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Weighted fit of optical spectra

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Abstract

Optical power spectra obtained from experiments or from numerical simulations are probabilistic in nature. When fitting such spectra to few-parameter analytical line shapes, the results from a weighted nonlinear least squares fit are significantly better than those from an unweighted fit. This is demonstrated by fitting a Lorentzian to directly simulated power spectra and to power spectra obtained from a rate-equation simulation of a diode laser output.

1. Introduction

Fitting of optical power spectra is an important tool for laser physicists and spectroscopists [1–3]. In simulations of the dynamic behaviour of a laser one often calculates the optical power spectrum in order to fit it with a theoretical curve so as to determine certain relevant parameters, e.g. linewidth and central frequency. Such numerical spectra are often obtained from a fast-fourier-transform (and then are called periodogram) of a noisy time series and, hence, are usually very noisy themselves. Even after averaging over several ensemble-members of time series the spectrum is still noisy and the question arises how one can best fit the expected theoretical shape to such a spectrum, the former usually being smooth. Similarly, theoretical shapes containing few parameters can be fitted to a measured spectrum in order to estimate these parameters and also here one is confronted with the inherent probabilistic nature of a spectrum. In fact, in the fitting it is necessary to take into account the probabilistic properties consistently. Only by such a procedure, the residuals of the fit can be evaluated and the model adequacy established [4].

In particular, the measurement of the power spectral density at a certain frequency must be regarded as proportional to a sample from a χ^2-distribution [5] which implies a standard deviation proportional to the mean. Carroll and Ruppert (Ref. [6](p.16)) say: "if the standard deviations vary by a factor of 3:1 or more, then weighting will generally be called for". Here we want to investigate quantitatively the importance of weighting in fitting optical spectra. Even though in one of the above mentioned papers [2] a weighted fit is mentioned, yet to our best knowledge the importance of a weighted fit seems not to be generally known. It is therefore the purpose of this letter to demonstrate quantitatively the advantages of the weighted fit by means of a simulation study. As an application a simple Lorentzian line shape will be fitted to a series of power spectra of a single-mode semiconductor laser obtained by numerical integration of the rate equations.

2. Stochastic description of the spectrum

Let a power spectrum with theoretical spectral profile $W(\nu;\theta)$, where ν is the frequency, depend upon several parameters contained in the vector θ. In case of the Lorentzian profile here studied, W has the explicit form

$$W(\nu;\theta)=\theta_3/[1+(2(\nu-\theta_1)/\theta_2)^2]\,, \qquad (1)$$

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where $\theta=(\theta_1, \theta_2, \theta_3)$ consists of three parameters: the central frequency θ_1, the linewidth θ_2, and the amplitude θ_3. This model is termed nonlinear because the derivative of W with respect to a parameter still depends on at least one of the parameters [4]. Two ways of estimating the unknown parameters θ will be compared: (a) unweighted nonlinear least squares, and (b) weighted nonlinear least squares with weights $1/W^2(\nu;\theta)$. According to Carroll and Ruppert [6] when the data are distributed according to the χ^2-distribution this weighted least squares estimate is equal to the maximum likelihood estimate, which is the best possible estimate. As W is usually not known beforehand, for the actual weighted fit we must proceed iteratively: first we take as weighting function the profile estimated from an unweighted fit, second we use the resulting profile to perform a refined weighted fit (so called iteratively reweighted least squares [6]).

In order to illustrate the method in a direct simulation, data points w_n are produced by multiplying the theoretical spectral profile (of which (1) is an example) by a sample drawn from a χ^2-distribution according to [5]

$$w_n = W(\nu_n;\theta)\chi^2_{d,n}/d\,, \quad n=1, \ldots, N\,, \tag{2}$$

where $W(\nu_n;\theta)$ is the spectral profile at frequency ν_n. $\chi^2_{d,n}$ is the nth sample drawn from a χ^2-distribution with d degrees of freedom. N is the total number of simulated data points. For an ensemble average over k periodograms we have $d=2k$. The expectation value of w_n is given by

$$E[w_n] = W(\nu_n;\theta)\,, \tag{3}$$

since $E[\chi^2_{d,n}]=d$. Furthermore the variance of w_n is proportional to the square of the mean:

$$\begin{aligned}\mathrm{var}(w_n) &= (W(\nu_n;\theta)/d)^2\,\mathrm{var}(\chi^2_{d,n})\\ &= (2/d)W^2(\nu_n;\theta)\end{aligned} \tag{4}$$

since $\mathrm{var}(\chi^2_{d,n})=2d$. Note that the variance is highest at the top of the spectrum. Thus, it can be seen that for a single, unaveraged spectrum ($d=2$ in (2) and (4)) the standard deviation at a given frequency is equal to the expectation value. This explains why the fluctuations cannot be made smaller by increasing the frequency resolution.

3. Fit of directly simulated spectra

For the direct simulation study we use a Lorentzian profile (1) with parameters inspired by the application to be described in section 4. We choose the central frequency $\theta_1=0$ MHz, the full linewidth at half maximum $\theta_2=50$ MHz, the amplitude $\theta_3=100$ and the sampling frequencies $\nu_n=(n-201)0.5$ MHz, $n=1, \ldots, N=401$. A typical simulated power spectrum according to (2) using a χ^2-distribution with $d=16$ degrees of freedom is shown in Fig. 1A. The weighted

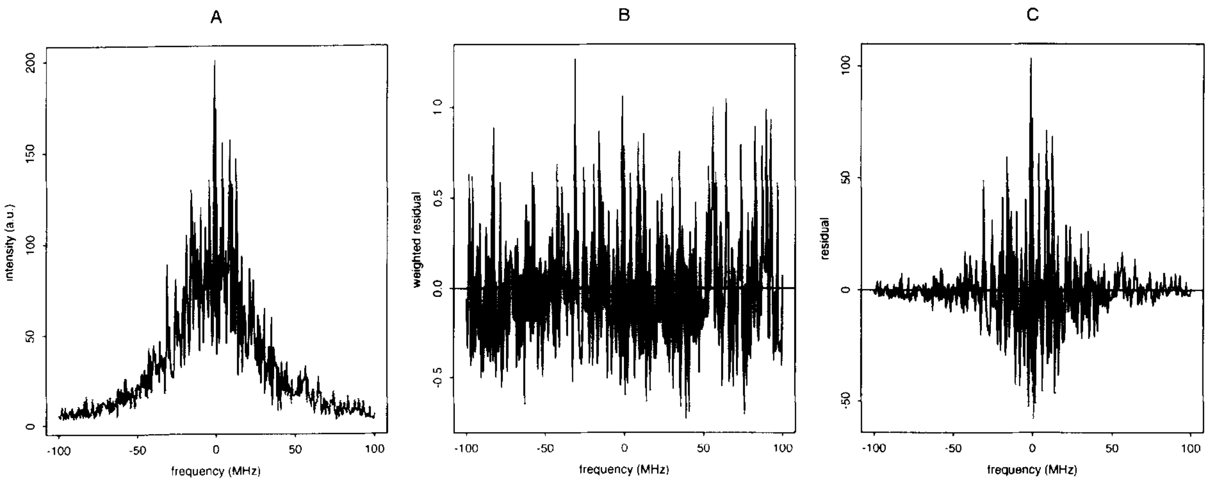

Fig. 1. (A) Directly simulated power spectrum, $N=401$ data points, (B) weighted residuals resulting from weighted fit, (C) residuals resulting from unweighted fit.

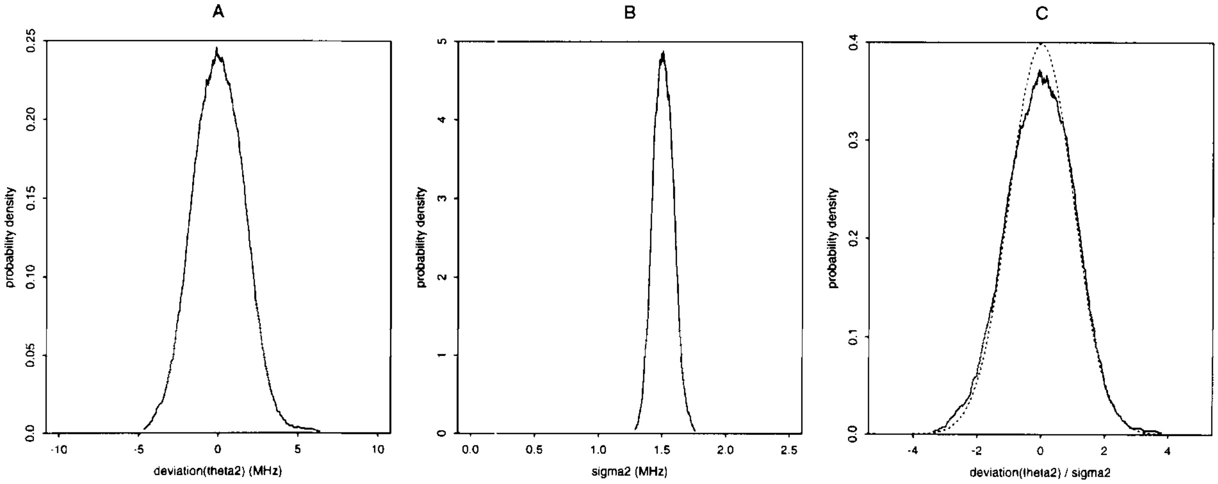

Fig. 2. Distributions estimated from weighted fit, (A) deviation of estimated linewidth parameter $\hat{\theta}_2 - \theta_2$, (B) approximate standard error $\hat{\sigma}_2$, (C) ratio of these two $(\hat{\theta}_2 - \theta_2)/\hat{\sigma}_2$ (solid line) and t_{df} distribution (dotted line). Further explanation in text.

residuals of a weighted fit are satisfactory, i.e. they behave randomly and show constant variance (Fig. 1B), whereas the residuals of an unweighted fit possess a variance which depends upon the function value (Fig. 1C). Note that there are more negative residuals, which is explained by the asymmetry of the χ^2-distribution. In order to investigate quantitatively the properties of a weighted versus an unweighted fit we performed 1001 simulations. This resulted in 1001 realizations of the estimates $(\hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_3)$ and their standard errors $(\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3)$ (for the calculation of these standard errors see e.g. [4]). We summarize the resulting estimates for the parameters and their standard errors by estimating smoothed probability densities using the Splus function *ksmooth* [11]. Fig. 2A depicts the distribution of deviations in the linewidth parameter $\hat{\theta}_2 - \theta_2$ (the difference between the estimated and the real value) of a weighted nonlinear least squares fit. It is symmetric around zero with a width of about 4 MHz. The distribution of the standard error $\hat{\sigma}_2$ (Fig. 2B) is narrowly peaked around 1.5 MHz. The ratio of the deviation and the estimated standard error should be distributed approximately as a Student's t-variable with degrees of freedom df equal to the number of data points (N) minus the number of parameters (3) (in this case, $df = 398$, the t_{df} distribution is close to the normal distribution). The distribution of this ratio is depicted by the solid line in Fig. 2C, whereas the dotted line represents the t_{df} distribution. There is a large similarity. The small differences which are present are attributed to the linear approximation of the standard errors [4].

Let us now make a comparison with the results of an unweighted fit for which the residuals do not behave well (Fig. 1C). The linewidth parameter summary for this case is shown in Fig. 3. We note that the distribution of the deviation in Fig. 3A is wider by about a factor of 1.5 compared with Fig. 2A. Likewise the estimated standard errors are on average larger (compare Fig. 2B and Fig. 3B) and are more broadly peaked around 1.8 MHz. Furthermore, the differences between solid and dotted lines are much more pronounced in Fig. 3C than in Fig. 2C, note the tails in Fig. 3C, which means that for large deviations the unweighted fit predicts more precise results than are actually achieved. We have investigated the differences between weighted and unweighted fit as a function of the number of data points N (and thus the spectral resolution $\Delta\nu$) and the signal to noise ratio (which is proportional to the square root of the number of degrees of freedom d of the χ^2-distribution). The results shown in Table 1 confirm that the weighted fit is superior to the unweighted fit for all conditions investigated. For sample sizes ranging from small ($N = 25$) to large ($N = 1601$) and different signal to noise ratios the root mean square deviation (of θ_2) of the unweighted fit is about 1.5 times as large as from the weighted fit. Only with the weighted fit the root mean square standard error σ_2 is about equal to the rms deviation of θ_2, which is necessary for a consistent fit.

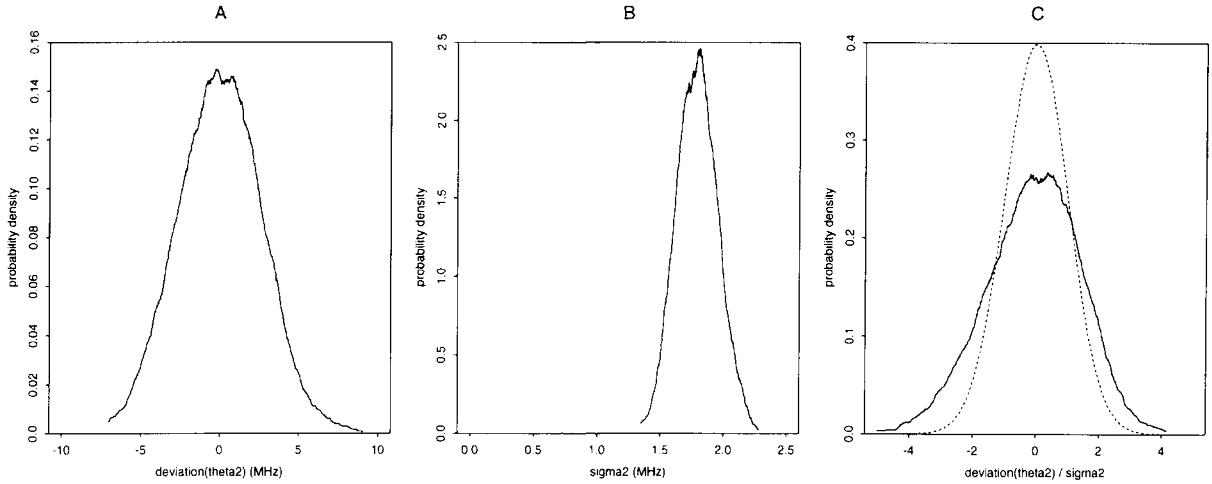

Fig. 3. Distributions estimated from unweighted fit. Lay out as in Fig. 2.

We conclude from this direct simulation study that the weighted fit is to be preferred for three reasons: (a) the weighted residuals behave well when the model is adequate; in contrast, if systematic deviations of these weighted residuals from randomness or constant variance are observed, this indicates model inadequacy, (b) the weighted fit is more accurate and results in smaller deviations of the estimated parameters, and (c) the ratio of the deviation and the standard error is closer to the t_{df} distribution, meaning a larger probability that the estimated parameters are correct [4].

4. Fit of the power spectrum of a simulated diode laser

As an application we consider the fit of the power spectrum of a single-mode semiconductor laser. In this type of laser the spontaneous emission is responsible for a central Lorentzian line shape [7] with sidebands at the relaxation oscillation frequency [8,9]. The dynamic behaviour of the intracavity optical field and the carrier-inversion is described by the standard rate equations [10] where Langevin noise terms account for spontaneous emission. These coupled nonlinear stochastic differential equations are numerically integrated using a 6th order Runge-Kutta algorithm with a step size of 1/60 of the relaxation oscillation period (the smallest time scale involved in the model). The resulting optical field can be Fourier transformed using an FFT to yield the periodogram that represents a single unaveraged spectrum. We can also divide the time series in a number of smaller blocks and perform an FFT on each block separately. The resulting power spectra will then loose resolution, as the latter is inversely proportional to the block length. If one then averages those FFT power spectra, thereby increasing the number of degrees of freedom d in (2) and (4), a spectrum with smaller variance is obtained. This illustrates the trade off between variance and resolution.

Table 1
Root mean square deviation and root mean square standard error σ_2 (between parentheses) of linewidth parameter θ_2 as a function of number of data points N, resolution $\Delta\nu$ and degrees of freedom d

N	$\Delta\nu$	$d=16$, W	$d=16$	$d=64$, W	$d=64$
25	8	6.9(6.0)	10.1(6.1)	3.3(3.0)	6.0(3.2)
101	2	3.1(3.0)	5.0(3.5)	1.5(1.5)	2.7(1.8)
401	0.5	1.5(1.5)	2.5(1.8)	0.8(0.8)	1.3(0.9)
1601	0.125	0.8(0.8)	1.2(0.9)	0.4(0.4)	0.6(0.5)

Unit is MHz. W indicates from weighted fit.

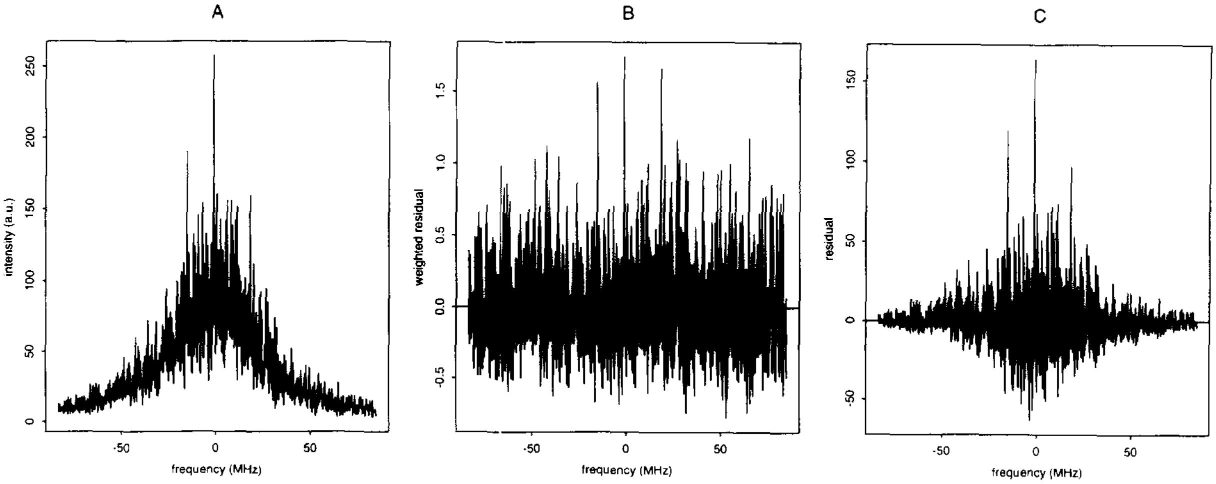

Fig. 4. (A) Power spectrum of a simulated semiconductor laser, $N = 1201$ data points, (B, C) as in Fig. 1.

First we discuss one fit in detail, thereafter we will summarize the results of a series of fits in which the pump current was varied. Dividing the time series in eight blocks of 32768 samples and taking the average of their respective periodograms results in the power spectrum whose central part is shown in Fig. 4A. In this figure we have shifted the frequency axis in such a way that the resonance frequency of the laser without noise lies at 0 MHz. The residuals resulting from a weighted nonlinear least squares fit are shown in Fig. 4B. No systematic deviations are visible in the weighted residuals, and the variance of the weighted residuals appears constant, indicating a satisfactory description of the data by a Lorentzian. The root mean square error of the residuals is equal to 0.356, which is close to the theoretical value of $\sqrt{2/d} = \sqrt{2/(2\times 8)} = 0.354$ (Eq. (4), with 8 periodograms averaged). Thus it is concluded that the fit is excellent, and that the estimated parameters of this central line are $\hat{\theta}_1 = (-1.7 \pm 0.4)$ MHz, $\hat{\theta}_2 = (53.0 \pm 1.0)$ MHz and $\hat{\theta}_3 = 94 \pm 3$. The residuals from an unweighted nonlinear least squares fit are shown in Fig. 4C. The nonconstant variance results in an incomplete description of the data and precludes proper conclusion about the adequacy of the model function. Just for comparison the parameters estimated from an unweighted fit are $\hat{\theta}_1 = (-0.5 \pm 0.4)$ MHz, $\hat{\theta}_2 = (53.5 \pm 1.2)$ MHz and $\hat{\theta}_3 = 93 \pm 2$, which in this particular case is not significantly different from the parameters estimated from the weighted fit. We investigated the linewidth θ_2 as a function of the pump current J for an eight times shorter time series. The estimates resulting from the weighted and the unweighted fit are depicted in Fig. 5A and Fig. 5B, respectively. According to Henry [7] and van Exter [9] the linewidth is proportional to $1/(J/J_{th} - 1)$ where J_{th} is the threshold pump current. The solid lines in Fig. 5 result from a weighted linear regression fit. The quality of this fit is considerably better in Fig. 5A than in Fig. 5B, as can be judged from the root mean square error of 0.94 versus 2.97. The effective slope parameters are (29.0 ± 0.4) MHz and (27.7 ± 0.7) MHz, respectively. Note in passing that both results differ from the theoretical value of 25 MHz predicted by [7] and [9]. This is an intriguing and confusing byproduct of our study, since it is the more reliable result that produces the largest deviation. This could indicate a fundamental shortcoming in the theory or in the numerical integration scheme. A more systematic study would be necessary, but is outside the scope of this paper.

5. Discussion

It has been demonstrated that a weighted fit is necessary for a complete description of a line in a power spectrum. With any number of data points available and with any signal to noise ratio the weighted fit produces superior estimates of the parameters and of their standard errors (Table 1). Hence, these results are relevant for spectra obtained from both simulation and experiment. Although we focused here on Lorentzian

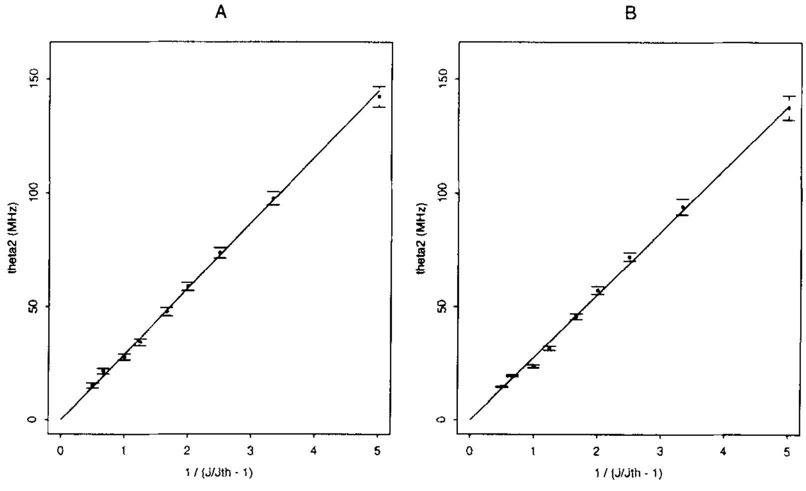

Fig. 5. Estimates of linewidth parameter θ_2 as a function of $1/(J/J_{th}-1)$ where J is the pump current, (A) from weighted fit, (B) from unweighted fit. The lines resulted from a (weighted) linear regression fit.

profiles, the conclusions are also valid for more general profiles. Thus for an adequate fit, which includes evaluation of the adequacy of the line profile used through a test of the residuals, a weighted fit is mandatory.

Summarizing: when fitting optical spectra the variance of the measurements usually is intensity dependent. A description with multiplicative noise (2) is often appropriate and it has been shown that for such cases the results from a weighted nonlinear least squares fit are significantly better than those from an unweighted fit (Fig. 2, Fig. 3, Table 1, Fig. 5). Moreover, taking into account the noise properties produces well distributed weighted residuals (Fig. 1B, Fig. 4B), thus the spectrum is described satisfactorily.

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