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OEFPIL: An Alternative Method for Curve Fitting

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Summary: In recent years, as measurement processes have grown increasingly complex, curve fitting has become a vital tool for aligning theoretical models with observed data. As instrumentation improves, previously overlooked uncertainties must now be addressed for more precise measurements. Uncertainties as well as correlation in both dependent and independent variables should be taken into account. This is illustrated by applying the algorithm OEFPIL to the determination of the internal resistance of an AC source from its loading characteristics.

Keywords: curve fitting, errors-in-variables

Background, Motivation and Objective

Modern metrology extensively uses curve fitting, with non-linear least squares (NLS) being the most common method, although it assumes negligible uncertainties in the independent variable and no data correlation. Errors-in-variables (EIV) addresses these limitations by symmetrically treating uncertainties in both variables as well as taking into account possible correlations. Several approaches can be found in literature e.g. [1, 2, 3] which implement different methods for the estimation of the covariance matrix of the fitted parameters, The Monte Carlo method (MCM) constitutes yet another alternative for the uncertainty estimation. For some of the approaches software implementations are available, e.g. [2, 3] although neither one of them is fully general. In this contribution we present a method named Optimum Estimate of Function Parameters by Iterated Linearization (OEFPIL), which allows a general covariance matrix of the input variables as well as a general function of an arbitrary number of variables, both in implicit and explicit form, and illustrate its use by determining the internal resistance of an AC voltage source from its load characteristics. The internal resistance of the source must be known with high accuracy as it is needed for measurements with different voltmeters.

Method

OEFPIL is based on iterative linearizations of the EIV model with nonlinear parameter constraints specified in implicit form written as

$$\mathbf{X} = \beta + \epsilon, \qquad \mathbf{f}(\mu, \beta) = 0. \tag{1}$$

Here, $\mathbf{X}$ is the vector of direct measurements, μ the (unknown) expectations of $\mathbf{X}$, β the unknown parameters and ϵ the measurement errors. The expectation value of the measurement errors is assumed to be zero and their covariance matrix is assumed to be known. The constraint f is a general, continuous vector function. In terms of curve fitting, β corresponds to the parameters of the fitted curve, $\mathbf{X}$ to the input variables x_i and y_i and f is the function to be fitted (in implicit form). If the constraint is linear in the form of

$$\mathbf{B_1}\mu + \mathbf{B_2}\beta + \mathbf{b} = 0 \tag{2}$$

the estimates of the parameters β and measurements μ can be found using Best Linear Unbiased Estimation (BLUE) [4] as:

$$\hat{\beta} = -\mathbf{U}\mathbf{B_1}^T\mathbf{Q_{11}}\mathbf{b} + \left(\mathbf{I} - \mathbf{U}\mathbf{B_1}^T\mathbf{Q_{11}}\mathbf{B_1}\right)\mathbf{X} \tag{3}$$

$$\hat{\mu} = \mathbf{Q_{21}}\mathbf{b} - \mathbf{Q_{21}}\mathbf{B_1}\mathbf{X}, \tag{4}$$

where $\mathbf{I}$ is a unit matrix and the matrices $\mathbf{Q}_{ij}$ are blocks of the matrix $\mathbf{Q}$ defined as

$$\mathbf{Q} = \begin{pmatrix} \mathbf{Q}_{11} & \mathbf{Q}_{12} \\ \mathbf{Q}_{21} & \mathbf{Q}_{22} \end{pmatrix} = \begin{pmatrix} \mathbf{B}_1\mathbf{U}\mathbf{B}_1^T & \mathbf{B_2} \\ \mathbf{B}_2^T & \mathbf{0} \end{pmatrix}^{-1}. \tag{5}$$

If the constraint is nonlinear we iteratively linearize it at specific values μ_0 and β_0 and apply the BLUE procedure at each of these steps. Iteration is stopped when a specified criterion, such as the relative change in the parameter estimates, is met within a pre-defined tolerance.

Results

We shall demonstrate the use of OEFPIL on the determination of the internal resistance of an AC voltage source (SineWaveGenerator by CMI) from its load characteristic. The SWG was subjected to various loads by adding loading resistance R_s, and the resulting voltage drop on the output terminals was measured. Commercially available component resistors were used as the load. The output voltage was measured using a programmable josephson quantum standard (PJVS), which operated in the mode of an

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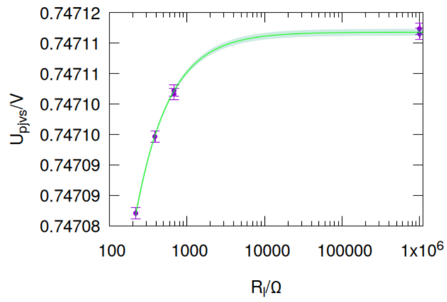

Fig. 1: Graph of relationship between the voltage measured by the PJVS and the applied load, including expanded uncertainties and bands.

AC quantum voltmeter. The PJVS itself introduces a load on the measured source through input impedance, R_d, of the sampling card (part of PJVS), so the total load on the SWG is the parallel combination of R_s and R_d. The SWG was modeled as a combination of an ideal voltage source U_s and the internal resistance R_s. The relationship between the voltage measured by the PJVS U_PJVS and the load R_l can be expressed as

$$U_\mathrm{PJVS} = U_\mathrm{s} R_\mathrm{l} / (R_\mathrm{l} + R_\mathrm{s}) \quad (6)$$

where U_s and R_s are the voltage and internal resistance of the source and the total load R_l is given by the parallel sum of the input impedance of the sampling card R_d and the resistance of the component resistor R_s as $R_\mathrm{l}^{-1} = R_\mathrm{s}^{-1} + R_\mathrm{d}^{-1}$. The uncertainties in the measured data arise from the calibration of the resistors, the estimation of the input impedance of the card based on literature, and the measurement of the AC voltage using the PJVS. An interesting question is the correlation of the data. Since we measure all voltage values with the same instrument, we can expect some correlation between them. The same holds for the resistance. However, the exact quantification remains an open question. In order to assess the effect correlation has on estimates and their uncertainties we considered constant correlation coefficients between any pair of resistances (denoted as ρ_R and any pair of voltage (denoted as ρ_V). Voltage and resistance values were assumed to be uncorrelated because of different traceability chains.

The data were fitted by OEFPI to the function (6). The fitted curve including expanded uncertainty bands is shown in Fig. 1. We verified the correspondence between the results obtained by OEFPIL and Monte Carlo method and found excellent agreement, see 1. It can be also seen that difference between NLS and OEFPIL without correlations is neglectable. The correlation between data obviously has a noticeable impact on the uncertainties whereas its effect on the estimated values is within error margins. This can be further elaborated creating maps for both estimated values as well as their uncertainties by varying the correlation coefficients. An example of such a map for the uncertainty of the resistance of the source is shown in fig. 2.

	R_s/mΩ	$u(R_\mathrm{s})$/mΩ
NLS	8.79364	0.148
OEFPIL (uncorr.)	8.79616	0.164
MC (uncorr.)	8.79636	0.164
OEFPIL (corr.)	8.79600	0.053
MC (corr.)	8.79619	0.053

Tab. 1: Internal resistance of the source obtained different fitting procedures: NLS, OEFPIL and Monte Carlo without correlations and OEFPIL and Monte Carlo with strong correlation $\rho_\mathrm{R} = \rho_\mathrm{V} = 0.9$.

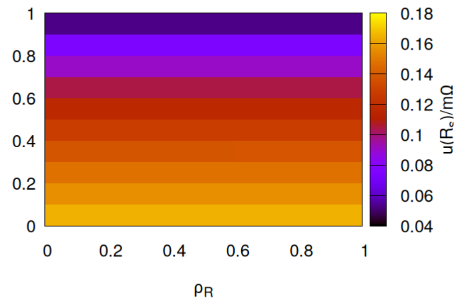

Fig. 2: Map of source resistance uncertainty depending on the correlation coefficients for voltage and resistance.

Conclusions

The use of OEFPIL has been illustrated on the determination of the internal resistance of an AC source. Uncertainty maps for different correlation assumptions can help to assess the impact of the correlation on the results.

Acknowledgements

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