled up pulses having optical intensity magnitudes of 100, 500, 1000 and 1500 photo-electrons per optical pulse were constructed. Figure 5 depicts the optical intensity for two piled up optical pulses. Note that the optical intensity of each incident pulse is still exponentially shaped with 20 nsec rise and 50 nsec decay components. Figures 6 and 7 contain the estimated mean and covariance of the PM tube's response to a pair of exponential optical pulses with a mean magnitude of 500 photo-electrons and 29.7% pulse overlap. An overlap of 29.7% was depicted because the 50% overlap case forms only a single peak.

Using the single pulse mean and covariance function of Equations (2) and (3), the double pulse WLS arrival time estimator of Equation (4) was applied to the piled up detector responses. The standard deviations were again calculated for each of the four intensity magnitudes and are given in Table 2 along with the pulse overlap and double pulse CR lower bound on the timing error.

IV. Discussion

The single pulse arrival time estimator results of Table 1 indicate that WLS arrival time estimation has improved timing performance over leading edge and constant fraction timing. The WLS estimator obtains a 30% improvement in timing resolution for 100 photo-electron pulses and much larger improvements for the 500 and 1500 photo-electron optical pulses. As one would expect, all of the estimators perform better as the photo-electron intensity increases. However, the WLS estimator's performance improves more rapidly than the leading edge or constant fraction timers. As the photo-electron intensity continues to increase, we would expect the relative improvement associated with the WLS estimator to again start to decline. The performance improvement is a consequence of the fact that the WLS estimator incorporates the statistical properties of the detector response into the estimator structure. This increases the complexity of the estimator but also improves the overall timing resolution.

The timing errors summarized in Table 2 show that the WLS estimator has the added advantage of being able to simultaneously estimate the arrival times of multiple pulses when the number of incident pulses is known. If the number of incident pulses is unknown, then they must be estimated prior to applying the WLS estimator. Good timing resolution was obtained using the WLS estimator even when significant pile up (*i.e.* 50% pulse overlap) was present and both leading edge and constant fraction timing proved ineffective. This ability to simultaneously estimate the arrival times of multiple pulses is the main advantage of the WLS implementation.

However, the WLS does have some limitations. The main problem being that it is computationally complex. If the number of piled up pulses increases by one, the computational complexity increase by an order of magnitude. Therefore, the WLS implementation is impractical for more than a few overlapping pulses. A second drawback with the WLS implementation is its strong dependence on the covariance estimate. Slight mismatches in the covariance were found to severely degrade the timing resolution of the estimator. This indicates that an alternative method for estimating the covariance may be useful. A possible method may be to derive the general form of the covariance from the shot noise model for the output signal of a PM tube developed by Wright [8] and Hero *et al.* [5].

The CR lower bounds on the single and double pulse timing resolution are also summarized in Tables 1 and 2. The WLS results only start to approach the lower bound calculations in the single pulse case as the photo-electrons intensity increases to 1500 per pulse, and is not close at all for the double pulses. The discrepancy may be due to two factors. First, the detector response may not be modeled well by a Gaussian distribution when the photo-electron intensity is low. In the single pulse case, the timing resolution of the WLS estimator approaches the CR bound as the photo-electron intensity increases. This indicates that the Gaussian assumption is only valid in the high intensity regime. A second possibility may again be due to mismatches in the covariance estimate reducing the achievable WLS timing resolution. When the true covariance for the data was used in the WLS implementation, the results did approach the CR bound values for all of the photo-electron intensities with the best results seen at the higher intensities.

V. CONCLUSION

While the WLS estimator is computationally complex, it has been shown to out perform the leading edge and constant fraction timers for detecting single and piled up optical pulses. This indicates that the WLS estimator can be used for detecting the arrival times of individual gamma rays using scintillation type detectors. Further research for improving implementation speed of the WLS algorithm is currently under way along with continued investigation of lower bounds on arrival time estimator performance.

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