



# Threshold estimation for least-squares fitting in impedance spectroscopy

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## ARTICLE INFO

### Keywords:

Impedance spectroscopy  
Threshold estimation  
Least-squares error function  
Parameter identification

## ABSTRACT

The estimation of circuit component values in impedance spectroscopy applications usually requires the minimization of a least-squares cost function. Independently of the minimization method used, a threshold value should be used as a stopping criteria for the iterative minimization procedure. This paper presents a new estimator for the threshold value to be used in least-squares minimization problems applied to electrical circuit impedance component values estimation. The new estimator is an improvement of a previous work that is more general as it can take into account different measurement system uncertainties for each measured value. Comparison between the threshold obtained with constant uncertainties and with varying uncertainties is presented to show the usefulness of this new method. Simulated impedance responses are used to validate the method, which is further confirmed using measurement results. The effects of correctly choosing a threshold in the fitting of a circuit impedance response to a set of measurements is presented by analyzing the convergence properties and the uncertainties of the estimated component values.

## 1. Introduction

The concept of impedance spectroscopy [1] continues to offer challenges both in new scientific developments and in available and new impedance based measurement applications [2,3] such as biomedical applications [4,5], food industry [6], corrosion studies [7–9] and battery analysis [10–12]. Until recently, it relied on specialized equipment [11–13] and software [14]. However, the advent of low-cost and reliable data acquisition systems along with powerful signal processing algorithms such as sine-fitting algorithms [15,16] has boosted the interest in impedance spectroscopy applications and developments. Examples of signal processing algorithms include the adaptation of evolutionary methods such as genetic algorithms [17] and gene expression programming [18], or the use of bilinear transformation [19] for impedance parameter identification.

Impedance spectroscopy usually starts with the measurement of the impedance amplitude and phase frequency response in a band of interest. This can be performed with a dedicated frequency response analyzer or a lock-in amplifier, but the option used here, without loss of generality, relies on an automated setup based on a sine wave generator, a data acquisition board and a reference impedance [20]. The voltage sine signals across the impedance, device or process under test and across the reference impedance are acquired. Sine-fitting algorithms are then applied to the acquired samples to estimate the amplitude, phase

and fundamental frequency of each acquired sine wave. Next, this information is used to estimate the amplitude and phase, at various frequencies, of the impedance under test. With the measured impedance frequency response it is possible to analyze it in terms of equivalent circuit which is very useful in many different applications.

When the impedance equivalent circuit is known, the task of finding the circuit component values can be performed by fitting, for example, in a least-squares (LS) sense, the impedance frequency response of the equivalent circuit to the measured data. However, minimization of the least-squares cost function is not a trivial task since it often has many local minima and spans a large search space (e.g., resistances from 0.1  $\Omega$  up to 10 M $\Omega$ ; capacitors from 1 pF up to 1 F, and so on). Genetic based algorithms have been successfully used to overcome this problem [17]. A more difficult problem occurs if the circuit topology is not known, but even this has been successfully addressed using a technique called gene expression programming (GEP) [18] that simultaneously searches for an adequate equivalent circuit and its component values. However, in both situations, the minimum value of the cost function is different from zero (i.e., a perfect fitting is not possible due to measurement uncertainty). This is usually tackled by traditional search methods by defining cost function and parameter tolerances, but in multi-dimensional cost functions with multiple minima it may mean that the search algorithm will settle in a local minimum instead of the global minimum. Therefore, it is important, if possible, to correctly set the cost function

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threshold so that the search algorithm recognizes that it is close to the global minimum. This is the topic addressed in this paper: how to estimate the threshold value to be used (in any least-squares minimization method) for impedance spectroscopy circuit parameter estimation. It has been shown in [21] that, in some situations, this minimum only depends on the uncertainty of the measurement system. Therein, an analytical formulation was developed to set the threshold for the optimization of least-squares cost functions in impedance circuit parameter estimation. Simulation of measurements showed promising results, but lacked experimental confirmation. Under real impedance measurements the variation of the measurement uncertainties for each measured value induced a deviation in the predicted threshold that should be used. This paper addresses this issue by developing a new estimator and presents simulation and measurement results to validate this new approach. It should be noted that this estimator can be used as a stopping criteria independently of the cost-function minimization algorithm used.

The paper is divided into six sections, including the introduction and the conclusions. Section 2 presents the general problem of fitting measurement results to a circuit impedance frequency response along with the need for the definition of a threshold for convergence decision. The new estimator is described in Section 3, where the least-squares cost function is defined and its expected value and standard deviation are derived along with a closed form expression for threshold definition. In Section 4, the performance of the new estimator is tested through simulation results of a circuit impedance response that includes changing uncertainties for the impedance values. Final validation is presented in Section 5 with measured impedance responses. Comparison between the new method and the previously constant uncertainties method from [21] and with measurement results is performed in this section. An analysis regarding the number of frequencies in the measured frequency response is also shown. Finally, as the main objective of this method is to define an adequate threshold for circuit parameter estimation, a study of the convergence properties along with the uncertainties of the estimated component values as a function of the threshold value is presented.

## 2. Impedance spectroscopy parameter identification

In impedance spectroscopy applications it is often important to know the equivalent circuit and component values that result in an impedance frequency response that models the impedance measurements. This is of particular importance for example in sensor characterization [18], fuel cell characterization [22] or corrosion analysis [7]. After the measurement of the impedance frequency response at selected frequencies, if a suitable equivalent circuit is known, a fitting procedure can be used to find the component values that correctly

reproduce the measured response. This is illustrated in Fig. 1 where the circles show the measured impedance amplitude (a) and phase (b) and the dashed line represents the full impedance response of the system or process under measurement. The solid line represents the impedance response of the equivalent circuit with circuit component values that are not yet optimized. A minimization algorithm attempts to fit the response of the equivalent circuit to the measured frequency response by searching for a set of component values that minimize the least-squares error between the estimated frequency response and the measurement results. However, due to the inherent measurement uncertainty, the fitting error has a minimum value which is not zero. This leads to the problem of deciding on a threshold value below which it is possible to say that the circuit component values have been found in the fitting procedure. The main objective of this paper is to develop an estimator to define this threshold value.

Fig. 2 illustrates the drawbacks of incorrectly choosing a threshold for the fitting of an estimated frequency response to a set of measurements. For the sake of simplicity, the situation depicted in Fig. 2 corresponds to a one-dimensional problem optimization scenario. In the situation shown in Fig. 2(a), the threshold is set quite high in relation to the minimum value and this causes the algorithm to converge easily but a better (lower) value of the cost function could be achieved – the problem with this scenario is that better estimates of the circuit parameters could be obtained. In case (b), the threshold is set lower than the achievable by the cost function and the algorithm will never converge. Situation (c) depicts the setting of a correct threshold which obtains a smaller interval for the possible final values. Note that, the tolerance of the cost function or the tolerance of the input parameter cannot be used for convergence since the cost function may have multiple local minima – as shown in Fig. 2(d).

## 3. Threshold estimation

In impedance parameter identification problems the measurement model is typically fitted to the measurements results through a least-squares cost function

$$\varepsilon = \frac{1}{N_f} \sum_{i=1}^{N_f} \left| \frac{Z_{meas}(\omega_i) - Z_{real}(\omega_i)}{Z_{real}(\omega_i)} \right|^2 \tag{1}$$

where  $Z_{meas}(\omega_i)$  is the measured impedance response and  $Z_{real}(\omega_i)$  is the true impedance response at angular frequency  $\omega_i$ , with  $N_f$  frequency points. Each measurement is a complex number (impedance amplitude and impedance phase) with associated measurement uncertainty in both amplitude and phase. Assuming that the measurement uncertainties of the relative amplitude and phase follow normal distributions with zero mean and variances  $u_{iZ}^2(\omega_i)$  and  $u_{i\phi}^2(\omega_i)$  (which can change for each measured frequency  $\omega_i = 2\pi f_i$ ), then the measured

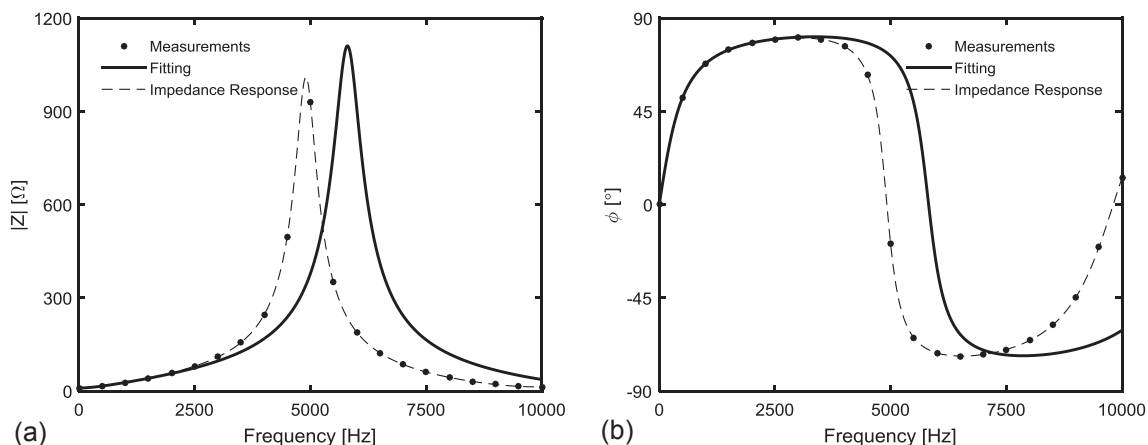


Fig. 1. Example of impedance spectroscopy fitting error.

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