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Optimal filtering of calorimeter signals

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Abstract

A technique based on the Wiener filter is presented for filtering calorimetric signals. The filter was applied to a simulated calorimetric signal with three different signal-to-noise levels. Smoothing takes place in the frequency domain using windows that allow the power spectrum of the signal noise to be estimated *a priori*. In addition, the filter removes the parasitic oscillations that the fast Fourier transform introduces during deconvolution.

INTRODUCTION

All the deconvolution processes recently applied to conduction calorimetry [1–6] contain a smoothing step in their formalism, either implicitly or explicitly. There have also been studies of sophisticated signal smoothing procedures which are applied after the deconvolution step [7,8]. Most of these techniques operate in the time domain using digital or analogous low-pass filters that remove the high frequencies due to noise. For deconvolution with a fast Fourier transform (FFT), filtering is carried out in the frequency domain by cutting off at a particular point in the Fourier spectrum of the signal; this creates parasitic oscillations, which then have to be removed [7]. Other smoothing procedures require a laborious study of each calorimeter to get as much information as possible about the autocorrelation function of the noise [8].

This article discusses a smoothing technique based on the classical Wiener filter, for which the power spectrum of the noise contaminating the signal must normally be modelled or at least partially known. The salient point is that cutting the frequency spectrum of the noisy signal at a certain frequency, above which we suppose there is only noise, can be made relatively independently of what is known about the calorimetric noise. A single parameter is needed to define the filter completely.

It is important to know the degree of smoothing, since trying to improve the signal leads to deformations in it which must be quantified. For this

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method it is straightforward, since the single filter parameter determines the cut-off frequency and the degree of attenuation for each frequency that is allowed to pass (of great importance for calorimetric studies of oscillating phenomena [9]). Furthermore, comparing the power spectra of the unfiltered and filtered signals gives a measure of the "energy" lost in smoothing.

In the following section we will show how the calorimetric signals used to test the filters were generated and why the classical application of the Wiener optimal filter does not provide a satisfactory solution to the problem. In the second section three filters will be postulated and their effects in the time and frequency domains will be studied.

CLASSICAL FREQUENCY FILTERING

Let $x(t)$ be the power dissipated in the calorimetry cell and $y(t)$ be the corresponding thermogram. Assuming the use of a digital system to process these signals, let $x[k]$ and $y[k]$ be the values of these temporal functions at $t = kT$, where T is the sampling period of the signal. The thermogram will contain noise, which is assumed to be independent of $x[k]$ and $y[k]$. In Fig. 1(a), a thermogenesis and its corresponding thermogram are shown simulated for a calorimeter with parameter $\tau_1 = 200$, $\tau_2 = 90$, $\tau_3 = 10$, $\tau_1^* = 20$ s (already used elsewhere [6]) and sensitivity 5 (this parameter is not important here; this value was chosen to unify the scales on the graphs). To reproduce an experimental signal, noise was added to the thermogram using the IMSL software package to generate pseudo random numbers with a normal distribution, which were added to the thermogram with signal-to-noise ratios of 100, 80 and 60 dB.

Performing the deconvolution of the three simulated thermograms gave the signals shown in Figs. 1(b), 1(c) and 1(d) for 100, 80 and 60 dB signal/noise, respectively. The deconvolution technique developed in ref. 1 was used, making the value of the compensation poles as small as possible to give a stable system without introducing deformations into the signal. Two pulses of 0.5 s were used for the 100 dB signal, two of 1.0 s for the 80 dB signal, and two of 2.5 s for the 60 dB signal. These values could be increased to give smoother signals, but this type of temporal filter rapidly distorts the signal.

The noisy signal can be treated as the sum of two other signals

$$z[k] = x[k] + n[k] \tag{1}$$

where $x[k]$ is the real thermogenesis we want to reconstruct from the measurement $z[k]$, eliminating the unknown noise $n[k]$. Let $f[k]$ be the optimal filter that gives $\hat{x}[k]$ as the best approximation to $x[k]$, hence

$$\hat{X}(w) = F(w)Z(w) \tag{2}$$

where the capitals stand for the Fourier transforms of the functions represented by the corresponding small letters and w is the frequency. By best approximation here we mean that $\hat{X}(w)$ is closest to $X(w)$ in the least-squares sense, i.e.

$$\int_{-\infty}^{\infty} |\hat{x}(t) - x(t)|^2 \, dt = \int_{-\infty}^{\infty} |\hat{X}(w) - X(w)|^2 \, dw \qquad \text{is a minimum} \quad (3)$$

Using eqns. (1) and (2), this condition becomes

$$\int_{-\infty}^{\infty} |X(w)[F(w) - 1] + N(w)F(w)|^2 \, dw \qquad \text{is a minimum} \quad (4)$$

Multiplying out the integrand (because integration is over all frequencies, $X(w)$ and $N(w)$ are not correlated)

$$\int_{-\infty}^{\infty} (|X(w)|^2 |1 - F(w)|^2 + |N(w)|^2 |F(w)|^2) \, dw \qquad \text{is a minimum} \quad (5)$$

The integral is a minimum if and only if the integrand is a minimum with respect respect to $F(w)$ for any frequency w. Hence, the optimal filter is defined as

$$F(w) = \frac{|X(w)|^2}{|X(w)|^2 + |N(w)|^2} \quad (6)$$

It is seen that both $f(t)$ and $F(w)$ are real functions. Because $x[k]$ and $n[k]$ are unknown, it is necessary to estimate their power spectra. With regard to the denominator of eqn. (6) it is reasonable to make the approximation

$$|X(w)|^2 + |N(w)|^2 \simeq |Z(w)|^2 \quad (7)$$

The power spectrum of $z[k]$, for the signal with signal-to-noise ratio of 80 dB (corresponding to Fig. 1(c)), is shown in Fig. 2(a) on a logarithmic scale. To estimate the numerator it is necessary to estimate the noise. A simple way is to suppose that the noise corresponds to all the frequencies above a cut-off frequency w_c, so that the spectrum above w_c corresponds to $|N(w)|^2$ and that below corresponds to $|\hat{X}(w)|^2$. This describes an optimal rectangular filter (Fig. 2(a))

$$F(w) = \begin{cases} 1 & w \leq w_c \\ 0 & w > w_c \end{cases} \quad (8)$$

In the figure, $w_c = 34/256$ Hz; that is, the spectrum is cut off at the point $m = 34$. The spectrum is calculated from a FFT of $N = 256$ points with a signal sampling period $T = 1$ s (in general $w = m/NT$).

Applying the filter defined in eqn. (8) to the signal in Fig. 1(c) (80 dB signal/noise) gives the filtered signal shown in Fig. 2(b). It can be seen that the noise has been reduced dramatically, but that a parasitic oscillation has

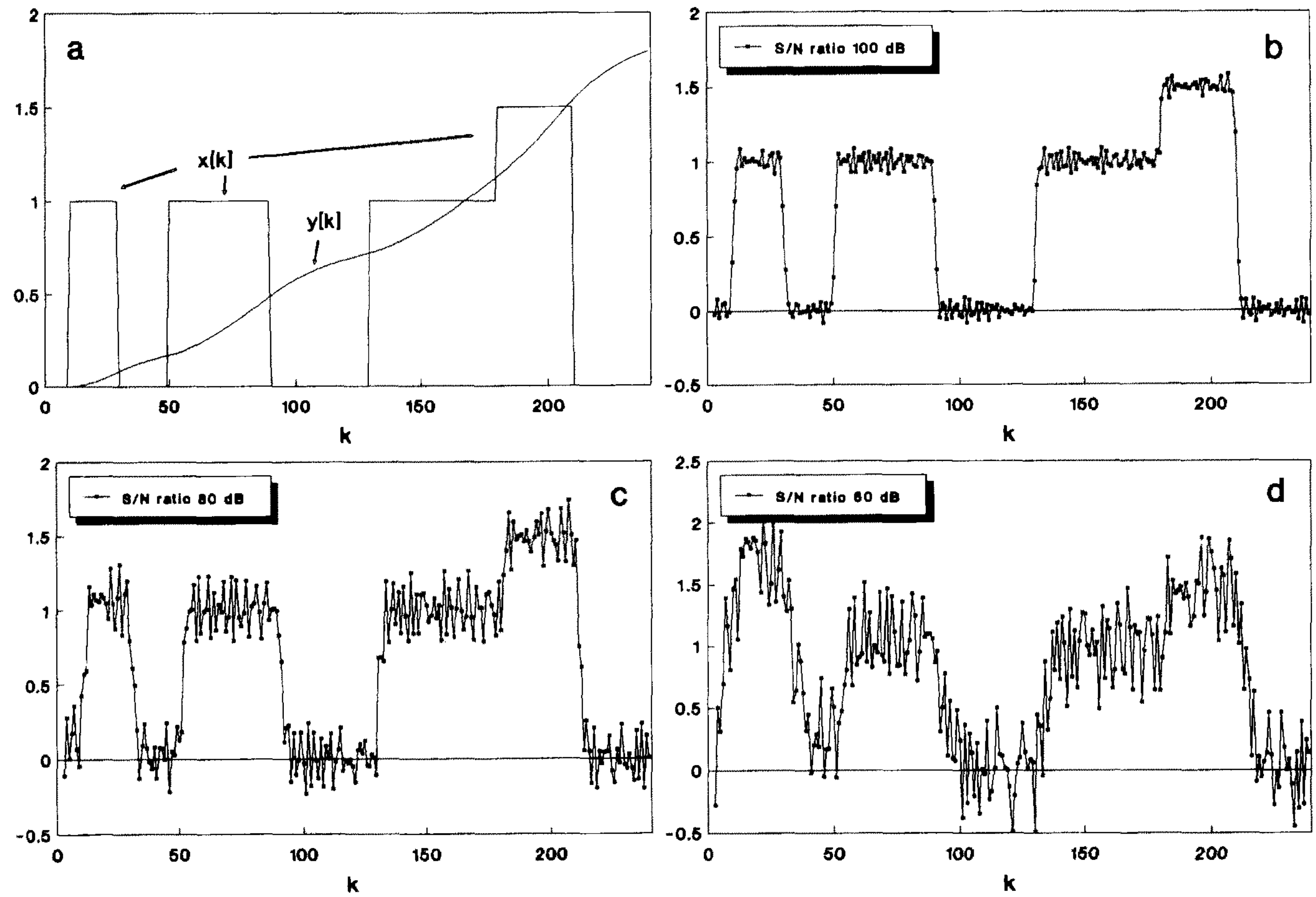

Fig. 1. (a) Simulation of calorimetry signals where $x[k]$ is the input signal and $y[k]$ the output thermogram. (b), (c), (d) Deconvolution of $y[k]$ with 100 dB, 80 dB and 60 dB of signal/noise, respectively.

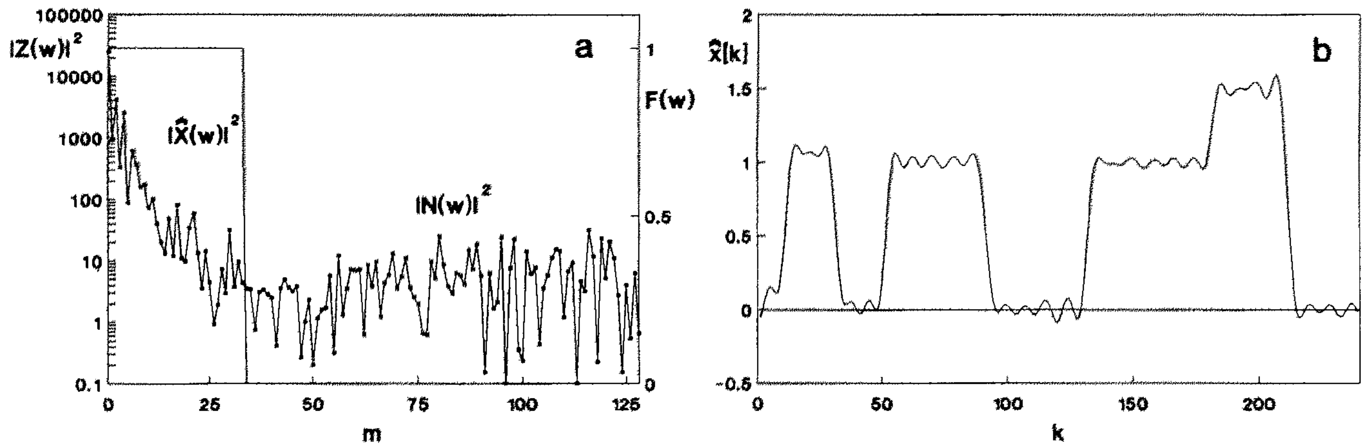

Fig. 2. (a) Power spectrum of $z[k]$ on a logarithmic scale. The rectangular filter $F(w)$ divides the spectrum into two parts: inside $F(w)$ estimation of the power spectrum of $x[k]$; outside $F(w)$ estimation of the noise power spectrum. On the X axis the frequency w is a function of the index m ($w = m/NT$), where N is the number of points used to calculate the FFT and T is the sampling period. (b) Estimation of $x[k]$ from the $z[k]$ of Fig. 1(c) with the rectangular filter.

appeared due the filter's action of abruptly cutting the power spectrum. This effect has been described for the deconvolution of calorimetric signals by an FFT technique [7]. A better system can be obtained by modifying the filter that has been developed.

NON-RECTANGULAR WINDOWS

Three ways of "softening" the filter constructed will be studied

The Welch window

$$F(j) = 1 - [2(j-1)B/N]^2 \tag{9}$$

the Parzen window

$$F(j) = 1 - |2(j-1)B/N| \tag{10}$$

and the Hanning window

$$F(j) = \frac{1}{2}\left\{1 - \cos 2\pi\left[\frac{(j-1)B + N/2}{N}\right]\right\} \tag{11}$$

where $F(j) \equiv F(w = j/NT)$, N is the number of points used to calculate the FFT (a power of 2) and T is the sampling period of the signal. The parameter B defines the cut-off frequency of the filter

$$w_c = j_c/NT \text{ con } j_c = N/2B + 1 \tag{12}$$

Putting $B = 0$ gives no filtering, at $B = 1$ (Fig. 3) no frequency is cut-off, but the signal is attenuated, whilst $B = 3.909$ gives a cut-off at $m = 34$ (Fig. 3), which corresponds to the same frequency used for filtering with the rectangular window [eqn. (8)].

These filters are applied in an unconventional way here. The defining equations (9)–(11) correspond to the classical forms of these windows, but here they are used in the frequency domain, where it is normal to use the

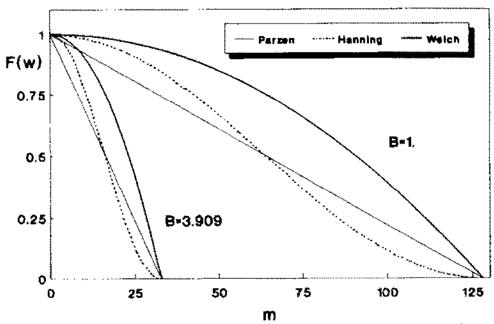

Fig. 3. The non-rectangular windows used as optimal filters for two values of the parameter B; w, N and T are defined as before (in this case $N = 256$ and $T = 1$ s).

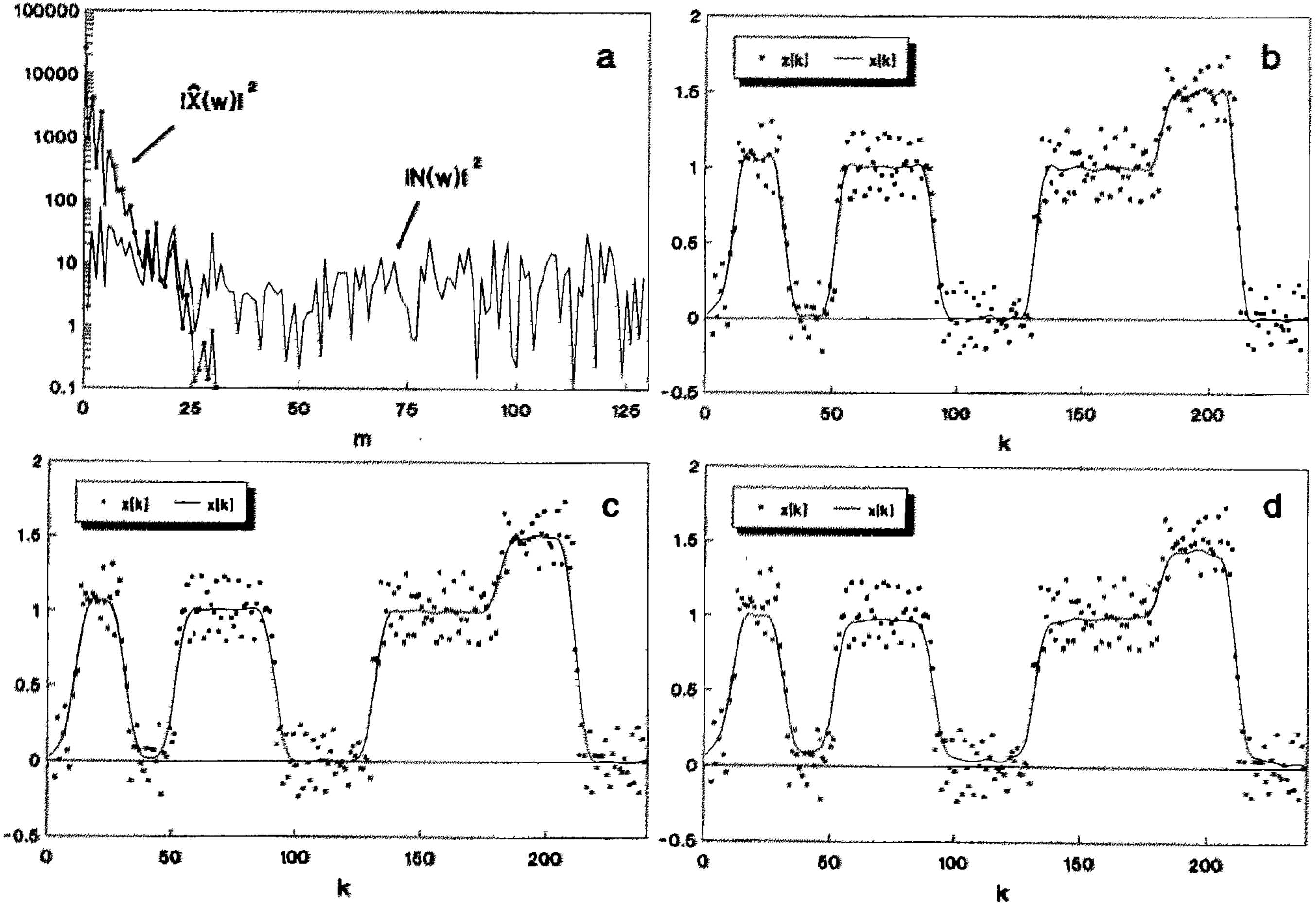

Fig. 4. (a) Estimation of the power spectra of $x[k]$ and $n[k]$ from the signal $z[k]$ with 80 dB signal/noise and the Welch window. (b), (c), (d) Reconstruction of $x[k]$ from the signal $z[k]$ with 80 dB signal/noise using the Welch, Hanning and Parzen windows, respectively.

Fourier transforms of the same filters [10]. Other filters could be employed [10,11], but they differ little from those used here. The three filters vary in their treatment of the frequency spectrum: the Welch window weakly filters low frequencies and rapidly falls to zero at high frequencies; the Parzen window has the most abrupt behaviour at low frequencies; the Hanning window treats low frequencies more gently but descends more rapidly at high frequencies.

RESULTS

Using the Welch window as an example, the effect of the non-rectangular windows on the estimated signal and the noise power spectra that were used in Fig. 2(a) for the rectangular window (80 dB signal/noise) is shown (Fig. 4(a)). The noise power spectrum is no longer cut off at frequency w_c but is practically constant across the whole frequency range; the signal power spectrum falls gently to zero. The reconstructed signal (Fig. 4(a)) has been cleaned of most noise, giving the shape of the original signal, and the parasitic oscillation has been removed. Comparing the areas under the power spectra before and after filtering, for the value $B = 3.909$ used here, shows that 97.5% of the "energy" of the original signal is conserved (practically the same value as with the rectangular window).

Using the two other filters gives the results shown in Figs. 4(c) (Hanning window) and 4(d) (Parzen window). The same parameter B has been used as before, which gives the same cut-off frequency, and, given the nature of the two windows, greater smoothing of the signal (the energy loss approaches 3%). A smaller value of B (equal to a higher cut-off frequency) could be used in these two cases, since there is no oscillation and the signal is excessively distorted (above all for the Parzen window).

Similar results were obtained for the other signal-to-noise ratios (using larger values of B in accordance with increasing signal-to-noise ratio). With B fixed, the Welch window gives the gentlest filtering, followed by the Hanning window and then the Parzen window, which treats the signal more severely.

CONCLUSIONS

Frequency filters that abruptly cut the frequency spectrum of a signal introduce an oscillation that limits their use. All of the non-rectangular filters described here are free from this drawback. A single parameter completely defines the filters, establishing the cut-off frequency and the fraction of energy of the power spectrum of the signal that is lost in the smoothing process.

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