Final Publishable JRP Summary for NEW04 – Uncertainty
Novel mathematical & statistical approaches to uncertainty evaluation

Overview

Measurement uncertainty evaluation is fundamental to metrology because without it no assessment of the reliability of a measurement can be given and no comparisons of measurement results, either among themselves or with reference values given in a specification or a standard are possible. The project has established ways of dealing with uncertainty in three different cases which are not covered by the guidelines in the definitive international document on uncertainties, the *Guide to the expression of uncertainty in measuremen*t (GUM)[1], or its supplements: (i) regression and inverse problems; (ii) uncertainty evaluation for computationally expensive models and (iii) conformity assessment and reliable decision making. This project developed new mathematical and statistical approaches which will be important for many new metrology applications such as biochemistry, biotechnology and transport processes. New guidelines have been issued for the three situations, with generic advice and a number of useful case studies. *MATHMET* – A *European Centre for Mathematics and Statistics in Metrology* has been founded during the project and will serve as a future platform for European cooperation in mathematics for metrology (see ***www.mathmet.org*** for more details).

Need for the project

The evaluation of measurement uncertainty is a critical part of quality management systems in all industries that employ measurement technology. Inaccurate evaluation of measurement uncertainty has important economic consequences for calibration and measurement activities. In calibration reports, the magnitude of the uncertainty is often taken as an indication of the quality of the laboratory, and smaller uncertainty values generally are of higher value and of higher cost.

In many cases best practice is covered by the existing GUM guidelines. There are, however, commonly encountered situations for which the GUM guidelines are not suitable. Development of guidance for these situations presents a significant mathematical challenge but brings benefit to a wide range of end users in fields such as biochemistry, biotechnology, transport processes, industry and regulation. The situations considered in this project were inverse and regression problems, uncertainty evaluation in computationally expensive problems and the role of measurement uncertainty in conformity assessment (i.e. testing compliance with standards) and decision making.

The current lack of guidelines means that in some cases uncertainty is not being considered, which can potentially lead to risky decisions. In other cases they are over-estimating uncertainty in order to be safe, and so better uncertainties would reduce costs. The lack of uncertainty evaluation can be a barrier to use of mathematical models as part of certification processes (e.g. aerospace) which would reduce R&D costs.

The specific needs require a co-ordinated effort to obtain reliable uncertainties, to ensure harmonisation and to develop a consistent application framework throughout Europe. A long-term infrastructure, such as a European Centre, to enable cooperation on mathematical and statistical topics relevant to metrology is needed to ensure dissemination of mathematical and statistical expertise for uncertainty evaluation for European NMIs and European industry.

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[1] The GUM is published jointly by: Bureau International des Poids et Mesures (BIPM); International Electrotechnical Commission (IEC); International Federation of Clinical Chemistry (IFCC); International Organization for Standardization (ISO);International Union of Pure and Applied Chemistry (IUPAC);International Union of Pure and Applied Physics (ISPAP); International Organization of Legal Metrology (OIML)

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Scientific and technical objectives

This project focused on three areas where new uncertainty analysis methods are needed with the following scientific and technical objectives:

- To develop methods for the evaluation of uncertainty in the context of inverse problems and regression problems that arise throughout metrology.
- To develop methods for uncertainty evaluation in metrological applications with computationally expensive model functions
- To develop methods for conformity assessment and reliable decision-making that incorporate knowledge of the measurement uncertainties;

The project also focused on applying these methods to challenging applications by carrying out case studies where there was a pressing need for new uncertainty evaluation methods.

Finally, the project aimed to build on an existing network of mathematical experts active in the *EURAMET Focus Group Mathematical and Software Tools for Metrology* project and lay the foundation for a *European Centre for Mathematics and Statistics in Metrology.* The Centre would disseminate state of the art methods to European NMIs, industry and other organisations and ensure that the momentum developed by the project is carried forward and that impact can be realised way beyond the end of the project.

Results

The three objectives have been completed and three Good Practice Guides have been produced and the MATHMET centre has been established.

Novel method for uncertainty evaluation in regression and inverse problems

Inverse problems are cases where the quantity of interest to the metrologist is not measured directly, but is instead a parameter in some relationship between the control and response variables of the measurement process. For example, immunoassay tests in biochemistry where testing for a molecule in solution is done through the use of an antibody. Regression problems are a type of inverse problem where the quantities of interest are parameters of a function linking the control and response variables that will then be used to estimate values of one variable at points where measurements have not been made. Calibration problems are the most commonly used instances of regression problems in metrology, and this project allows more accurate uncertainty calculations to be made.

A Good Practice Guide “A Guide to Bayesian inference for regression problems” has been developed and is freely available for download. It provides a general introduction about how to deal with uncertainty evaluation in regression and inverse problems and suggests a Bayesian treatment based on conditional probability.

The guidelines were used to develop a novel statistical method for the analysis of immunoassay tests. As a result, novel informative prior distributions have been developed which allow for a significantly improved analyses of such tests. These are often used for diagnosis of potential diseases in routine check-up tests of apparently healthy people as well as in diagnosis of specific diseases eg. myocardial infarction for which troponin is an indicator that is commonly tested with the enzyme-linked immunoassay tests studied in this project. In addition, the method serves as an illustration for the application of Bayesian inferences for non-linear regression in metrology. This is an example of a regression problem, not covered by GUM.

Novel methods for computationally expensive systems

Uncertainty evaluation for applications which are described by equations, such as fluid or heat flow, are often non-linear and can require considerable computational resource. Using the GUM gives a linear approximation which is often crude or inaccurate. A model was used to assess and compare different sampling methods and different surrogate modelling methods.

Work on uncertainty evaluation for computationally expensive models focused on smart sampling methods and surrogate models. Smart sampling methods aim to capture the behaviour of the quantity of interest in a small number of model evaluations by careful choice of input parameter values. Surrogate models build an approximation to the full model based on a small number of model evaluations.

A Best Practice Guide “Uncertainty evaluation for computationally expensive models” was produced and published in 2015 and is available for free download. The guide provides a walk-through of the steps in the uncertainty evaluation process and compares multiple smart sampling methods and surrogate models using a simple test problem. Software has been created and tested for implementation of two of the sampling methods investigated. The guidance was illustrated using a set of real-world case study problems; fluid flow through an installation of pipes and through a nozzle, thermal diffusivity and scatterometry methods important in the manufacture of a wide range of products such as photomasks that are widely used in microelectronic element production where a better analysis of measurement uncertainty supports the optimisation or improvement of manufacturing processes by better quality control. The fluid flow case study led to a much improved estimation of systematic errors in flow meters in everyday installations and is therefore beneficial to consumers as well as water suppliers who could get a more accurate estimate of the water consumption, if the findings are applied to the positioning and correction of flow meters in practical situations.

Novel methods for conformity assessment and reliable decision-making that incorporate knowledge of the measurement uncertainties

New perspectives on measurement uncertainty in conformity assessment and decision making have been gained by extending existing approaches to multivariate, qualitative data, computationally expensive systems and the inclusion of measures of impact.

A Best Practice Guide “A guide to decision-making and conformity assessment” and new software for assessing the conformance probability in different circumstances was published is freely available for download. Quality-assured measurements based on traceability and accurate evaluation of the measurement uncertainty are a valuable contribution to the technological infrastructure throughout the innovation process for many products and services.

Best-practice in making multivariate conformity assessment and decision-making was illustrated in case studies of healthcare products. Mathematical and statistical approaches to uncertainty evaluation were introduced in studies where typically there was no simple theory of how the perceived (‘response’) properties depend on the physical material (‘explanatory’) properties of the material. This is needed when dealing with properties important for consumers, such as smoothness of material surfaces (skin) as perceived in measurements by human panellists, which in turn depend on the surface topography, friction and hardness, of interest to the manufacturer wishing to fashion the product to the consumer’s satisfaction.

The research on a case study on the conformance assessment of electrical utility meters contained a description of the impact of today´s regulation and possible proposed changes. The case study on fire engineering provided a scientifically challenging example for conformity assessment based on a computationally expensive model and employs a hybrid approach. Decisions on conformity are important for environmental monitoring and product safety testing, but there is often no clear or harmonised basis for sharing the risks that arise from measurement uncertainty between the consumer and the supplier. Measurements requiring multivariate approaches (e.g. in healthcare products) are commonly required in conformity assessment. In these cases, two or more quantities and the associated probability density functions are used in conformity assessment and decision making, and current guidelines do not address these cases.

European Centre for Mathematics and Statistics in Metrology

The European Centre for Mathematics and Statistics in Metrology was set up with the support from the NMIs for a long term commitment to scientific collaboration between the members of the consortium. It is a European platform for metrologists, academia and industry for mathematical statistical research in metrological areas to meet future industrial needs.

Actual and potential impact

General dissemination has been achieved through 22 scientific journal papers, 47 conference contributions, and 8 trade journal articles. In summer 2015, a training course provided the first opportunity for experts from European NMIs, as well as interested stakeholders from industry, universities, regulatory bodies and NMIs outside Europe. This interaction will help encourage the application of mathematics and statistics to challenging uncertainty evaluation problems beyond the partners of the project. MATHMET2014, an International Workshop on Mathematics and Statistics for Metrology was held in PTB which gathered about

75 scientists from NMIs in Europe and overseas as well as colleagues from universities and research institutes in a lively exchange on metrology-related mathematical research themes.

Dissemination is also achieved by free distribution of 3 Best Practice Guides and 4 software packages through the project website and the MATHMET website. Best practice guides on the three topic areas give comprehensive summaries of the main findings in combination with tutorial introduction for practitioners, and are available for free download from the project website. The results of this project will strengthen European capabilities for innovation by enabling traceability for modern metrology and measurement techniques and by strengthening European NMIs role in international organisations (eg in the Joint Committee for Guides in Metrology (JCGM) – Working Group 1 on Uncertainty in Measurement). Product testing, safety regulations, medical diagnosis and drug testing will benefit from the procedures for reliable uncertainty evaluation, decision-making and conformity assessment that were developed in this project.

In the long term it is likely that this new guidance will be incorporated into GUM suite of documents, probably as a supplement; although the revision of the GUM is a long complicated process and will take many years.The BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP and OIML, which are representative bodies for the standards in different sector of industry and research, had identified the need for this work for their sectors. Their nominated representatives constitute the JCGM Working Group 1 (JCGM/WG1) on the Expression of Uncertainty in Measurement.

The European NMI scientists involved in the project are in dialogue with international and national technical committees and the wider metrological community. The results of the project were forwarded regularly to stakeholders, which included large energy generators, industrial companies, SMEs, instrument makes and research groups, and feedback has been received. The case studies have been developed in intensive exchange and resulted in seven joint publications.

Collaboration between European NMIs with mathematical and statistical expertise is essential to ensure wide take-up of the project outputs and to maintain Europe's current leading role in mathematics for metrology. Four key members of the consortium founded *MATHMET – A European Centre for Mathematics and Statistics in Metrology* as a platform to support and encourage such collaboration. MATHMET will continue to disseminate results internationally through its webpage (www.mathmet.org), and via conferences and workshops.

List of publications

A. Good practice guides:

1. C. Elster, K. Klauenberg, M. Walzel, G. Wuebbeler, P. Harris, M. Cox, C. Matthews, I. Smith, L. Wright, A. Allard, N. Fischer, S. Cowen, S. Ellison, P. Wilson, F. Pennecchi, G. Kok, A. van der Veen and L. R. Pendrill. A Guide to Bayesian Inference for Regression Problems, Good practice guide (WP1), available on https://www.ptb.de/emrp/new04-home.html (2015).

2. K. Rasmussen, J. B. Kondrup, A. Allard, S. Demeyer, N. Fischer, E. Barton, D. Partridge, L. Wright, M. Bär, A. Fiebach, H. Gross, S. Heidenreich, M.-A. Henn, R. Model, S. Schmelter, G. Kok and N. Pelevic. Novel mathematical and statistical approaches to uncertainty evaluation: Best practice guide to uncertainty evaluation for computationally expensive models, Good practice guide (WP2), available on https://www.ptb.de/emrp/new04-home.html (2015).

3. L. R. Pendrill, H. Karlsson, N. Fischer, S. Demeyer and A. Allard. A guide to decision-making and conformity assessment, Good practice guide (WP3), available on https://www.ptb.de/emrp/new04-home.html (2015).

B. Refereed Journal Papers:

1. A. Weissenbrunner, A. Fiebach, S. Schmelter, M. Bär, P. Thamsen, and T. Lederer. Simulation-based determination of systematic errors of flow meters due to uncertain inflow conditions. **Flow Measurement and Instrumentation**, approved for publication (2016).
   DOI: 10.1016/j.flowmeasinst.2016.07.011.

2. S. Heidenreich, H. Gross, M. Bär, and L. Wright. Uncertainty propagation in computationally expensive models: A survey of sampling methods and application to scatterometry. **Measurement**, approved for publication (2016). DOI: 10.1016/j.measurement.2016.06.009.

3. K. Klauenberg and C. Elster. Markov chain Monte Carlo methods: an introductory example **Metrologia** 53 (1), 32--39 (2016).

4. L. R. Pendrill and N. Petersson. Metrology of human-based measurements. Meas. Sci. Tech. 27, 094003 (2106). DOI: 10.1051/metrology/20150017001

5. S. Schmelter, A. Fiebach and A. Weissenbrunner. Polynomchaos zur Unsicherheitsquantifizierung in Strömungssimulationen für metrologische Anwendungen. **tm-Technisches Messen** 83 (2), 71--76 (2016).

6. K. Klauenberg, G. Wübbeler, B. Mickan, P. Harris, and C. Elster. A tutorial on Bayesian Normal linear regression. **Metrologia** 52 (6), 878-892 (2015). DOI: 10.1088/0026-1394/52/6/878.

7. K. Klauenberg, M. Walzel, B. Ebert and C. Elster. Informative prior distributions for ELISA analyses **Biostatistics** 16 (3), 454--464 (2015). DOI: 10.1093/biostatistics/kxu057.

8. S. Schmelter, A. Fiebach, R. Model and M. Bär. Numerical prediction of the influence of uncertain inflow conditions in pipes by polynomial chaos. **Int. J. Comp. Fluid. Dyn.** 29 (6-8), 411-422 (2015). DOI: 10.1080/10618562.2015.1112899.

9. S. Heidenreich, H. Gross and M. Bär. Bayesian approach to the statistical inverse problem of scatterometry: Comparison of three surrogate models. **Int. J. Uncertainty Quantification** 6, 511-526 (2015).

10. A. Allard, N. Fischer, G. Ebrard, P. Harris, L. Wright, D. Rochais and J. Mattout. A multi-thermogram-based Bayesian model for the determination of the thermal diffusivity of a material. **Metrologia** 53, 1--9 (2015). DOI: 10.1088/0026-1394/53/1/S32.

11. L. R. Pendrill and W.P. Fisher. Counting and quantification: Comparing psychometric and metrological perspectives on visual perceptions of number. **Measurement** 71, 46--55 (2015).

12. H. Gross, S. Heidenreich, A. Rathsfeld, M. A. Henn and M. Bär. Modeling aspects to improve the solution of the inverse problem in scatterometry. **Cont. Dyn. S.** (8), 497--519 (2015).

13. G. Kok, A. van der Veen, P. Harris, I. Smith and C. Elster. Bayesian analysis of a flow meter calibration problem. **Metrologia** 52 (2), 392--399 (2015).

14. L. R. Pendrill. Man as a measurement instrument. **NCSLI Measure J. Meas. Sci.** 9, 24--35 (2014)

15. O. Bodnar and C. Elster. On the adjustment of inconsistent data using the Birge ratio **Metrologia** 51 (5), 516--521 (2014).

16. L. R. Pendrill. Using measurement uncertainty in decision-making and conformity assessment. **Metrologia** 51 (4), 191--196 (2014)

17. G. Mana and C. Palmisano. Interval estimations in metrology. **Metrologia** 51 (3), 191--196 (2014).

18. H. Gross, S. Heidenreich, M. A. Henn, F. Scholze and M. Bär. Modelling line edge roughness in periodic-line space structures by Fourier optics to improve scatterometry. **JEOS** 9, 14003 (10pp) (2014). DOI: 10.2971/jeos.2014.14003.

19. S. Heidenreich, H. Gross, M. A. Henn, C. Elster and M. Bär. A surrogate model enables a Bayesian approach to the inverse problem of scatterometry. **J. Phys.: Conf. Ser.** 490, 012007(4pp) (2014). DOI: 10.1088/1742-6596/490/1/012007.

20. G. Wübbeler and C. Elster. Simplified evaluation of magnetic field fluctuation thermometry. **Meas. Sci. Tech.** 24, 115004 (8pp) (2013). DOI: 10.1088/0957-0233/24/11/115004.

21. A. Malengo and F. Pennecchi. A weighted total least-square algorithm for any fitting model with correlated variables. **Metrologia** 50, 654-662 (2013). DOI: 10.1088/0026-1394/50/6/654

22. M. A. Henn, S. Heidenreich, H. Gross, C. Elster and M. Bär. Improved grating reconstruction by determination of line roughness in extreme ultraviolet scatterometry. Opt. Lett. 37 (24), 5229-5231 (2012). DOI: 10.1364/OL.37.005229.

C. Trade Journal and Conference Papers

23. H. Karlsson, A.A. Falnes Olsen and L. R. Pendrill. Conformance assessment of electrical energy meters investigated by risk analysis – a case study. OIML - Bulletin LVII (2) (2016).

24. P.G. Spazzini, F. Pennecchi, E. Pessana and A. Piccato. Analysis of Flow Meters Calibration Proceedings of the 9th ISFFM Symposium Arlington (2015). http://library.ceesi.com/...&orgid=16&eid=424

25. S. Demeyer, N. Fischer, F. Didieux and M. Binacchi
Statistical methods for conformity assessment when dealing with computationally expensive systems: application to a fire engineering case study. Advanced Mathematical and Computational Tools in Metrology and Testing X. F. Pavese et al. (Eds.), World Scientific, Singapore (2015).

26. A. Weissenbrunner, A. Fiebach, S. Schmelter, M. Straka, M. Bär and T. Lederer.
Numerical prediction of the flow rate through a flow meter with uncertain inflow profile
Proceedings of Imeko 2015 XXI World Congress Measurement in Research and Industry (2015).
https://www.imeko.org/pub...MEKO-WC-2015-TC21-389.pdf.

27. L. R. Pendrill and N. Petersson. Metrology of human-based measurement (2015). DOI: http://dx.doi.org/10.1051/metrology/20150017001;http://cfmetrologie.edpsciences.org/articles/metrology/abs/2015/01/metrology_metr2015_17001/metrology_metr2015_17001.html.

28. S. Heidenreich, H. Gross and M. Bär. Alternative methods for uncertainty evaluations in EUV scatterometry. Proc. SPIE: Modeling aspects in Optical metrology IV 8789, 87890T-1 (8pp) (2013) DOI: 10.1117/12.2020677.

29. M. Bär, C. Elster, S. Heidenreich, C. Matthews, L. R. Pendrill and L. Wright.
Novel mathematical and statistical approaches to uncertainty evaluation: introducing a new EMRP research (2013). DOI: 10.1051/metrology/201304010; http://www.metrologie2013.com/index_en.php.

30. C. Elster, K. Klauenberg, M. Bär, A. Allard, N. Fischer, G. Kok, A. van der Veen, P. Harris, I. Smith, L. Wright, S. Cowen, P. Wilson and S. Ellison. Novel mathematical and statistical approaches to uncertainty evaluation in the context of regression and inverse problems (2013). DOI: 10.1051/metrology/201304003; http://www.metrologie2013.com/index_en.php.

C. Papers submitted to Refereed Journals

1. L. Wright, A. Allard, L. Chapman, S. Demeyer, N. Fischer, and D. Partridge. Laser flash experiment on layered materials: parameter estimation and uncertainty evaluation. Submitted, 2015.

2. S. Demeyer, D. Marquis, and N. Fischer. Surrogate-model based sequential sampling estimation of conformance probability for computationally expensive systems: application to fire safety science. Submitted, 2015.

3. P. Wilson and S. L. R. Ellison. Extending digital PCR analysis by modelling quantification cycle data. Submitted, 2015.

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