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Methods of uncertainty evaluation using virtual experiments with the example of the tilted-wave interferometer

Manuel Stavridis[1], *Manuel Marschall*[1], *Finn Hughes*[1], *Ines Fortmeier*[1] *and Clemens Elster*[1]
[1] *Physikalisch-Technische Bundesanstalt Braunschweig and Berlin*

Summary:

This paper uses virtual experiments to present a simplified uncertainty analysis for non-linear measurement methods. For these, the dependencies of the measured value on the uncertainty sources can often be regarded as sufficiently linear. This statement is examined for the example of a complex optical application based on the simplified version of the tilted-wave interferometer (TWI) by comparing the results of a simplified uncertainty evaluation with those of a Bayesian reference method.

Keywords: Uncertainty Evaluation, Virtual Experiments, Tilted-Wave Interferometer, Bayes, GUM, SimOptDevice

Bayesian uncertainty analysis (reference method)

In [1], a method for calculating the uncertainty for the TWI using virtual experiments (VEs) was presented. The Bayesian method described there includes an approximation, which leads to a Monte Carlo sampling procedure. For each sampling step, a call to the VE of the TWI is required, and a high-dimensional regression problem is solved.

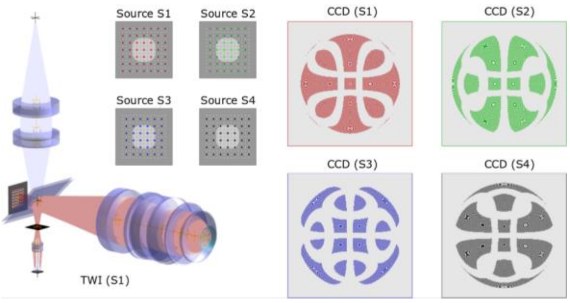

Figure 1: VE: Tilted-wave interferometer (left) and its simulated interferograms (right), (from [2], CC BY 4.0).

The VE of the TWI, as seen in Figure 1, includes a physical modelling of the measurement using ray tracing by SimOptDevice [2] up to the generation of the measurement data (interferograms).

The subsequent data analysis, with the aim of reconstructing the form of a sphere-, asphere- or freeform surface, again calls to the VEs in the context of a non-linear inverse problem.

Using the Bayesian uncertainty evaluation in [1], the point-wise standard uncertainty shown in Figure 2 was obtained for the polynomial fit (intermediate reconstruction step).

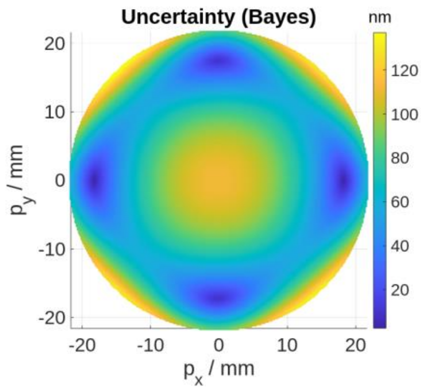

Figure 2: Point-wise standard uncertainty for the intermediate reconstruction step using the Bayesian method from [1].

Consideration of the uncertainty sources as linear

The GUM [3] serves as the de facto standard for uncertainty evaluation in metrology, and it propagates the uncertainties associated with the so-called input quantities to the quantity of interest, i.e. the measurand. Often a linearisation of this relationship is sufficient to provide an adequate uncertainty evaluation. An uncertainty evaluation using the linearised model and the "Law of propagation of uncertainty" (LPU) also requires the determination of the sensitivities or gradients of the VE. However, whether such a linearisation is sufficient or not needs to be checked.

Determination of the gradients for the sources of uncertainty using VEs

In the TWI, the VE is embedded in the measurement data reconstruction process. As a result, the VE models a physical-technical state in silico, in which the deviations from the real measured values (interferograms) have to be minimised within a numerical optimisation arising from an inverse problem.

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The VE can then represent the dependencies between the actual measurand and the input quantities. In the linearised form, gradients can be calculated numerically by varying the input quantities and repeating the VE. SimOptDevice [2], a library for optical simulations, is also able to output these gradients analytically [4]. This is used to calculate the dependencies of optical elements or element groups regarding input quantities such as positioning or direction.

The basis for this is the change in the optical path length OPL with respect to the position of the surface $\frac{\partial OPL}{\partial p} = n_o\vec{e}_o - n_i\vec{e}_i$, where $\vec{e}_o$,$\vec{e}_i$ are the direction vectors of the beam and n_o, n_i are the refractive indices of the media before and after the surface, respectively [4]. The chain rule could also be used here to analyse dependencies on other quantities such as lens radii, directions, etc. [4].

Linearisation of the VE

After exporting the above sensitivities for the measurement, a linear model can be created:

$$x = G(y, z, \epsilon) \approx A_Y y + A_Z z + \epsilon \qquad (1)$$

x is the measurement data generated by the virtual or real experiment $G(y, z, \epsilon)$, y is a value for the measurand Y, and ϵ is a realization of observation noise, modelled as multivariate Gaussian distributed with covariance $\sigma^2 I$. The value z of a quantity Z represents additional input quantities that affect the measurement. With the TWI, x corresponds to the optical path length differences, which are simulated using the model or calculated accordingly from the measurement data.

In the simplified model (1), the matrices A_Y and A_Z represent the linear dependence of the measured value with respect to the measurand Y and the additional input quantities Z. In the simplified TWI, Y denotes the difference to the known design topography as well as the lateral position of the specimen. Z contains, for example, the positioning of the specimen along the optical axis and its tilt.

With consideration to (1), a possible approach for the linear reconstruction of the measurand Y and for setting up a measurement model according to GUM is as follows:

$$Y = A_Y^{-1}(X - A_z Z) \qquad (2)$$

Uncertainty according to GUM using LPU

According to GUM, the covariance V of the measurand Y can be determined with linear propagation using the following formula.

$$V = JUJ^T \qquad (3)$$

Here, J is the derivative of (2) with respect to X and Z, such that

$$J = [A_Y^{-1} \quad -A_Y^{-1} A_Z] \qquad (4)$$

and U is set up as follows:

$$U = \begin{bmatrix} U_x & 0 \\ 0 & U_Z \end{bmatrix}. \qquad (5)$$

Here, $U_X = \sigma^2 I$ is the assumed covariance of the measurement data and U_Z denotes the covariance of the additional quantities Z.

Applying this method to the analogue setting from [1], the point-wise standard uncertainty is obtained for the greatly simplified TWI method. If this result is compared with the corresponding case of the Bayesian method [1], it becomes clear that the uncertainty evaluation method presented here adequately replicates the Bayesian method. Furthermore, regarding computation time, the method presented here took significantly less time to achieve adequate results, which renders the usage in live applications much more feasible.

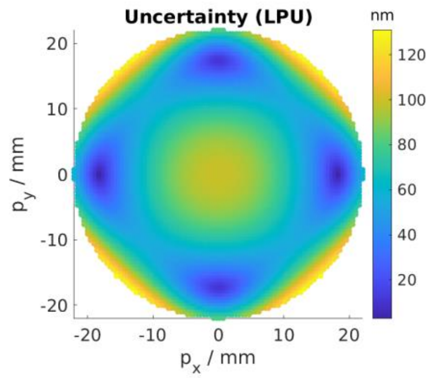

Figure 3: Point-wise standard uncertainty for the intermediate reconstruction step using the linearised model around the measured value.

Conclusion

We demonstrated for the example of the TWI that the uncertainty evaluation with a linear approximation of the influence of the input quantities essentially corresponds to that of a Bayesian reference method. The calculation of the linearised approach is significantly less time-consuming as Monte Carlo analyses with VEs are not required.

Acknowledgements

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