Parameter Identification and Measurement Uncertainty for Dynamic Measurement Systems

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1 Introduction

The analysis of dynamic measurements requires new approaches to the estimation of the value of the measurand as well as for the evaluation of measurement uncertainty. In static measurements the value of the measurand is represented by a single value or a tuple of values, and estimation of the measurand typically requires solving algebraic equations. In dynamic measurements the value of the measurand varies with time. In addition, the response of the measurement device depends on the frequency content in the measured time series.

A typical workflow in the analysis of a dynamic measurement is shown in figure 1. The measurand is the system input signal and the available data the corresponding output signal. Estimation of the measurand requires a mathematical model for the dynamic system which covers its frequency-dependent response in the relevant frequency range. This cannot be accomplished by algebraic equations.

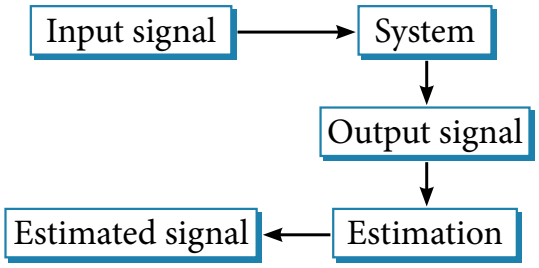

Figure 1: Work flow in the analysis of dynamic measurements.

An appropriate mathematical model for most dynamic systems is given by the state-space system model

$$\dot{z}(t) = f(z(t), y(t), t) \tag{1}$$

$$x(t) = g(z(t), y(t), t)\,, \tag{2}$$

with (1) being the state equation modelling the dynamics of the system, and (2) the observation equation modelling the data acquisition [1]. Such state-space system models cover single sensors [2] as well as complex measurement set-ups [3] or sensor networks. Sometimes the system model can be determined based on physical reasoning and the calibrated parameters then give insights into the physical properties of the measurement system. For instance, in a shock-force calibration experiment the measurement system may be modelled by means of coupled mass-spring-damper elements such that estimated spring stiffness values correspond to the stiffness of the coupling of the measurement system components [4].

The goal of dynamic calibration is to provide a characterization of the system dynamics and the influence of the measurement itself. Both can be achieved by means of parameterization of the functions f and g in (1)–(2). A parametric characterization has the benefit that it allows versatile application of the calibration result. For instance, a calibrated parametric model of a force transducer can be applied as part of a model of a fatigue testing machine [3], or a model of a torque sensor can be incorporated into a model of an engine test stand [5].

For the state-space model (1)–(2), special cases exist which allow a simplified treatment in certain scenarios. For instance, if the complete measurement system can be modelled by a linear time-invariant (LTI) system with single input and single output, then equations (1)–(2) can be transformed to a transfer function model in the Laplace domain [1]

$$H(s) = \frac{\sum_{k=0}^{K} b_k s^k}{\sum_{l=0}^{L} a_l s^l}\,. \tag{3}$$

The relation between input and output of the dynamic system is then given by

$$L\{x(t)\} = H(s) L\{y(t)\}\,, \tag{4}$$

where $L\{x(t)\}$ denotes the Laplace transform of the time signal $x(t)$. In order to emphasize the dependence of the transfer function on its parameters we write $H(s; \boldsymbol{\theta})$ with $\boldsymbol{\theta} = (b_0, \ldots, b_K, a_0, \ldots, a_L)^{\mathrm{T}}$ as the vector of parameters.

In the following, the task of calibrating a linear time-invariant dynamic system by means of identification of the transfer function model parameters (3) is considered. In section 2 generic methods for parameter estimation are discussed. In section 3 and 4, estimation is addressed for calibration data available in the frequency and time domain, respectively. The evaluation of uncertainty for parameter estimation in line with GUM [6] is discussed in section 5.

2 Generic Parameter Identification

An important step in the process of parameter identification is to set up the statistical measurement model

$$H(s_k; \boldsymbol{\theta}) = H_0(s_k; \boldsymbol{\theta}) + \varepsilon_k \,, \tag{5}$$

where H_0 denotes the (unavailable) error-free value and the ε_k denote statistical measurement errors. The statistical model takes into account all sources of uncertainties in the calibration experiment, (cf. [7]) for an example, in the field of acceleration using sophisticated statistical modelling.

The aim of parameter identification is to determine the parameter vector $\boldsymbol{\theta}$ which provides the best explanation of the data given the statistical model (5). One possibility to achieve that goal is to carry out a maximum likelihood estimation [9]. In this approach the statistical model (5) is employed to define the likelihood function $l(\boldsymbol{\theta}, \boldsymbol{H})$ as a probabilistic expression of the likelihood of the data $\boldsymbol{H}$ for a given parameter vector $\boldsymbol{\theta}$. Parameter estimation in this context corresponds to determining the solution of

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} l(\boldsymbol{\theta}, \boldsymbol{H}) \,. \tag{6}$$

Consider, for instance, the case which the measurement errors ε_k in (5) follow a normal distribution with zero mean and known covariance $\boldsymbol{\Sigma}$. In this case, the likelihood function is proportional to $\exp(-0.5\|\boldsymbol{H} - H(s; \boldsymbol{\theta})\|_{\boldsymbol{\Sigma}}^2)$ and the application of the maximum likelihood method becomes the weighted least squares estimation [8]

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \|\boldsymbol{H} - H(s; \boldsymbol{\theta})\|_{\boldsymbol{\Sigma}}^2 \,, \tag{7}$$

with $\|\boldsymbol{A}\|_{\boldsymbol{W}}^2 = \boldsymbol{A}^{\mathrm{T}} \boldsymbol{W}^{-1} \boldsymbol{A}$.

It is worth noting that least squares estimation is often applied for parameter estimation irrespective of the statistical model (5). However, although the resulting parameter vector estimate then satisfies (7), it may not be the optimal solution for the model (5). Moreover, assignment and interpretation of measurement uncertainty becomes problematic if the statistical properties of the data are ignored.

Maximum likelihood estimation can be considered as a numerical optimization problem [9]. The optimization merit function is given by equation (6) and is typically non-linear. In contrast to linear optimization, the solution space of non-linear problems can be very complex and many (local) solutions may exist. In general, non-linear optimization has many pitfalls that have to be considered in order to obtain a reliable parameter estimate. For instance, stopping of the iterations is decided, based on user-defined tolerances, and numerical calculation of the model function's Jacobian requires appropriately small step sizes. Convergence of optimization routines is typically proven under the assumption of an appropriate choice of method parameters. Hence, reliable parameter estimation requires a careful usage of the applied non-linear optimization method.

An often applied optimization method in the case of non-linear least squares is the Levenberg-Marquardt method [9]. This is an iterative method where in each step the Jacobian of the model function $H(s; \boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$ is employed in order to progress to a solution of (7). In many software environments, such as LabView, Matlab and SciPy, the Levenberg-Marquardt method is the default method for non-linear least squares problems. However, like all iterative solution methods, the Levenberg-Marquardt method requires defining an initial starting point $\boldsymbol{\theta}^{(0)}$ and only provides local solutions to problem (7). That is, for a different starting point, the outcome of the optimization might differ. It is thus advisable to repeat the optimization process with different initial parameter estimates.

An alternative approach to the maximum likelihood method for parameter estimation is the application of Bayesian inference [10, 11]. Therefore, in addition to the likelihood function, a probability distribution function (PDF) modelling the *a priori* knowledge about the parameters is employed. Parameter estimation in this context is then applied in terms of a probability calculus using Bayes' Theorem, carried out numerically, e.g. by means of Markov Chain Monte Carlo (MCMC) sampling [11]. The result of such a Bayesian inference is a *posterior* PDF modelling the (probabilistic) knowledge about the parameter values after taking into account the measurement data. The benefit of the Bayesian approach here is that no numerical optimization has to be applied and that uncertainties associated with the parameter estimate can be directly obtained from the posterior PDF. However, care has to be taken when no actual prior knowledge about the model parameters is available, and a careful convergence analysis of the MCMC sampling has to be carried out in order to obtain reliable results [11]. In the following, we focus on the maximum likelihood estimation and refer

the reader interested in details about the Bayesian approach to parameter estimation to [10, 11] and references therein.

3 Frequency Domain Identification

The transfer function model (3) gives rise to a frequency domain representation of the dynamic system by replacing the variable s with $j\omega$ with $j = \sqrt{-1}$ and the radial frequency $\omega = 2\pi f$ giving

$$H(j\omega) = \frac{\sum_{k=0}^{K} b_k (j\omega)^k}{\sum_{l=0}^{L} a_l (j\omega)^l} \,. \tag{8}$$

Identification of the system parameters in the frequency domain requires measurements of the frequency response of the dynamic system over the whole range of relevant frequencies [12]. This can be achieved either frequency-by-frequency using sinusoidal excitations [13] or by application of the discrete-time Fourier transform (DFT) to a time domain calibration measurement of input and output signal [14].

In any case, parameter identification based on equation (8) requires measurement of the complex-valued frequency response values $\boldsymbol{H} = (H(f_1), \ldots, H(f_N))^{\mathrm{T}}$, represented either by means of the real and the imaginary part of $\boldsymbol{H}$ or of the corresponding amplitude and phase values. The uncertain knowledge about these values is modelled by a (multivariate) probability density function (PDF) or is given as an estimate of the values and an associated matrix $\boldsymbol{U}$ of (mutual) uncertainties.

When the frequency response measurements are carried out by means of a sinusoidal excitation experiment, amplitude and phase values $\tilde{\boldsymbol{H}} = (|H(f_1)|, \ldots, \measuredangle H(f_N))$ with associated uncertainties are typically available [13, 15]. In general, the values at different frequencies are correlated, for instance, due to being obtained with the same measurement set-up. However, in practice the correlation between the estimates at different frequencies is often considered to be negligible. The corresponding statistical model for the measurement errors in equation (5) is then given by $\boldsymbol{\varepsilon} \sim N(0, \boldsymbol{\Sigma})$ with known diagonal matrix $\boldsymbol{\Sigma}_{ii} = u_i^2$, where u_i denotes the uncertainty associated with the i-th component of the vector $\tilde{\boldsymbol{H}}$. Depending on the type of the transfer function model (3), a linear or non-linear least squares method can then be applied for the determination of transfer function parameter estimates [13, 16].

In the case of time domain measurement and subsequent application of the discrete Fourier transform (DFT) to obtain frequency response values, the model (5) depends on the statistical model of the time domain measurements [14]. Determination of the likelihood function for frequency domain maximum likelihood estimation is thus more complicated than for the case of sinusoidal excitation and the time domain estimation might be more appropriate then. In addition, systematic errors introduced by the non-ideal DFT itself have to be taken into account in the subsequent uncertainty analysis [17].

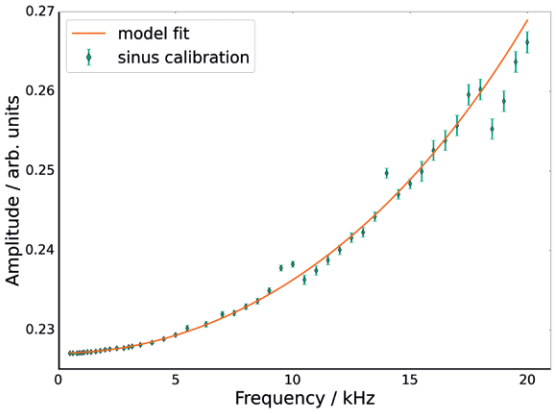

Figure 2:
Estimated transfer function for sinusoidal excitation data.

4 Time Domain Identification

The time domain description of a transfer function model is obtained by taking the inverse Laplace transform of equation (4)

$$x(t) = (h_{\boldsymbol{\theta}} * y)(t) \,, \tag{9}$$

where $h_{\boldsymbol{\theta}}(t) = h(t; \boldsymbol{\theta})$ denotes the system's impulse response function and '$*$' means convolution [1]. The statistical models

$$y(t) = y_0(t) + \varepsilon_y \,, \tag{10}$$

$$x(t) = x_0(t) + \varepsilon_x \tag{11}$$

have to be set up by taking into account measurement noise, systematic influences of the involved measurement devices and other sources of uncertainty [18]. When the uncertainty in y is negligible and the statistical model (11) for x is covered by a normal distribution with known covariance matrix $\boldsymbol{\Sigma}$, then the parameter estimation becomes the least squares problem

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \| \boldsymbol{x} - (h_{\boldsymbol{\theta}} * \boldsymbol{y}) \|_{\boldsymbol{\Sigma}}^2 \tag{12}$$

with vector $\boldsymbol{x} = (x(t_1), \ldots, x(t_N))^{\mathrm{T}}$ of system output values and the corresponding input values $\boldsymbol{y} = (y(t_1), \ldots, y(t_N))^{\mathrm{T}}$.

Note that a non-parametric estimation of the impulse response $h(t)$ from measured system input $y(t)$ and output $x(t)$ requires a deconvolu-

tion, which is an ill-posed inverse problem [19]. The corresponding model for the estimation of the impulse response in the time domain is given by

$$h(t) = (x * y^{\dagger})(t) + \varepsilon, \tag{13}$$

where $y^{\dagger}$ denotes the regularized inverse of y [19, 20]. It is worth noting that (13) is typically applied in the frequency domain for ease of calculation.

For the more general dynamic system model (1)-(2) an ordinary differential equation (ODE) has to be solved. When the uncertainty in $y(t)$ can be neglected, the statistical model is then given by

$$x(t) = g(y(t), z(t; \boldsymbol{\theta}), t; \boldsymbol{\theta}) + \varepsilon_x, \tag{14}$$

which is derived from the measurement equation (2). Note that in order to calculate $z(t)$, the differential equation

$$\dot{z}(t; \boldsymbol{\theta}) = f(z(t; \boldsymbol{\theta}), y(t), t; \boldsymbol{\theta}) \tag{15}$$

has to be solved. To this end, typically numerical integration, such as the backward differentiation formula or a Runge-Kutta method can be applied [21]. Software tools for this task are available in almost all major scientific software packages. However, the numerical optimization in conjunction with numerical ODE integration requires careful selection of the step size tolerances of the ODE solver and of the numerical differentiation in the optimization routine. For instance, the application of the Levenberg-Marquardt method for the optimization problem

$$\hat{\boldsymbol{\theta}} = \arg\min_{\theta} \| \boldsymbol{x} - g(\boldsymbol{y}, \boldsymbol{z}, \boldsymbol{\theta}) \|_{\Sigma}^{2}, \tag{16}$$

in the case of normally distributed errors ε_x with known covariance $\boldsymbol{\Sigma}$ requires differentiation of g with respect to $\boldsymbol{\theta}$ which itself requires solving the ODE (15). Hence, at each iteration in the optimization process a numerical differentiation of the ODE integration method has to be carried out with precision being high enough for a reliable parameter estimation result. In some cases, this may require use of an optimization routine which does not require differentiation, such as the Powell method [4, 9].

Figure 3 shows the outcome of a time domain parameter estimation for a shock force calibration experiment. In this example, the system model equation (1) models the dynamics of the measurement system as a series of mass-spring-damper elements. Measured data (14) in this case is the sensor output signal and the acceleration of one of the involved masses, see [4] for details.

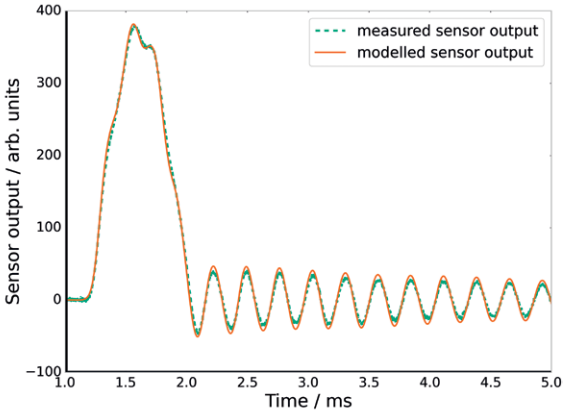

Figure 3:
Time domain parameter estimation for shock calibration of a force sensor.

5 Evaluation of Uncertainty

In order to provide the parameter estimates as part of a calibration result, reliable uncertainties have to be associated with the estimated parameters in line with GUM [6, 22]. Statistically speaking, the task of parameter estimation is a regression. Although this task is very common in metrological applications, so far there is no generally accepted approach to the corresponding GUM-compliant evaluation of uncertainties. The GUM itself provides an example for uncertainty evaluation for linear least squares, see H.3 in [6] or example 3 in 6.2.2 in [22]. There are a number of publications which assess the applicability of the GUM framework to regression models. For instance, in [23] a Bayesian inference approach is compared to an application of GUM-S1 Monte Carlo. The authors conclude that GUM-S1 does in general not provide a Bayesian solution, opposed to what is stated in the introduction of GUM-S1 [22]. Furthermore, the authors in [23] point out that the measurement model is ambiguous in contrast to the assumptions made by the GUM as it depends on the actual data and not the physical model alone.

Despite the pitfalls of the application of GUM to least squares and other regression problems, this task is routinely considered in many metrological applications. Therefore, the statistical model (5) has to be replaced by a GUM-compliant measurement model. For the linear least squares problem, i.e. a linear mathematical model and normally distributed data with known covariance $\boldsymbol{\Sigma}$, the measurement model is

$$\hat{\boldsymbol{\theta}} = \arg\min_{\theta} \| \boldsymbol{y} - \boldsymbol{H}\boldsymbol{\theta} \|_{\Sigma}^{2} \tag{17}$$

which can also be written as

$$\hat{\boldsymbol{\theta}} = (\boldsymbol{H}^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}\boldsymbol{H})^{-1}\boldsymbol{H}^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}\boldsymbol{y}\,. \tag{18}$$

The uncertainty associated with this estimate is then calculated as the variance of this expression and results in

$$\boldsymbol{U}_{\hat{\theta}} = (\boldsymbol{H}^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}\boldsymbol{H})^{-1}\,. \tag{19}$$

For a non-linear optimization often an approach is chosen that mimics the linear least squares case. Therefore, the Jacobian of the optimization merit function at the final iteration is employed together with the covariance matrix associated with the data points [16, 24]. Another approach is the utilization of the Hessian matrix of the least squares cost functional [24]. However, the resulting uncertainties may be underestimated in the case of uncertainties in the independent variables (time or frequency in the here considered scenarios), see [24]. To this end, the authors in [16] propose the application of a Monte Carlo method instead of a linearized propagation with closed formulas. In a Monte Carlo propagation of uncertainties for a parameter estimation problem, the input quantities and their associated uncertainty are given by the calibration data. As a measurement model, equation (6) is considered and propagation of uncertainties is carried out according to GUM-S2 [22]. As discussed in section 3, non-linear optimization requires careful choice of the numerical method and its parameters. This is of particular importance for the application of Monte Carlo where the optimization has to be repeated many times in an automated way.

Irrespective of whether closed formulae are applied or a Monte Carlo propagation is carried out, the ambiguity of the measurement model and the difference to the result of a full Bayesian treatment remain. This makes a general GUM-compliant approach for uncertainty evaluation in parameter estimation based on statistical arguments very challenging. However, this has been recognized by the BIPM JCGM working groups and a supplement addressing this issue for the case of least squares regression is in preparation [25].

6 Conclusions

The characterization of a dynamic system in terms of a parametric model allows a versatile utilization of the calibration result. In its mathematical description, parameter estimation is a regression problem which itself can be interpreted as a numerical optimization problem. Both are well-established disciplines in mathematics and statistics and many scientific software packages contain efficient tools for their application. However, care has to be taken in the determination of the statistical model of the measured data and in the application of the estimation method in order to obtain a reliable calibration result.

Unfortunately, there is no general commonly accepted GUM-compliant approach yet. To this end, some authors have proposed approaches for certain non-linear least squares scenarios. A more general approach would be to fully embrace the Bayesian framework, and to carry out Bayesian inference not only for the interpretation of uncertainty, but for parameter estimation, too.

Acknowledgements

This work was supported by the EMRP program of the European Union. The EMRP is jointly funded by the EMRP participating countries within EURAMET and the European Union.

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