Optimizing Pulse-Pileup Detection for Soft-X-ray Spectroscopy

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ABSTRACT

The problem of optimizing detection of the pileup of randomly occurring exponential tail pulses in white noise is considered. An attempt is made to reduce the process to an algorithm that could practically be performed in real time. Quantitative estimates are made for the performance of such an "optimum" detector. The relation to a more general pattern recognition problem is mentioned.

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Introduction

The problem of the pileup of randomly occurring events has received considerable attention over the years.^{1,2} Interest remains high at the Plasma Physics Laboratory due to the desire to improve the performance of a basic plasma diagnostic³ utilizing the time resolved spectral analysis of soft Xrays. Since failure to detect and reject events which are piled up leads to distortion of the spectrum, the performance of the pileup detection sets an upper limit on the rate of Xrays that can be measured without distortion. This, in turn, sets the best time resolution that can be obtained for a spectrum with a given statistical precision.

We begin by repeating the oft quoted results on the optimum detection or pulse height measurement of a single pulse in noise.^{1,2} A Si(Li) detector and preamplifier can be adequately modelled by a circuit with equivalent series and parallel white noise generators at its input (neglecting $1/f$ noise). These equivalent noise sources define an optimum time constant T_c such that if the preamplifier has a suitable transfer function, Xray induced events appear as tail pulses with time constant T_c in a background of white noise.

The best pulse shape for high count rate spectroscopy is the finite cusp.² A more practical choice is to shape the tail pulse into a triangle with a baseline of $2\sqrt{3} T_c$ since this shape is practically realizable, and has a signal to noise ratio close to optimum, together with a rapid return to the baseline.^{4,5}

Now let us imagine that we accurately digitized the tail pulse signal and noise waveform, $f(t)$, at a suitably high rate and then could analyze it at our leisure on a digital computer. The accepted procedure would be to fit the data to a single exponential tail pulse and then compute Chi Square. Chi Square is a discrete sum,

$$\chi^2 = \sum_{i=1}^N \frac{(f_i - y_i)^2}{\sigma_i^2}, \quad (1)$$

where y_i is the expected value for f_i , σ_i is the average error of f_i , and the errors in f_i for different i are uncorrelated.

The presence of a finite bandwidth in the measurement both limits the noise and causes $f(t)$ to be autocorrelated. We choose to define χ^2 in this paper to be a continuous integral of correlated squares as a practical measure of the fit.

$$\chi^2(T_E) = \frac{1}{\sigma^2} \left[\int_{T_1}^{T_E} |f(t)|^2 dt + \int_{T_E}^{T_2} \left| f(t) - A e^{\left(\frac{-(t - T_E)}{T_c} \right)} \right|^2 dt \right]. \quad (2)$$

The limits of integration are chosen to encompass the pulse and potential disturbing neighbors. In χ^2 we have factored σ^2 , the square of the average error in $f(t)$, outside the integral because it is due to the noise, which is independent of time. We would then choose an upper limit for χ^2 beyond which we would reject the hypothesis that $f(t)$ was represented by a single tail pulse arriving at T_E . This procedure would form an optimum pileup detector under the principle of Maximum Likelihood.

Real Time Algorithm

Next, we ask if there is a reasonable algorithm for the computation of χ^2 in real time.

Motivated by the theory of Young and Huggins,⁶ let us consider using a transversal filter shown in Fig. 1a. The transfer function (LaPlace Transform of the impulse response) of the filter is

$$\frac{e^{-sT_D} (1 + sT_C)}{(1 - sT_C)} \quad (3)$$

In Fig. 1b, the impulse response of the filter is shown together with its response to tail pulses. It has the effect of turning tail pulses around in time. This filter is an all pass filter which means that the white noise spectrum comes out as white with the same power with which it entered.

Young and Huggins⁶ proved some general results from which we extract the first term, time reverse it, delay it by T_D , take some liberties with the limits of integration, and restate it as Young and Huggins' Theorem:

$$\int_{T_E}^{T_2} |f(t) - Ae^{-\frac{(t - T_E)}{T_C}}|^2 dt = \int_{T_E + T_D}^{T_2 + T_D} |\tilde{f}(t)|^2 dt, \quad (4)$$

where $\tilde{f}(t)$ is the output of the transversal filter. In other words, $\tilde{f}(t)$, which Young and Huggins refer to as the present instant error, contains the same signal energy following the epoch of arrival T_E plus the filter delay T_D as one side of the error energy in the fit (See Fig. 2). Young and Huggins pointed out the usefulness of this result for related waveform recognition problems but despaired of its real time realization. Miller and Robinson⁷ have pointed out the practicality of transversal filter approximations, and similar filters have been built.^{8,9}

Figure 3 then shows a block diagram for such a pileup detection scheme arranged for real time processing. On the left, a single exponential tail pulse of amplitude K and time constant T_C enters riding on stationary white Gaussian noise of zero mean and standard deviation of a (volt/ $\sqrt{\text{radian/sec}}$). A Y-H transversal filter is used to form $\tilde{f}(t)$. Equivalent bandpass filters are shown in the f and $\tilde{f}$ channels before each is squared. These may be either real filters to limit the bandwidth or schematic for the band limiting already

produced by the preamplifier and filter circuits. After being filtered the subscript of B is added. The $|f_B(t)|^2$ is delayed by $T_D + \sqrt{3} T_C$ so that both contributions to the integral may be computed at the same time. The block labeled $(1 - e^{-s\sqrt{3} T_C})/sT_C$ continuously computes the integral over the past inspection interval of, $\sqrt{3} T_C$. Its output is $\chi^2(t)$ times a constant. In parallel with this computation is a filter that turns the tail pulse into a triangle of base $2\sqrt{3} T_C$. The triangle is then delayed such that its peak occurs at the same time as the calculation of χ^2 . Referring to Fig. 4, $\chi^2(t)$ indicates a misfit before and after the peak of the triangle but drops down at the peak time to indicate a good fit. In the case of a piled up event, $\chi^2(t)$ never drops low enough to indicate a good fit during the piled up peak.

Because of the finite bandwidth, B , we expect that for times of the order of $1/(\pi B)$, the computation is inexact, and a single tail pulse will produce an error energy contribution to $\chi^2(t)$ indistinguishable from two closely spaced tail pulses. In order to prevent a large single pulse from rejecting itself, an adaptive threshold in which the peak of the triangle predicts and automatically adjusts for this error is used.

Figure 5 shows a running integrator circuit that may perform the integral over the past T_I . It consists of a single delay line differentiator followed by an integrator. Assuming that it is driven by a circuit with negligible output impedance, R_2 would be adjusted to equal the characteristic impedance of the delay line. R_1 would be adjusted such that $R_1/R_3 = R_2/R_L$, where R_L is the lossy impedance of the delay line. The same transfer function may also be formed by a transversal filter with a total delay of T_I and equal tap weights.

The squaring functions must be fast and stable. However, they need not be accurately in conformance with a square law. In fact, it might be advantageous purposely to avoid a square law for large signals since this may avert a potential dynamic range problem for the circuit.

In building a prototype, it would not be surprising to find that one needed an active baseline restorer and another delay gated by detection of the slow Triangle's peak in order to get rid of low frequency noise and hum before the squaring device.

Now, let us begin to examine the performance of the pileup detector. Figure 6a shows the shape of the signal error contribution to $\chi^2(t)$. The shape can be deduced geometrically from Fig. 2. The pileup inspection interval is $\pm\sqrt{3} T_C$. For a tail pulse entering in Fig. 3 with a step of K volts in the absence of noise, the $\chi^2(t)$ signal error approaches $K^2/2$ volts at its maximum. We can see from Fig. 6a that sensitivity falls off at small separation times. While this is the Maximum Likelihood solution, it causes a spectroscopic problem. Since the pulse pair resolution time is a function of pulse height, the measured spectrum becomes distorted; i.e., the detector is more efficient at rejecting events that are large. This is a more difficult effect to correct for in computer analysis than if the pileup was pulse height independent. Also some of the energy slops past the pileup inspection interval and unnecessarily rejects good events.

We suggest here that the "optimum" pileup detector is in fact not the Maximum Likelihood solution, but a variant which trades energy sensitivity for invariance of pulse pair resolution with pulse height. Figure 6b shows the ideal time waveform for a modified $\chi^2(t)$, $M\chi^2(t)$. At $\pm\sqrt{3} T_C$ the $M\chi^2(t)$ rapidly rises to its flat top, falling steeply at $\pm\sqrt{3} T_C$ the bandwidth limited pulse pair resolution time. Figure 7 shows a signal processing scheme for accomplishing this. An all pass filter with transfer function $(1-sT_C/2)/(1 + sT_C/2)$ is added following the computation of $|\tilde{f}_B(t)|^2$. This has the effect on large single events of turning them around in time again so that they look like normal tail pulses. A zero is

added to square up the waveform and a pole is put in at four times the prior bandwidth B. This pole is arbitrarily chosen so as to limit additional noise lobes caused by the zero while producing little degradation in the B limited pulse pair resolution.

The delay in the $|f_B(t)|^2$ leg is adjusted until a gap appears between the rectangular lobes of just the amount to match the actual pulse pair resolution time.

Figure 8 shows a circuit with the all pass function needed.

Expected Sensitivity

Let us now attempt to estimate the sensitivity of the "optimum" pileup detector quantitatively.

For a tail pulse entering Fig. 7 with amplitude K in the absence of noise, a double rectangular output error signal of height $K^2/2$ volts is formed. At the input we also have zero mean Gaussian noise. The noise power spectrum at the input to the squaring device is

$$S_{f_B}(\omega) = \frac{a^2}{2[1 + (\omega/2\pi B)^2]} ; -\infty < \omega < \infty , \quad (5)$$

and the corresponding autocorrelation function is

$$R_{f_B}(\tau) = \frac{a^2}{4\pi} \int_{-\infty}^{\infty} \frac{e^{i\omega\tau} d\omega}{[1 + (\omega/2\pi B)^2]} \quad (6)$$

$$= \frac{a^2 B \pi}{2} e^{-2\pi B |\tau|} . \quad (7)$$

It can be shown¹⁰ that the autocorrelation function of the square of f_B is related to the autocorrelation of f_B by

$$R_{|f_B|^2}(\tau) = (R_{f_B}(0))^2 + 2 (R_{f_B}(\tau))^2, \quad (8)$$

and hence the power spectral density of $|f_B|^2$ is

$$S_{|f_B|^2}(\omega) = \int_{-\infty}^{\infty} R_{|f_B|^2}(\tau) e^{-j\omega\tau} d\tau \quad (9)$$

$$= \left(\frac{\pi a_B^2}{2}\right)^2 \left[2\pi\delta(\omega) + \frac{1}{\pi B [1 + (\omega/4\pi B)^2]} \right], \quad (10)$$

which represents a D.C. noise power term and A.C. white noise power with bandwidth $2B$.

After the final pole/zero compensation, the power spectral density of M_X^2 is

$$S_{M_X^2} = \left(\frac{\pi a_B^2}{2}\right)^2 \left[2\pi\delta(\omega) + \frac{1}{(\pi B) [1 + (\omega/4\pi B)^2]} \right] [2] \frac{(2)[1 - \cos(\sqrt{3} \omega \tau_c)]}{(\omega \tau_c)^2} \frac{[1 + (\omega \tau_c/2)^2]}{[1 + (\omega/8\pi B)^2]}. \quad (11)$$

(The factor of [2] is due to the sum of Fig. 7 and would be correct if the noise from the two paths were uncorrelated. In fact, it is a bit correlated.)

Of interest to us are the mean modified Chi Square noise voltage, $\bar{V}_{M_X^2}$, and the variance, $\sigma_{M_X^2}^2$. The mean noise voltage is equal to the square root of the D.C. noise power.

$$\bar{V}_{M\chi^2} = \text{SQRT} \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} 2 \left(\frac{\pi a^2 B}{2} \right)^2 2\pi \delta(\omega) \frac{2 [1 - \cos(\sqrt{3} \omega T_c)]}{(\omega T_c)^2} \frac{[1 + (\omega T_c/2)^2]}{[1 + (\omega/8\pi B)^2]} d\omega \right] \quad (12)$$

$$= \sqrt{3/2} \pi a^2 B . \quad (13)$$

The variance is equal to the integrated A.C. power

$$\sigma_{M\chi^2}^2 = \frac{1}{2\pi} \int_{-\infty}^{\infty} 2 \left(\frac{\pi a^2 B}{2} \right)^2 \frac{1}{\pi B [1 + (\omega/4\pi B)^2]} \frac{2[1 - \cos(\sqrt{3} \omega T_c)]}{(\omega T_c)^2} \frac{[1 + (\omega T_c/2)^2]}{[1 + (\omega/8\pi B)^2]} d\omega . \quad (14)$$

This integral may be evaluated by Cauchy's Residue Theorem and yields

$$\sigma_{M\chi^2}^2 = \frac{a^4 \pi B^2}{2} \left[\frac{\sqrt{3}}{BT_c} + \frac{1}{12\pi B^2} \left[(1 - e^{-4\sqrt{3}\pi B T_c}) \left((4\pi B)^2 - \left(\frac{2}{T_c} \right)^2 \right) - \frac{1}{8} (1 - e^{-8\sqrt{3}\pi B T_c}) \left((8\pi B)^2 - \left(\frac{2}{T_c} \right)^2 \right) \right] \right] . \quad (15)$$

For realistic values of BT_c ,

$$\sigma_{M\chi^2}^2 \approx \frac{\pi a^4 B^2}{2} \left[\frac{\sqrt{3}}{BT_c} + \frac{2\pi}{3} \right] , \quad (16)$$

and

$$\frac{\sigma_{M_X^2}}{\bar{V}_{M_X^2}} = .5 \sqrt{1 + .8/BT_c} \quad (17)$$

Let us find the threshold setting for the M_X^2 comparator of Fig. 7. The threshold should be set as low as possible for maximum sensitivity to pileup while causing no more than a tolerable amount of false alarm pileup detections. A probability of false alarm pileup detection of .1 is about the right order of magnitude since randomly throwing away 10% of the single unpiled up events has no effect on the spectral shape and negligible effect on the count rate statistics. We approximate the M_X^2 distribution as a Gaussian with mean and variance equal to those calculated above. We can see from a table of Normal Error that a threshold set at $1.3 \sigma_{M_X^2}$ above the mean will yield the .1 false alarm probability so the threshold voltage, V_{Thresh} , is

$$V_{Thresh} = \bar{V}_{M_X^2} + 1.3 \sigma_{M_X^2} \quad (18)$$

$$\frac{V_{Thresh}}{\bar{V}_{M_X^2}} = 1 + .65 \sqrt{1 + .8/BT_c} \quad (19)$$

Next, we wish to define and compute the pile up detection sensitivity. An incident tail pulse with step K volts will produce error lobes which in the absence of noise have height $K^2/2$. For signals large compared to the noise, the detection of a fraction of the pileup events are missed due to the finite pulse pair resolution $\tau_R = 1/(\pi B)$ as mentioned above. This large signal probability of missed pileup detection is then

$$P_{mpud} = \frac{\text{Probability of undetected pileup}}{\text{Probability of pileup}} \quad (20)$$

$$= \frac{[1 - e^{-(2x/\pi B)}]}{[1 - e^{-(2x/\sqrt{3} T_c)}]} ; \text{ where } x \text{ is the event rate} \quad (21)$$

$$\approx \frac{1}{\pi\sqrt{3} BT_c} \quad (22)$$

$$\approx \frac{.2}{BT_c} . \quad (23)$$

Let us define the sensitivity as that signal to noise ratio in triangular pulse height to $FWHM_{en}$ such that there is a contribution to missed pileup detection from noise approximately equal to the finite pulse pair resolution contribution. Here the $FWHM_{en}$ is the electronic noise contribution to the full width at half maximum resolution in measuring a monoenergetic Xray with a perfect triangle amplifier. In order to find this signal to noise ratio, we must look at the statistics of $M\chi^2$ when there is a signal in the noise. Now admittedly, we have not shown that $M\chi^2$ is truly Chi Square distributed with some N degrees of freedom. However, if it isn't, intuitively it must be close. Hence, we shall treat it statistically as if it were Chi Square distributed. It has been shown¹¹ that when one adds a signal to Gaussian noise and then squares and sums, the distribution that results is known as a Noncentral Chi Squared Distribution, and the mean of the error signal in the presence of noise is the sum of the signal and the noise means,

$$\bar{v}_K = \bar{v}_{M\chi^2} + \frac{K^2}{2} \quad (24)$$

$$\frac{\bar{v}_K}{\bar{v}_{M\chi^2}} = 1 + \frac{K^2}{2\bar{v}_{M\chi^2}} , \quad (25)$$

and the variance is

$$\sigma_K^2 = \sigma_{M\chi^2}^2 [1 + K^2/\bar{V}_{M\chi^2}] \quad (26)$$

$$\frac{\sigma_K}{\bar{V}_{M\chi^2}} \approx .5 \text{ SQRT} \left((1 + .8/BT_C) (1 + K^2/\bar{V}_{M\chi^2}) \right) \quad (27)$$

Again, we will approximate this Noncentral Chi Squared Distribution by a Gaussian with the same mean and variance. This time we choose $K^2/\bar{V}_{M\chi^2}$ such that the probability of having a voltage lower than the threshold is equal to $.2/BT_C$, the large signal probability of missed pileup detection. The only remaining variable is the dimensionless constant BT_C . The performance of the pileup detector is summarized in Table 1 as a function of BT_C . The sensitivity is listed as the ratio of the height of a triangular pulse corresponding to the sensitivity input value K to the $FWHM_{en}$. This ratio can be shown to be

$$\frac{\text{Triangle height}}{FWHM_{en}} \approx .35/\sqrt{BT_C} \text{ SQRT} (K^2/\bar{V}_{M\chi^2}) \quad (28)$$

As is expected, the energy sensitivity of pileup detection decreases as the bandwidth increases. This is less a function of the noise increasing with increased bandwidth, than it is a reflection of our definition of sensitivity; namely, as the bandwidth goes up, the large signal probability of missed pileup detection goes down, and only successively higher energy pulses are enough above the noise to avoid "spoiling" the large signal probability.

For good commercial cooled Si(Li) detector/preamplifier, the $FWHM_{en}$ is ~ 150 eV with an optimum time constant of ~ 5 μ sec. Table 2 then gives the expected performance of an "optimum" detector used with the Si(Li). Considering the approximations made in this paper and deviation of any real

circuit from the ideal, these numbers should be taken as order of magnitude only.

The limiting circuit elements in how high a BT_C one could attain for a practical implementation are in both the transversal filter and the delay lines. We might estimate that in order for the transversal filter to achieve a bandwidth of B , it might have to sample at $8B$. In order to contain a reasonable amount of an exponential tail pulse of time constant T_C , its delay, T_D , should be $4T_C$. Therefore, the number of samples in the transversal filter must be $\geq 32 BT_C$. Thus, if one wanted to achieve a large signal probability of missed pileup detection $< .05$, one would need a transversal filter with 128 samples memory taken at 6.4 million samples/sec. This is not far from the performance of commercially available products. (Reticon Corp. has a printed circuit board, model TC32A-02, which samples at 5 million samples/sec with 32 samples of memory and 32 adjustment potentiometers. Further, it can be cascaded.) The delays needed are proportionally more or less demanding.

Pattern Recognition in the Time Domain.

There is a general problem¹³ in pattern recognition of classifying a time domain signal in noise as being acceptable given the expected shape. Pileup detection is a special case of the pattern recognition problem and the above treatment may be extended to the general case.

Figure 9 shows an expected time domain signal $h(t)$, with LaPlace Transform $H(s)$, entering a signal recognition circuit. As is normal, a matched filter would have an output indicating that an event had occurred. A linear filter, possibly another transversal filter, with transfer function $1/[H(s)(s+a)]$ would also transform the incoming signal of the expected shape into an exponential tail pulse. This could then be followed by a χ^2 computer

as described above. The variable, a , would be chosen to maximize sensitivity for a given problem.

Conclusions

An implementation in real time of an "optimum" algorithm for the detection of pileup of randomly occurring tail pulses in white noise seems practical with commercially available components. Its sensitivity has been estimated.

We must emphasize that for X-ray spectra of ~ 1 keV and above, ad hoc pileup rejection schemes containing less circuitry^{1,12} provide adequate performance. It is only for the analysis of sub keV X-rays at high rate or related problems that such an "optimum" pileup detector would be justified. Such a potential application is the planned use of a windowless Si(Li) on the PDX tokamak to analyze Carbon and Oxygen impurity X-rays.

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Figure Captions

Fig. 1 Y-H Transversal Filter.

Fig. 2 Illustration of Young and Huggins' Theorem.

Fig. 3 Maximum Likelihood Pileup Detection Scheme.

Fig. 4 $\chi^2(t)$ With and Without Pileup.

Fig. 5 Integral Over Past T_I (Running Integrator) Implementation.

Fig. 6 $\chi^2(t)$ and $M\chi^2(t)$ for a Single Event.

Fig. 7 "Optimized" Pileup Detection Scheme.

Fig. 8 Allpass Filter Implementation.

Fig. 9 General Signal Detection

Tables

Table 1 Pileup Detection Sensitivity as a Function of BT_C .

Table 2 Expected Performance for Cooled Si(Li).

Table 1

Pileup Detection Sensitivity as a Function of BT.

BT _C	$\frac{\sigma_{M_X}^2}{\bar{V}_{M_X}^2}$	$\frac{V_{\text{Threshold}}}{\bar{V}_{M_X}^2}$	Large signal probability of missed pileup detection	$\frac{K^2}{\bar{V}_{M_X}^2}$	$\frac{\bar{V}_K}{\bar{V}_{M_X}^2}$	$\frac{\sigma_K}{\bar{V}_{M_X}^2}$	Sensitivity given as <u>Triangular Pulse Height</u> FWHM electronic noise
1	.7	1.9	.2	4.3	3.2	1.5	.7
2	.6	1.8	.1	5.5	3.8	1.5	1.2
4	.5	1.7	.05	6.3	4.1	1.5	1.8
8	.5	1.7	.025	7.4	4.7	1.5	2.7
16	.5	1.7	.013	8.2	5.1	1.5	4.0

Table 2

Expected Performance for Cooled Si(Li)

B (MHz)	Large Signal Probability of missed pileup detection	Pileup Sensitivity (eV)
.2	.2	110
.4	.1	180
.8	.05	270
1.6	.025	410
3.2	.013	600

FWHM electronic noise taken as 150 eV with $T_c = 5\mu s$

81E0004

(a)

(b)

Fig. 1

808109

Fig. 2

MAXIMUM LIKELIHOOD PILEUP DETECTION SCHEME

81E0005

Fig. 3

81E0008

Fig. 4

(a)

81E0002

(b)

Fig. 5

(a) Maximum Likelihood

#808090

(b) Optimum

Fig. 6

"OPTIMIZED" PILEUP DETECTION SCHEME

808094

Fig. 7

(a)

81E0001

(b)

Allpass Filter

Fig. 8

Fig. 9