PROPAGATION OF MEASUREMENT UNCERTAINTY FOR SURFACE
TEXTURE PARAMETERS

J. K. Brennan¹, X. Jiang¹, A. Crampton¹ and R. K. Leach²
¹University of Huddersfield, Queensgate, Huddersfield, HD1 3DH, UK
²National Physical Laboratory, Teddington, Middlesex, TW11 0LW, UK

ABSTRACT

This paper outlines a proposal for research into fulfilling the need for reliable software algorithms to compute the standard uncertainty of surface texture parameters. The target will be to develop a library of software algorithms for the sole purpose of safely calculating surface parameters from ISO standards. The research pays particular attention to the propagation of measurement uncertainty through each parameter, something which has not been thoroughly addressed in this field. By taking existing methodologies to express the uncertainty of measurement the endeavour is to tailor a new method that will specifically address the special issues concerned with determining surface texture parameters from nano-scale surfaces.

Keywords metrology uncertainty surface texture parameter

1 INTRODUCTION

Examining the surface of an object under magnification will reveal a complex terrain that is a result of the structure of the material surface and the processes used to manufacture it. This complex topography is called surface texture and plays a vital role in the functionality of engineered products, since it affects the performance, quality and life of such products. For many years surface texture has been measured in order to quantify and control the surface characteristics of products.

A set of parameters provides a readily compared group of values that quantify aspects of a surface. In the case of two-dimensional measurement, for example, a parameter can be thought of as a function that can be applied to a measured surface profile. The current ISO specification standard, ISO 4287: 1997 [1], lists eleven parameters for two-dimensional measurements. However, it has been shown that some, if not all, of these published standard parameters exhibit an element of ambiguity in their definition [2, 3]. Recent comparisons of surface texture measurement results (parameters) have shown an alarming spread in the results [4], which highlights the need for the concept of the software measurement standard, introduced in ISO 5436-2 [5], in order to eliminate the scope for (mathematically) differing implementations of the same parameter. Research carried out [6, 7] has already provided unambiguous mathematical algorithms for some of these parameters; although without a statement of uncertainty for a calculated surface texture parameter it is difficult to assess the quality of any value given for a parameter.

The calculation of the uncertainty associated with the measurement of surface texture is a very complicated task. This is because the measurement of surface texture itself is a complicated procedure. The most common method of measuring a surface is by using a stylus instrument whereby a sharp tip (the stylus) is drawn across the surface at a constant speed (Figure 1). From movement of the stylus an electrical signal is obtained and amplified, much more so in the vertical direction, to produce an outline of the surface called a profile. Software filters are applied to this digitised profile to extract the roughness element of the profile, to which parameter-estimation software is applied. There are many variables involved in the measurement of surface texture: not just the calibration of the stylus instrument and traceability issues, but also the effects of using a different sized stylus, the part of the artefact that is measured, the measurement environment and also the software developer’s interpretation of the filters and parameters involved. It can be seen that the repeatability and reproducibility of results present problems and that the evaluation of the measurement uncertainty associated with a surface texture parameter is, therefore, difficult. Considerable benefit would result if (a) software measurement standards could be used to improve this process and (b) approaches were developed by which the uncertainty could reliably be evaluated.
In comparison with software measurement standards there has been little progress on the reliable evaluation of measurement uncertainty for these parameters. Current literature only provides an approach that tends to overestimate uncertainty [8]. At present no standard exists that caters specifically for the complex measurement process of surface texture parameters. There is however a generic guide [9] for the evaluation of uncertainty in all fields of metrology.

A genuine need exists for the development of robust algorithms for this purpose. Algorithms are required that can:

1. handle large sets of data at the nano-scale as calculations using a large volumes of data that is of a very small magnitude can result in ill conditioning without due care and attention
2. compute reliably and stably the uncertainty associated with an estimated surface texture parameter, possibly using approaches that are dedicated exclusively to that parameter function.

2 THE PROJECT

This proposal is for a three-year research study in which uncertainty evaluation techniques for surface texture parameters by a combination of new surface metrology research and sound mathematical theory will be investigated. The research will facilitate the development of a complete software library containing algorithms for the reliable evaluation of the uncertainty associated with current surface texture parameters.

This proposed project is based on principles derived from initial research recently carried out at the University of Huddersfield under an EPSRC CASE award studentship in close collaboration with the National Physical Laboratory (NPL). Some highlights of that research are listed below:

(1). It has been presented that the definitions of measurement parameters, and subsequently the implementation of software for their evaluation, will benefit greatly from a mathematical treatment founded on sound approximation theory and numerical analysis [1]. The previous research showed that it will be necessary for the development of a deeper understanding of uncertainty evaluation in the processes applied to measured surface profiles, to extract and quantify desired characteristics, in order to provide traceable and reliable measurement results in the calculation of surface parameters.

(2). An approach to surface profile data fitting was presented [10] that overcomes the apparent ineffectiveness of the Gaussian profile filter with non-uniformly spaced profile points [11]. This process allows more efficient and more reliable computation of the surface profile parameters because it represents the discrete profile as a series of continuous functions. This feature permits definite integrals and other mathematical quantities found in the definition of surface profile parameters to be calculated exactly from these functions rather than approximated using numerical quadrature.

(3). The result of propagating uncertainty through surface texture profile parameters, using the developed method of data fitting, was presented in [12]. This method of data fitting was used in conjunction with existing methods for the evaluation of uncertainty [9, 13] and provided a better approximation to both the measurand (parameter value) and its associated uncertainty value.

The initial investigation of previous work carried out was published at the international Euspen conference series [2, 6]. The research into surface profile data fitting was published in Journal of Physics: Conference Series [10], and the results of this method with the propagation of uncertainty was published in the illustrious series of Advanced Mathematical and Computational Tools in Metrology [12].

3 AIMS & OBJECTIVES OF THE PROPOSED PROJECT

This project aims to explore the evaluation of stable and reliable evaluation of measurement uncertainty associated with standard surface texture parameters by whatever methods are deemed necessary.
Objectives

- To design and develop a complete software library of algorithms for the evaluation of uncertainty for all surface texture parameters with particular focus on two-dimensional profiles
- To determine those methods that are best suited to evaluate the measurement uncertainty associated with estimates of the parameters
- To develop robust mathematical algorithms based on established theoretical knowledge with the focus firmly on numerical reliability
- To produce a comprehensive software library with full documentation to a level suitable of being associated with software measurement standards

4 PROGRAMME AND METHODOLOGY

4.1 FORMULATE THE PROBLEM

The first task to be undertaken for this project will be a formulation of the given problem. The aim here is to identify the sources of uncertainty and quantify these sources in terms of standard uncertainty values or, more comprehensively, in terms of probability distributions. These sources can include:

- The standard uncertainty of the measurement instrument
- The correlation effect introduced by the filtration process
- The element of non-linearity caused by the arcial movement of the measuring stylus

It is not in the nature of this project to state how such contributing uncertainties can be solved or eradicated from the process but to quantify their contribution to the standard uncertainty of the parameters. All measurements have uncertainties and some may have a negligible effect on further calculations of the measurement, such as our parameter values, but to know that a particular contribution has a negligible effect is a much safer place to be.

4.2 APPLICATION OF THE GUIDE

‘The Guide’ is the term used to refer to the authoritative document *the Guide to the expression of uncertainty in measurement* [9]. This is the key document in the area of uncertainty evaluation and provides a procedure for evaluating uncertainties. This procedure is formulated as one of propagating uncertainty through a measurement model; see Figure 2. The model has \( n \) sets of input quantities \( X_i \) and \( Z_i \), which are the profile co-ordinate values estimated by \( x_i \) and \( z_i \) with associated standard uncertainty \( u(z) \). There is a single output quantity \( Y \), estimated by the measurement result \( y \) with associated standard uncertainty \( u(y) \).

However, the nature of some of the standard surface texture parameters is inherently incompatible with the methodology stated in *the Guide*, especially those such as 

\[
Rp = \max(Z),
\]

which is discontinuous, and \( Rv \), which is non-linear.

The Guide approach applies the Law of Propagation on Uncertainty (LPU) and requires the following conditions to hold:

- the non-linearity of \( f \) must be insignificant
- the Central Limit Theorem (CLT) must apply and the output quantity be characterised by a Gaussian or \( t \)-distribution.

It has been shown that the second point cannot always be assumed [12]; however, this is largely a result of the first point not holding. When LPU is used in violation of the above conditions (one is usually unaware of this), the results produced can only be regarded as approximate, with an unquantified degree of approximation.

Further, *the Guide* is often applied by disregarding mutual dependencies in the input quantities. Here, however, the measured values constituting a profile have associated correlation due to the filtration process [14] and non-linearity as a result of the inherent nature of contact stylus measurement [15]. Additional information is needed to quantify these attributes.
4.3 APPLICATION OF A MONTE CARLO METHOD

The Guide does not refer explicitly to the use of a Monte Carlo method (MCM) [13]. However it does state in cases where the law of propagation of uncertainty cannot be applied that other analytical or numerical methods are required. MCM is a sampling technique that provides an implementation of the propagation of distributions. The process is undertaken numerically rather than analytically and it provides much richer information, by propagating the probability density functions (PDFs) for the input quantities $Z_i$ (rather than just the uncertainties associated with these values) through the measurement model $f$ to provide the PDF for the output quantity $Y$. A Supplement to The Guide concerned with MCM Error! Reference source not found., which is expected to be a highly influential document in the world of uncertainty evaluation, is at an advanced stage of development. This project would constitute one of the earliest serious applications of that Supplement, following its expected publication in 2007.

4.4 APPLICATION OF BAYESIAN INFERENCE

The application of Bayes' theorem to uncertainty evaluation [16, 17] is not widely known to metrologists and is virtually non-existent in the field of surface texture parameters. Bayesian inference provides a rigorous means of using all known prior information in calculating a measurand. It allows the current state of knowledge about the measurand to be refined in the light of new information acquired through the measurement process.

The Bayesian approach offers a systematic and flexible approach to the problem of uncertainty evaluation. By adopting an objective or non-informative prior, the Bayesian approach produces estimates and uncertainty measures comparable to the classical approach. However, particularly in the case of surface texture profile measurement, it is important to take into account either prior information or physical knowledge, or any underlying latent and unobservable processes, such as those that have been identified in 4.1. Thus, the Bayesian approach offers a viable and rigorous solution, though there is the added benefit of providing much needed uncertainty and probability assessments in non-linear situations in a valid and rigorous way.

A method using a Bayesian approach will also allow certain prior rules to be observed that could be overlooked using an analytical approach. In the case of an ultra flat surface, the magnitude of a parameter value could be overshadowed by that of the associated uncertainty. Figure 3 shows such a case where the probability density function (PDF) of the calculated $Ra$ value crosses over the zero threshold. Therefore, when determining a coverage interval for a parameter, it could lead to the belief that the parameter has a finite probability of being negative or taking some other infeasible value. A Bayesian method would not allow this as part of the prior knowledge would simply state that this value cannot be negative.

Bayesian inference also has the advantage of providing coverage intervals for parameters that are more in line with commonsense interpretations. The statement that a coverage interval for a parameter such as $5.0 \, \text{nm} \pm 0.5 \, \text{nm}$ for a coverage probability of 95 % is often interpreted that over many repeated instances the interval produced (in this case from 4.5 nm to 5.5 nm) will contain the parameter 95 % of the time. In other words the probability statement related to the coverage interval refers to the randomness of the sampling process. In Bayesian statistics an interval is also produced, but this is called a credible set or credible interval. The probability statement in a credible set is one practitioners seem ‘naturally’ to want; it is the probability that the parameter lies in the interval. At a glance these statements are easier to visualise and comprehend.

4.5 DETERMINATION OF RESULTS AND COMPARISON OF APPROACHES

Numerical results will be obtained for all surface texture parameters considered for actual profile data using the three approaches constituting the core of the research, the Guide, MCM and Bayesian inference. These three approaches and the results they provide will be compared and critically appraised. As far as possible, general conclusions will be drawn concerning the adequacy and suitability of the various approaches for each parameter.
4.6 CONSTRUCTION AND EVALUATION OF SOFTWARE LIBRARY AND KNOWLEDGE TRANSFER

Drawing upon the research carried out and the software developed in 4.1 – 4.4 a final version of each algorithm will be produced complete with documentation of the underlying mathematical analysis. The extent of the special care required when treating each parameter in order to evaluate the uncertainty associated with an estimate of it will be determined in the course of the study.

At appropriate stages the approaches used and the results obtained will be discussed with NPL and industrial instrument makers and users, and with experts concerned with the development of surface texture standards, to ensure the suitability of the approaches in practice.

5 INDUSTRIAL COLLABORATORS

The National Physical Laboratory (NPL) will support this project mainly in kind in terms of traceability research, time and knowledge to the total of three days per year (£8k), as the work aligns well to structure outlined in the next Software Support for Metrology1 (SSfM) programme; an initiative funded by the DTI.

REFERENCES


1 See http://www.npl.co.uk/ssfm/ for more information.

Figure 1. Path of a stylus in surface profile measurement.

Figure 2. Input-output model illustrating the propagation of uncertainty.

Figure 3. Part of the PDF indicates that the Ra value could be negative.