

Figure 13.3.1. Optimal (Wiener) filtering. The power spectrum of signal plus noise shows a signal peak added to a noise tail. The tail is extrapolated back into the signal region as a “noise model.” Subtracting gives the “signal model.” The models need not be accurate for the method to be useful. A simple algebraic combination of the models gives the optimal filter (see text).

Don’t waste your time on this line of thought. The scheme converges to a signal of $S(f) = 0$. Converging iterative methods do exist; this just isn’t one of them.

You can use the routine `four1` (§12.2) or `realft` (§12.3) to FFT your data when you are constructing an optimal filter. To apply the filter to your data, you can use the methods described in §13.1. The specific routine `conv1v` is not needed for optimal filtering, since your filter is constructed in the frequency domain to begin with. If you are also deconvolving your data with a known response function, however, you can modify `conv1v` to multiply by your optimal filter just before it takes the inverse Fourier transform.

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13.4 Power Spectrum Estimation Using the FFT

In the previous section we “informally” estimated the power spectral density of a function $c(t)$ by taking the modulus-squared of the discrete Fourier transform of some

finite, sampled stretch of it. In this section we'll do roughly the same thing, but with considerably greater attention to details. Our attention will uncover some surprises.

The first detail is power spectrum (also called a power spectral density or PSD) normalization. In general there is *some* relation of proportionality between a measure of the squared amplitude of the function and a measure of the amplitude of the PSD. Unfortunately there are several different conventions for describing the normalization in each domain, and many opportunities for getting wrong the relationship between the two domains. Suppose that our function $c(t)$ is sampled at N points to produce values $c_0 \dots c_{N-1}$, and that these points span a range of time T , that is $T = (N - 1)\Delta$, where Δ is the sampling interval. Then here are several different descriptions of the total power:

$$\sum_{j=0}^{N-1} |c_j|^2 \equiv \text{“sum squared amplitude”} \quad (13.4.1)$$

$$\frac{1}{T} \int_0^T |c(t)|^2 dt \approx \frac{1}{N} \sum_{j=0}^{N-1} |c_j|^2 \equiv \text{“mean squared amplitude”} \quad (13.4.2)$$

$$\int_0^T |c(t)|^2 dt \approx \Delta \sum_{j=0}^{N-1} |c_j|^2 \equiv \text{“time-integral squared amplitude”} \quad (13.4.3)$$

PSD estimators, as we shall see, have an even greater variety. In this section, we consider a class of them that give estimates at discrete values of frequency f_i , where i will range over integer values. In the next section, we will learn about a different class of estimators that produce estimates that are continuous functions of frequency f . Even if it is agreed always to relate the PSD normalization to a particular description of the function normalization (e.g., 13.4.2), there are at least the following possibilities: The PSD is

- defined for discrete positive, zero, and negative frequencies, and its sum over these is the function mean squared amplitude
- defined for zero and discrete positive frequencies only, and its sum over these is the function mean squared amplitude
- defined in the Nyquist interval from $-f_c$ to f_c , and its integral over this range is the function mean squared amplitude
- defined from 0 to f_c , and its integral over this range is the function mean squared amplitude

It *never* makes sense to integrate the PSD of a sampled function outside of the Nyquist interval $-f_c$ and f_c since, according to the sampling theorem, power there will have been aliased into the Nyquist interval.

It is hopeless to define enough notation to distinguish all possible combinations of normalizations. In what follows, we use the notation $P(f)$ to mean *any* of the above PSDs, stating in each instance how the particular $P(f)$ is normalized. Beware the inconsistent notation in the literature.

The method of power spectrum estimation used in the previous section is a simple version of an estimator called, historically, the *periodogram*. If we take an N -point sample of the function $c(t)$ at equal intervals and use the FFT to compute

its discrete Fourier transform

$$C_k = \sum_{j=0}^{N-1} c_j e^{2\pi ijk/N} \quad k = 0, \dots, N-1 \quad (13.4.4)$$

then the periodogram estimate of the power spectrum is defined at $N/2 + 1$ frequencies as

$$\begin{aligned} P(0) &= P(f_0) = \frac{1}{N^2} |C_0|^2 \\ P(f_k) &= \frac{1}{N^2} \left[|C_k|^2 + |C_{N-k}|^2 \right] \quad k = 1, 2, \dots, \left(\frac{N}{2} - 1 \right) \\ P(f_c) &= P(f_{N/2}) = \frac{1}{N^2} |C_{N/2}|^2 \end{aligned} \quad (13.4.5)$$

where f_k is defined only for the zero and positive frequencies

$$f_k \equiv \frac{k}{N\Delta} = 2f_c \frac{k}{N} \quad k = 0, 1, \dots, \frac{N}{2} \quad (13.4.6)$$

By Parseval's theorem, equation (12.1.10), we see immediately that equation (13.4.5) is normalized so that the sum of the $N/2 + 1$ values of P is equal to the mean squared amplitude of the function c_j .

We must now ask this question. In what sense is the periodogram estimate (13.4.5) a "true" estimator of the power spectrum of the underlying function $c(t)$? You can find the answer treated in considerable detail in the literature cited (see, e.g., [1] for an introduction). Here is a summary.

First, is the *expectation value* of the periodogram estimate equal to the power spectrum, i.e., is the estimator correct on average? Well, yes and no. We wouldn't really expect one of the $P(f_k)$'s to equal the continuous $P(f)$ at *exactly* f_k , since f_k is supposed to be representative of a whole frequency "bin" extending from halfway from the preceding discrete frequency to halfway to the next one. We *should* be expecting the $P(f_k)$ to be some kind of average of $P(f)$ over a narrow window function centered on its f_k . For the periodogram estimate (13.4.6) that window function, as a function of s the frequency offset *in bins*, is

$$W(s) = \frac{1}{N^2} \left[\frac{\sin(\pi s)}{\sin(\pi s/N)} \right]^2 \quad (13.4.7)$$

Notice that $W(s)$ has oscillatory lobes but, apart from these, falls off only about as $W(s) \approx (\pi s)^{-2}$. This is not a very rapid fall-off, and it results in significant *leakage* (that is the technical term) from one frequency to another in the periodogram estimate. Notice also that $W(s)$ happens to be zero for s equal to a nonzero integer. This means that if the function $c(t)$ is a pure sine wave of frequency exactly equal to one of the f_k 's, then there will be *no* leakage to adjacent f_k 's. But this is not the characteristic case! If the frequency is, say, one-third of the way between two adjacent f_k 's, then the leakage will extend *well* beyond those two adjacent bins. The solution to the problem of leakage is called *data windowing*, and we will discuss it below.

Turn now to another question about the periodogram estimate. What is the variance of that estimate as N goes to infinity? In other words, as we take more sampled points from the original function (either sampling a longer stretch of data at the same sampling rate, or else by resampling the same stretch of data with a faster sampling rate), then how much more accurate do the estimates P_k become? The unpleasant answer is that the periodogram estimates *do not become more accurate at all!* In fact, the variance of the periodogram estimate at a frequency f_k is always equal to the square of its expectation value at that frequency. In other words, the standard deviation is always 100 percent of the value, independent of N ! How can this be? Where did all the information go as we added points? It all went into producing estimates at a greater number of discrete frequencies f_k . If we sample a longer run of data using the same sampling rate, then the Nyquist critical frequency f_c is unchanged, but we now have finer frequency resolution (more f_k 's) within the Nyquist frequency interval; alternatively, if we sample the same length of data with a finer sampling interval, then our frequency resolution is unchanged, but the Nyquist range now extends up to a higher frequency. In neither case do the additional samples reduce the variance of any one particular frequency's estimated PSD.

You don't have to live with PSD estimates with 100 percent standard deviations, however. You simply have to know some techniques for reducing the variance of the estimates. Here are two techniques that are very nearly identical mathematically, though different in implementation. The first is to compute a periodogram estimate with finer discrete frequency spacing than you really need, and then to sum the periodogram estimates at K consecutive discrete frequencies to get one "smoother" estimate at the mid frequency of those K . The variance of that summed estimate will be smaller than the estimate itself by a factor of exactly $1/K$, i.e., the standard deviation will be smaller than 100 percent by a factor $1/\sqrt{K}$. Thus, to estimate the power spectrum at $M + 1$ discrete frequencies between 0 and f_c inclusive, you begin by taking the FFT of $2MK$ points (which number had better be an integer power of two!). You then take the modulus square of the resulting coefficients, add positive and negative frequency pairs, and divide by $(2MK)^2$, all according to equation (13.4.5) with $N = 2MK$. Finally, you "bin" the results into summed (not averaged) groups of K . This procedure is very easy to program, so we will not bother to give a routine for it. The reason that you sum, rather than average, K consecutive points is so that your final PSD estimate will preserve the normalization property that the sum of its $M + 1$ values equals the mean square value of the function.

A second technique for estimating the PSD at $M + 1$ discrete frequencies in the range 0 to f_c is to partition the original sampled data into K segments each of $2M$ consecutive sampled points. Each segment is separately FFT'd to produce a periodogram estimate (equation 13.4.5 with $N \equiv 2M$). Finally, the K periodogram estimates are averaged at each frequency. It is this final averaging that reduces the variance of the estimate by a factor K (standard deviation by \sqrt{K}). This second technique is computationally more efficient than the first technique above by a modest factor, since it is logarithmically more efficient to take many shorter FFTs than one longer one. The principal advantage of the second technique, however, is that only $2M$ data points are manipulated at a single time, not $2KM$ as in the first technique. This means that the second technique is the natural choice for processing long runs of data, as from a magnetic tape or other data record. We will give a routine later for implementing this second technique, but we need first to return to the matters of

leakage and data windowing which were brought up after equation (13.4.7) above.

Data Windowing

The purpose of data windowing is to modify equation (13.4.7), which expresses the relation between the spectral estimate P_k at a discrete frequency and the actual underlying continuous spectrum $P(f)$ at nearby frequencies. In general, the spectral power in one “bin” k contains leakage from frequency components that are actually s bins away, where s is the independent variable in equation (13.4.7). There is, as we pointed out, quite substantial leakage even from moderately large values of s .

When we select a run of N sampled points for periodogram spectral estimation, we are in effect multiplying an infinite run of sampled data c_j by a window function in time, one that is zero except during the total sampling time $N\Delta$, and is unity during that time. In other words, the data are windowed by a square window function. By the convolution theorem (12.0.9; but interchanging the roles of f and t), the Fourier transform of the product of the data with this square window function is equal to the convolution of the data’s Fourier transform with the window’s Fourier transform. In fact, we determined equation (13.4.7) as nothing more than the square of the discrete Fourier transform of the unity window function.

$$W(s) = \frac{1}{N^2} \left[\frac{\sin(\pi s)}{\sin(\pi s/N)} \right]^2 = \frac{1}{N^2} \left| \sum_{k=0}^{N-1} e^{2\pi i s k/N} \right|^2 \quad (13.4.8)$$

The reason for the leakage at large values of s , is that the square window function turns on and off so rapidly. Its Fourier transform has substantial components at high frequencies. To remedy this situation, we can multiply the input data c_j , $j = 0, \dots, N-1$ by a window function w_j that changes more gradually from zero to a maximum and then back to zero as j ranges from 0 to N . In this case, the equations for the periodogram estimator (13.4.4–13.4.5) become

$$D_k \equiv \sum_{j=0}^{N-1} c_j w_j e^{2\pi i j k/N} \quad k = 0, \dots, N-1 \quad (13.4.9)$$

$$\begin{aligned} P(0) &= P(f_0) = \frac{1}{W_{ss}} |D_0|^2 \\ P(f_k) &= \frac{1}{W_{ss}} \left[|D_k|^2 + |D_{N-k}|^2 \right] \quad k = 1, 2, \dots, \left(\frac{N}{2} - 1 \right) \\ P(f_c) &= P(f_{N/2}) = \frac{1}{W_{ss}} |D_{N/2}|^2 \end{aligned} \quad (13.4.10)$$

where W_{ss} stands for “window squared and summed,”

$$W_{ss} \equiv N \sum_{j=0}^{N-1} w_j^2 \quad (13.4.11)$$

and f_k is given by (13.4.6). The more general form of (13.4.7) can now be written in terms of the window function w_j as

$$W(s) = \frac{1}{W_{ss}} \left| \sum_{k=0}^{N-1} e^{2\pi i s k / N} w_k \right|^2 \quad (13.4.12)$$

$$\approx \frac{1}{W_{ss}} \left| \int_{-N/2}^{N/2} \cos(2\pi s k / N) w(k - N/2) dk \right|^2$$

Here the approximate equality is useful for practical estimates, and holds for any window that is left-right symmetric (the usual case), and for $s \ll N$ (the case of interest for estimating leakage into nearby bins). The continuous function $w(k - N/2)$ in the integral is meant to be some smooth function that passes through the points w_k .

There is a lot of perhaps unnecessary lore about choice of a window function, and practically every function that rises from zero to a peak and then falls again has been named after someone. A few of the more common (also shown in Figure 13.4.1) are:

$$w_j = 1 - \left| \frac{j - \frac{1}{2}N}{\frac{1}{2}N} \right| \equiv \text{“Bartlett window”} \quad (13.4.13)$$

(The “Parzen window” is very similar to this.)

$$w_j = \frac{1}{2} \left[1 - \cos \left(\frac{2\pi j}{N} \right) \right] \equiv \text{“Hann window”} \quad (13.4.14)$$

(The “Hamming window” is similar but does not go exactly to zero at the ends.)

$$w_j = 1 - \left(\frac{j - \frac{1}{2}N}{\frac{1}{2}N} \right)^2 \equiv \text{“Welch window”} \quad (13.4.15)$$

We are inclined to follow Welch in recommending that you use either (13.4.13) or (13.4.15) in practical work. However, at the level of this book, there is effectively *no difference* between any of these (or similar) window functions. Their difference lies in subtle trade-offs among the various figures of merit that can be used to describe the narrowness or peakedness of the spectral leakage functions computed by (13.4.12). These figures of merit have such names as: *highest sidelobe level (dB)*, *sidelobe fall-off (dB per octave)*, *equivalent noise bandwidth (bins)*, *3-dB bandwidth (bins)*, *scallop loss (dB)*, *worst case process loss (dB)*. Roughly speaking, the principal trade-off is between making the central peak as narrow as possible versus making the tails of the distribution fall off as rapidly as possible. For details, see (e.g.) [2]. Figure 13.4.2 plots the leakage amplitudes for several windows already discussed.

There is particularly a lore about window functions that rise smoothly from zero to unity in the first small fraction (say 10 percent) of the data, then stay at unity until the last small fraction (again say 10 percent) of the data, during which the window function falls smoothly back to zero. These windows will squeeze a little bit of extra narrowness out of the main lobe of the leakage function (never as

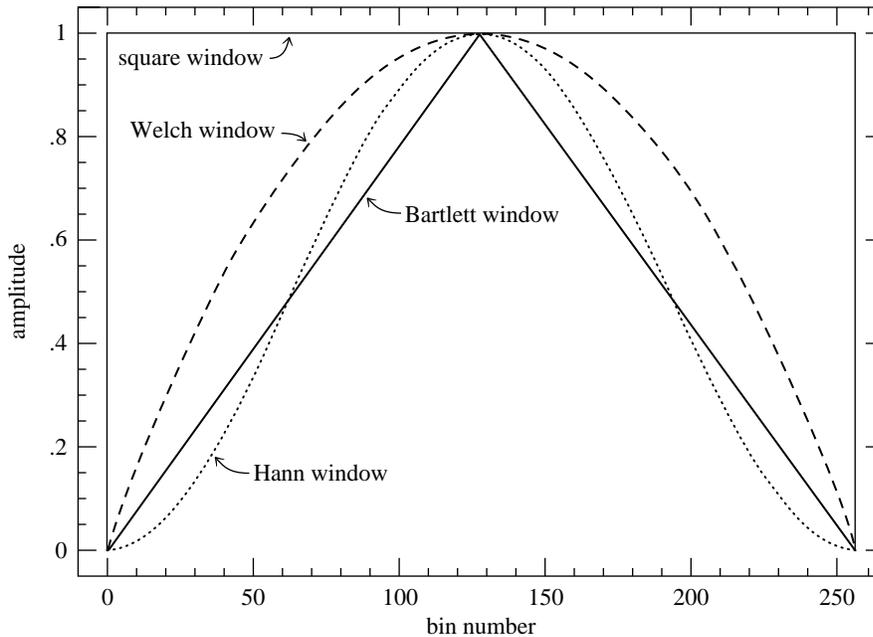


Figure 13.4.1. Window functions commonly used in FFT power spectral estimation. The data segment, here of length 256, is multiplied (bin by bin) by the window function before the FFT is computed. The square window, which is equivalent to no windowing, is least recommended. The Welch and Bartlett windows are good choices.

much as a factor of two, however), but trade this off by widening the leakage tail by a significant factor (e.g., the reciprocal of 10 percent, a factor of ten). If we distinguish between the *width* of a window (number of samples for which it is at its maximum value) and its *rise/fall time* (number of samples during which it rises and falls); and if we distinguish between the *FWHM* (full width to half maximum value) of the leakage function's main lobe and the *leakage width* (full width that contains half of the spectral power that is not contained in the main lobe); then these quantities are related roughly by

$$(\text{FWHM in bins}) \approx \frac{N}{(\text{window width})} \quad (13.4.16)$$

$$(\text{leakage width in bins}) \approx \frac{N}{(\text{window rise/fall time})} \quad (13.4.17)$$

For the windows given above in (13.4.13)–(13.4.15), the effective window widths and the effective window rise/fall times are both of order $\frac{1}{2}N$. Generally speaking, we feel that the advantages of windows whose rise and fall times are only small fractions of the data length are minor or nonexistent, and we avoid using them. One sometimes hears it said that flat-topped windows “throw away less of the data,” but we will now show you a better way of dealing with that problem by use of overlapping data segments.

Let us now suppose that we have chosen a window function, and that we are ready to segment the data into K segments of $N = 2M$ points. Each segment will be FFT'd, and the resulting K periodograms will be averaged together to obtain a

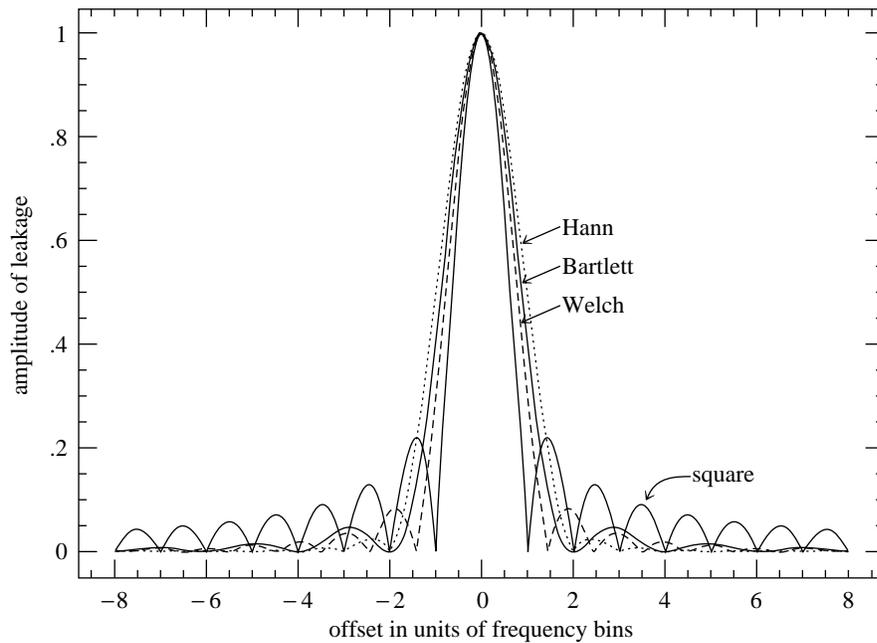


Figure 13.4.2. Leakage functions for the window functions of Figure 13.4.1. A signal whose frequency is actually located at zero offset “leaks” into neighboring bins with the amplitude shown. The purpose of windowing is to reduce the leakage at large offsets, where square (no) windowing has large sidelobes. Offset can have a fractional value, since the actual signal frequency can be located between two frequency bins of the FFT.

PSD estimate at $M + 1$ frequency values from 0 to f_c . We must now distinguish between two possible situations. We might want to obtain the smallest variance from a fixed amount of computation, without regard to the number of data points used. This will generally be the goal when the data are being gathered in real time, with the data-reduction being computer-limited. Alternatively, we might want to obtain the smallest variance from a fixed number of available sampled data points. This will generally be the goal in cases where the data are already recorded and we are analyzing it after the fact.

In the first situation (smallest spectral variance per computer operation), it is best to segment the data without any overlapping. The first $2M$ data points constitute segment number 1; the next $2M$ data points constitute segment number 2; and so on, up to segment number K , for a total of $2KM$ sampled points. The variance in this case, relative to a single segment, is reduced by a factor K .

In the second situation (smallest spectral variance per data point), it turns out to be optimal, or very nearly optimal, to overlap the segments by one half of their length. The first and second sets of M points are segment number 1; the second and third sets of M points are segment number 2; and so on, up to segment number K , which is made of the K th and $K + 1$ st sets of M points. The total number of sampled points is therefore $(K + 1)M$, just over half as many as with nonoverlapping segments. The reduction in the variance is not a full factor of K , since the segments are not statistically independent. It can be shown that the variance is instead reduced by a factor of about $9K/11$ (see the paper by Welch in [3]). This is, however,

significantly better than the reduction of about $K/2$ that would have resulted if the same *number* of data points were segmented without overlapping.

We can now codify these ideas into a routine for spectral estimation. While we generally avoid input/output coding, we make an exception here to show how data are read sequentially in one pass through a data file (referenced through the parameter `FILE *fp`). Only a small fraction of the data is in memory at any one time. Note that `spctrm` returns the power at M , not $M + 1$, frequencies, omitting the component $P(f_c)$ at the Nyquist frequency. It would also be straightforward to include that component.

```
#include <math.h>
#include <stdio.h>
#include "nrutil.h"
#define WINDOW(j,a,b) (1.0-fabs((((j)-1)-(a))*(b))) /* Bartlett */
/* #define WINDOW(j,a,b) 1.0 /* Square */
/* #define WINDOW(j,a,b) (1.0-SQR((((j)-1)-(a))*(b))) /* Welch */

void spctrm(FILE *fp, float p[], int m, int k, int overlap)
Reads data from input stream specified by file pointer fp and returns as p[j] the data's power
(mean square amplitude) at frequency (j-1)/(2*m) cycles per gridpoint, for j=1,2,...,m,
based on (2*k+1)*m data points (if overlap is set true (1)) or 4*k*m data points (if overlap
is set false (0)). The number of segments of the data is 2*k in both cases: The routine calls
four1 k times, each call with 2 partitions each of 2*m real data points.
{
    void four1(float data[], unsigned long nn, int isign);
    int mm,m44,m43,m4,kk,joffn,joff,j2,j;
    float w,facp,facm,*w1,*w2,sumw=0.0,den=0.0;

    mm=m+m;                                     Useful factors.
    m43=(m4=mm+mm)+3;
    m44=m43+1;
    w1=vector(1,m4);
    w2=vector(1,m);
    facm=m;
    facp=1.0/m;
    for (j=1;j<=mm;j++) sumw += SQR(WINDOW(j,facm,facp));
    Accumulate the squared sum of the weights.
    for (j=1;j<=m;j++) p[j]=0.0;                 Initialize the spectrum to zero.
    if (overlap)                                 Initialize the "save" half-buffer.
        for (j=1;j<=m;j++) fscanf(fp,"%f",&w2[j]);
    for (kk=1;kk<=k;kk++) {
    Loop over data set segments in groups of two.
        for (joff = -1;joff<=0;joff++) {         Get two complete segments into workspace.
            if (overlap) {
                for (j=1;j<=m;j++) w1[joff+j]=w2[j];
                for (j=1;j<=m;j++) fscanf(fp,"%f",&w2[j]);
                joffn=joff+mm;
                for (j=1;j<=m;j++) w1[joffn+j]=w2[j];
            } else {
                for (j=joff+2;j<=m4;j+=2)
                    fscanf(fp,"%f",&w1[j]);
            }
        }
    }
    for (j=1;j<=mm;j++) {                         Apply the window to the data.
        j2=j+j;
        w=WINDOW(j,facm,facp);
        w1[j2] *= w;
        w1[j2-1] *= w;
    }
    four1(w1,mm,1);                                Fourier transform the windowed data.
    p[1] += (SQR(w1[1])+SQR(w1[2]));              Sum results into previous segments.
}
```

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```

    for (j=2;j<=m;j++) {
        j2=j+j;
        p[j] += (SQR(w1[j2])+SQR(w1[j2-1])
                +SQR(w1[m44-j2])+SQR(w1[m43-j2]));
    }
    den += sumw;
}
den *= m4;
for (j=1;j<=m;j++) p[j] /= den;
free_vector(w2,1,m);
free_vector(w1,1,m4);
}

```

Correct normalization.
Normalize the output.

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13.5 Digital Filtering in the Time Domain

Suppose that you have a signal that you want to filter digitally. For example, perhaps you want to apply *high-pass* or *low-pass* filtering, to eliminate noise at low or high frequencies respectively; or perhaps the interesting part of your signal lies only in a certain frequency band, so that you need a *bandpass* filter. Or, if your measurements are contaminated by 60 Hz power-line interference, you may need a *notch filter* to remove only a narrow band around that frequency. This section speaks particularly about the case in which you have chosen to do such filtering in the time domain.

Before continuing, we hope you will reconsider this choice. Remember how convenient it is to filter in the Fourier domain. You just take your whole data record, FFT it, multiply the FFT output by a filter function $\mathcal{H}(f)$, and then do an inverse FFT to get back a filtered data set in time domain. Here is some additional background on the Fourier technique that you will want to take into account.

- Remember that you must define your filter function $\mathcal{H}(f)$ for both positive and negative frequencies, and that the magnitude of the frequency extremes is always the Nyquist frequency $1/(2\Delta)$, where Δ is the sampling interval. The magnitude of the smallest nonzero frequencies in the FFT is $\pm 1/(N\Delta)$, where N is the number of (complex) points in the FFT. The positive and negative frequencies to which this filter are applied are arranged in wrap-around order.
- If the measured data are real, and you want the filtered output also to be real, then your arbitrary filter function should obey $\mathcal{H}(-f) = \mathcal{H}(f)^*$. You can arrange this most easily by picking an \mathcal{H} that is real and even in f .