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# Uncertainty evaluation for the calculation of a surface texture parameter in the profile case

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March 2010

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# ABSTRACT

Knowledge of the topography of a machined surface is necessary in order to understand the functional performance of the surface, and is consequently essential to the manufacturing process. Surface texture parameters defined in ISO specification standards are widely used to associate numerical values to the measured topography. However, if the values of a parameter are to be used for the comparison of different surfaces and for the interpretation of surface texture tolerances on engineering drawings, it is essential that the values are accompanied by statements of uncertainty. Furthermore, it is important that those statements are reliable and convey meaningful information about the parameter. Consideration is given to the problem of uncertainty evaluation for a particular (amplitude) surface texture parameter, viz., the root mean square value of a surface profile. A formulation of the problem is given in terms of a measurement model that defines the mathematical relationship between all quantities involved in the measurement and the available information about those quantities. The applications of two approaches to solving the formulated problem, namely the conventional approach of 'uncertainty propagation' and a Monte Carlo method that provides a more generally-applicable approach, are described. The results obtained from the two approaches for simulated measurement data are compared.

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# 1 Introduction

Knowledge of the topography of a machined surface is necessary in order to understand the functional performance of the surface, and is consequently essential to the manufacturing process [6]. The use of a surface texture parameter to characterize numerically the measured topography was proposed many years ago [19], and a number of parameters have been adopted by standards bodies and are used in industry for this purpose. For example, the current ISO specification standard [14] lists eleven parameters for characterizing a surface profile, which are calculated in terms of the coordinates of points on the profile. However, if the values of a parameter are to be used for the comparison of different surfaces and for the interpretation of surface texture tolerances on engineering drawings, it is essential that the values are accompanied by statements of uncertainty that reflect the uncertainties associated with the coordinate values measured by surface measuring instruments. Furthermore, it is important that those statements are reliable and convey meaningful information about the parameter.

In this report the problem of uncertainty evaluation for a particular (amplitude) surface texture parameter, viz., the root mean square value of a surface profile, is considered. The aims of the work are summarized as follows.

1. To give a formulation of the problem of uncertainty evaluation in terms of (a) a measurement model that defines the mathematical relationship between all quantities involved in the measurement, and (b) the available information about those quantities;

2. To describe the applications of two approaches to solving the formulated problem, namely the conventional approach of 'uncertainty propagation' and a Monte Carlo method that provides a more generally-applicable approach, and to compare the results obtained from the two approaches;

3. To investigate the impact on the results of different information about the measured quantities in the measurement model, such as whether the quantities are correlated as a consequence of common (systematic) errors affecting the data provided by an instrument.

With regard to the first aim, the procedure for evaluating a surface texture parameter for a measured profile is a complicated one, involving a number of steps, including the application of filters to the profile. Furthermore, the relevant specification standards that define these steps do so in terms of continuous (analogue) representations of the profile, and the definitions need to be *interpreted* appropriately if they are to be applied to the discrete (digital) representations that are available in practice [5]. The definitions, which are typically presented as integrals of functions of the continuous profile, are formulated in this work as quadrature rules involving the measured coordinate values. This formulation allows for the consideration of uncertainties associated with both (abscissa and ordinate) coordinate values of the measured points.

Only one surface texture parameter is treated. However, similar considerations (in terms of approach) would apply to other such parameters. For some related material work, see, e.g., [11, 16].

The report is organized as follows. The measurement model in the form of the measurement functions that define the computational steps to evaluate a surface texture parameter for a measured surface profile is described in section 2. The uncertainties associated with the coordinate values of a measured profile are considered in section 3. The cases when there are uncertainties associated with the ordinate values only and there are uncertainties associated with both (abscissa and ordinate) coordinate values are treated. The uncertainties associated with the coordinate values provided by a particular instrument, NPL's NanoSurf IV [18], are also quantified. Approaches to measurement uncertainty evaluation, including the GUM uncertainty framework based on the law of propagation of uncertainty and a Monte Carlo approach as a generally-applied procedure, are described in section 4. The applications of these approaches to the problem of evaluating a surface texture parameter are presented in sections 5 and 6. The results of applying the approaches for simulated surface profile data are given and discussed in section 7. Finally, conclusions are given in section 8.

# 2 Measurement functions

The following steps are undertaken to calculate surface texture parameters for a measured surface profile:

1. Remove geometric form from the measured profile;
2. Mean centre the resulting profile;
3. Apply filters to obtain the primary, waviness and roughness profiles;
4. Evaluate surface texture parameters for the primary, waviness and roughness profiles [14].

Each of the steps is described below for a particular surface texture parameter. For each step, the corresponding measurement function to be used as the basis for the associated uncertainty evaluation is given. These measurement functions comprise the measurement model that describes the mathematical relationship between all quantities involved in the measurement.

## 2.1 Form removal and profile mean centering

Let $z(x)$ denote the function representing the surface profile as perceived by the measuring instrument. The first steps in evaluating surface texture parameters for $z(x)$ are to determine a profile $y(x)$ by (a) removing geometric form from $z(x)$, and (b) 'mean centering' the resulting profile so that the average 'height' is zero. In practice, knowledge of $z(x)$ takes the form of a set of measured points with coordinate values $(x_i, z_i)$, $i = 1, \ldots, n$, with $x$-coordinate values that are uniformly spaced, and these steps are undertaken in terms of these values.[1]

In (a), for example, (ordinary or orthogonal) least-squares fitting to the measured points may be used to remove geometric form. Because a number of different surface geometries, including planes, spheres, cylinders, etc., are measured in practice, and the treatment can depend on the geometry, it will be assumed in this work that geometric form has already been removed.

In (b), the step of mean centering consists of evaluating ordinate values $y_i$, $i = 1, \ldots, n$, given by

$$y_i = z_i - \frac{1}{n}\sum_{i=1}^{n} z_i. \tag{1}$$

The above formula[2] suggests the measurement functions

$$Y_i = Z_i - \frac{1}{n}\sum_{i=1}^{n} Z_i \tag{2}$$

for quantities $Y_i \equiv y(x_i)$ representing the ordinates of $y(x)$. The value $y_i$ given by formula (1) is an estimate of $Y_i$ calculated using the measurement function (2) for the estimates (measured values) $z_i$ of quantities $Z_i \equiv z(x_i)$ representing the ordinates of $z(x)$.

## 2.2 Filtering to obtain the primary, waviness and roughness profiles

The primary profile $p(x)$ is derived from the mean centred profile $y(x)$ by filtering $y(x)$ to remove short-wavelength components associated with measurement noise.[3] The filter used is defined by its cut-off wavelength $\lambda_{\rm s}$,[4] which is the wavelength of the sinusoidal

[1] In fact, these steps, which are not well defined in specification standards, are here *defined* in terms of the coordinate values that constitute a discrete (digital) representation of $z(x)$. In contrast, specification standards define the steps of filtering (section 2.2) and evaluating surface texture parameters (section 2.3) in terms of continuous (analogue) representations of profiles, and are subsequently *interpreted* in terms of discrete representations of those profiles.

[2] If the step of mean centering were to be defined in terms of a continuous representation of $z(x)$, the use of the arithmetic mean as an interpretation of that step might not be appropriate. A formulation in terms of a quadrature rule might be used instead: see sections 2.2 and 2.3.

[3] For stylus-based surface-texture measuring instruments, the use of a non-ideal stylus ball, i.e., one with a radius that is non-zero, leads naturally to the suppression of short-wavelength components. Consequently, filtering of the measured surface profile to remove short-wavelength components can be regarded as being performed 'mechanically' as part of the measurement of the profile. Nevertheless, it is usual to filter the profile 'numerically' to reduce the influence of measurement noise.

[4] For clarity, the notation $\lambda_{\rm s}$, $\lambda_{\rm c}$ and $\lambda_{\rm f}$ are used throughout to denote filter cut-off wavelengths in place of the (more familiar) notation $\lambda s$, $\lambda c$ and $\lambda f$ used in specification standards.

component of the profile for which $50\,\%$ of the amplitude of the component is transmitted by the filter, with shorter wavelength components attenuated to a greater extent and longer wavelength components to a lesser extent.

The waviness profile $w(x)$ and roughness profile $r(x)$, satisfying

$$p(x) = w(x) + r(x),$$

are derived from the primary profile $p(x)$ by suppressing the short-wavelength and long-wavelength components, respectively, of $p(x)$ using a filter with cut-off wavelength $\lambda_{\rm c}$, where $\lambda_{\rm c} > \lambda_{\rm s}$.[5]

A general form of linear filter applied to $y(x)$ is defined by

$$f(x) = \int_{-\infty}^{\infty} K(x, \xi) y(\xi)\,\mathrm{d}\xi,$$

where $f(x)$ is the filtered profile and $K(x, \xi)$ is the kernel of the filter. Furthermore, if $K(x, \xi) = k(x - \xi)$, i.e., the value of the kernel only depends on the difference between $x$ and $\xi$, the filter is defined by the convolution integral

$$f(x) = \int_{-\infty}^{\infty} k(x - \xi) y(\xi)\,\mathrm{d}\xi,$$

and $k(x - \xi)$ is called the weighting function of the filter. A linear filter widely used in the measurement of surface texture is the Gaussian filter [15] with weighting fuction

$$s(x - \xi, \lambda) = \frac{1}{\alpha\lambda} \exp\left[-\pi \left(\frac{x - \xi}{\alpha\lambda}\right)^2\right],$$

where $\alpha = \sqrt{\log 2/\pi}$. The filter suppresses short-wavelength components of $y(x)$ and gives $50\,\%$ transmission at the cut-off wavelength $\lambda$. Using this filter,

$$p(x) = \int_{-\infty}^{\infty} s(x - \xi, \lambda_{\rm s}) y(\xi)\,\mathrm{d}\xi, \tag{3}$$

$$w(x) = \int_{-\infty}^{\infty} s(x - \xi, \lambda_{\rm c}) p(\xi)\,\mathrm{d}\xi, \tag{4}$$

and

$$r(x) = p(x) - w(x). \tag{5}$$

[5]According to the specification standard [14], the waviness profile $w(x)$ is derived from the primary profile $p(x)$ by suppressing long-wavelength and short-wavelength components of $p(x)$ using filters with cut-off wavelengths $\lambda_{\rm f}$ and $\lambda_{\rm c}$, respectively, where $\lambda_{\rm f} > \lambda_{\rm c} > \lambda_{\rm s}$. The roughness profile $r(x)$ is also derived from $p(x)$ by suppressing only long-wavelength components of $p(x)$ using a filter with cut-off wavelength $\lambda_{\rm c}$. However, the value of $\lambda_{\rm f}$ is not well defined in specification standards (such as [13]) and, consequently, it is common practice not to apply this filter.

#### 2.2.1 Measurement functions for the case of uncertainties associated with the ordinate values only

In practice, knowledge of the profile $y(x)$ takes the form of a set of points with coordinate values $(x_i, y_i),\ i = 1, \ldots, n$ (section 2.1), with $x$-coordinate values that are uniformly spaced with spacing interval $h$, i.e., $x_{i+1} - x_i = h,\ i = 1, \ldots, n-1$. Then, the calculation of the primary profile at $x = x_i,\ i = 1+m_{\rm s}, \ldots, n-m_{\rm s}$, is implemented using the discrete convolution

$$\begin{aligned} p_i &= h \sum_{k=i-m_{\rm s}}^{i+m_{\rm s}} s(x_i - x_k, \lambda_{\rm s}) y_k \\ &= h \sum_{j=-m_{\rm s}}^{m_{\rm s}} s(x_i - x_{i+j}, \lambda_{\rm s}) y_{i+j} \\ &= h \sum_{j=-m_{\rm s}}^{m_{\rm s}} s(-jh, \lambda_{\rm s}) y_{i+j}, \end{aligned}$$

from which it follows

$$p_i = h \sum_{j=-m_{\rm s}}^{m_{\rm s}} s_{{\rm s},j} y_{i+j}, \qquad (6)$$

where

$$s_{{\rm s},j} = s(jh, \lambda_{\rm s}), \quad j = -m_{\rm s}, \ldots, m_{\rm s}.$$

It is assumed that $h$ is sufficiently small compared with $\lambda_{\rm s}$ and $m_{\rm s}$, which determines the number of points in the discrete convolution, is sufficiently large so that, to a good approximation,

$$s_{{\rm s},-m_{\rm s}} = s_{{\rm s},m_{\rm s}} = 0, \qquad (7)$$

and the filter is normalized, i.e.,

$$h \sum_{j=-m_{\rm s}}^{m_{\rm s}} s_{{\rm s},j} = 1. \qquad (8)$$

In terms of the results obtained from the discrete convolution (6), the primary profile is defined by the points with coordinate valuess $(x_i, p_i),\ i = 1 + m_{\rm s}, \ldots, n - m_{\rm s}$.

In the case that there is no uncertainty associated with the values $x_i,\ i = 1, \ldots, n$, the formula (6) suggests the measurement functions

$$P_i = h \sum_{j=-m_{\rm s}}^{m_{\rm s}} s_{{\rm s},j} Y_{i+j}, \qquad (9)$$

for quantities $P_i$ representing the ordinates of the primary profile. In these functions, $P_i$ are approximations to the quantities $p(x_i)$ defined by the continuous convolution (3). The value

$p_i$ given by formula (6) is an estimate of $P_i$ calculated using the measurement function (9) for the estimates $y_{i+j}$ of $Y_{i+j} \equiv y(x_{i+j})$, the (known) values $s_{\mathrm{s},j}$ of the Gaussian weighting function with cut-off wavelength $\lambda_\mathrm{s}$, and the (known) value $h$ of the spacing interval.

Similar considerations apply to the determinations of the waviness and roughness profiles from the primary profile. The calculation of these profiles is implemented using

$$w_i = h \sum_{j=-m_\mathrm{c}}^{m_\mathrm{c}} s_{\mathrm{c},j} p_{i+j}, \quad r_i = p_i - w_i, \tag{10}$$

where

$$s_{\mathrm{c},j} = s(jh, \lambda_\mathrm{c}), \quad j = -m_\mathrm{c}, \ldots, m_\mathrm{c}.$$

It follows that measurement functions for quantities $W_i$ and $R_i$ representing the ordinates of the waviness and roughness profiles at $x = x_i$, $i = 1 + m_\mathrm{s} + m_\mathrm{c}, \ldots, n - m_\mathrm{s} - m_\mathrm{c}$, take the form

$$W_i = h \sum_{j=-m_\mathrm{c}}^{m_\mathrm{c}} s_{\mathrm{c},j} P_{i+j}, \quad R_i = P_i - W_i. \tag{11}$$

### 2.2.2 Measurement functions for the case of uncertainties associated with both coordinates

Provided the conditions (7) hold, the discrete convolution (6) can be expressed in the alternative form

$$p_i = h \sum_{j=-m_\mathrm{s}}^{m_\mathrm{s}}{}'' s_{\mathrm{s},j} y_{i+j}, \tag{12}$$

where the double prime notation means that the first and last terms in the summation are multiplied by one half. The expression (12) corresponds to an application of the trapezoidal quadrature rule to the continuous convolution integral (3) for values $\xi \in [x_{i-m_\mathrm{s}}, x_{i+m_\mathrm{s}}]$.[6] It follows that

$$p_i = \sum_{k=-m_\mathrm{s}}^{m_\mathrm{s}-1} q_k, \quad q_k = \tfrac{1}{2} h (s_{\mathrm{s},k} y_{i+k} + s_{\mathrm{s},k+1} y_{i+k+1}), \tag{13}$$

in which $q_k$ is the value of the integral of the straight-line function joining the points $(x_{i+k}, s_{\mathrm{s},k} y_{i+k})$ and $(x_{i+k+1}, s_{\mathrm{s},k+1} y_{i+k+1})$. If the values $x_i$, $i = 1, \ldots, n$, are not uniformly spaced, a modest generalization [10] of the calculation (13) is

$$p_i = \sum_{k=-m_\mathrm{s}}^{m_\mathrm{s}-1} q_k, \quad q_k = \tfrac{1}{2} (x_{i+k+1} - x_{i+k})(s_{\mathrm{s},k} y_{i+k} + s_{\mathrm{s},k+1} y_{i+k+1}),$$

[6] An alternative to the trapezoidal quadrature rule would be to use the (simpler) midpoint quadrature rule, which would provide an approximation to the continuous convolution integral (3) for values $\xi$ in the (larger) interval $[x_{i-m_\mathrm{s}} - h/2, x_{i+m_\mathrm{s}} + h/2]$. The trapezoidal rule has been chosen here to be consistent with the choice of that rule for the evaluation of the surface texture parameter described in section 2.3. For the evaluation of that parameter, an integration is to be performed over a specified *finite* interval, and the use of the trapezoidal quadrature rule corresponds to integrating *exactly* a piecewise linear approximation to the integrand.

or, equivalently,

$$\begin{aligned} p_i = {} & \tfrac{1}{2}(x_{i-m_\mathrm{s}+1} - x_{i-m_\mathrm{s}}) s(x_{i-m_\mathrm{s}} - x_i, \lambda_\mathrm{s}) y_{i-m_\mathrm{s}} \\ & + \sum_{j=-m_\mathrm{s}+1}^{m_\mathrm{s}-1} \tfrac{1}{2}(x_{i+j+1} - x_{i+j-1}) s(x_{i+j} - x_i, \lambda_\mathrm{s}) y_{i+j} \\ & + \tfrac{1}{2}(x_{i+m_\mathrm{s}} - x_{i+m_\mathrm{s}-1}) s(x_{i+m_\mathrm{s}} - x_i, \lambda_\mathrm{s}) y_{i+m_\mathrm{s}}, \end{aligned} \tag{14}$$

in which the dependence of the values of the Gaussian weighting function on the values $x_i$ and $x_{i+j}$ has been made explicit.

In the case that there are uncertainties associated with the values $x_i$ and $y_i,\ i = 1, \ldots, n$, the formula (14) suggests the measurement functions

$$\begin{aligned} P_i^x = {} & X_i, \\ P_i^z = {} & \tfrac{1}{2}(X_{i-m_\mathrm{s}+1} - X_{i-m_\mathrm{s}}) s(X_{i-m_\mathrm{s}} - X_i, \lambda_\mathrm{s}) Y_{i-m_\mathrm{s}} \\ & + \sum_{j=-m_\mathrm{s}+1}^{m_\mathrm{s}-1} \tfrac{1}{2}(X_{i+j+1} - X_{i+j-1}) s(X_{i+j} - X_i, \lambda_\mathrm{s}) Y_{i+j} \\ & + \tfrac{1}{2}(X_{i+m_\mathrm{s}} - X_{i+m_\mathrm{s}-1}) s(X_{i+m_\mathrm{s}} - X_i, \lambda_\mathrm{s}) Y_{i+m_\mathrm{s}}, \end{aligned} \tag{15}$$

for quantities $P_i^x$ and $P_i^z$ representing the coordinates defining the primary profile at $x = x_i$, $i = 1 + m_\mathrm{s}, \ldots, n - m_\mathrm{s},$. The values $x_i$ and $p_i$ are estimates of $P_i^x$ and $P_i^z$ calculated using the (bivariate) measurement function (15) for the estimates (measured values) $x_i$ of $X_i$ and $y_i$ of $Y_i \equiv y(X_i)$.

Similar considerations apply to the determinations of the waviness and roughness profiles from the primary profile. Measurement functions for quantities $(W_i^x, W_i^z)$ and $(R_i^x, R_i^z)$, $i = 1 + m_\mathrm{s} + m_\mathrm{c}, \ldots, n - m_\mathrm{s} - m_\mathrm{c}$, representing the coordinates of the $i$th points defining the waviness and roughness profiles are given by, respectively,

$$\begin{aligned} W_i^x = {} & X_i, \\ W_i^z = {} & \tfrac{1}{2}(X_{i-m_\mathrm{c}+1} - X_{i-m_\mathrm{c}}) s(X_{i-m_\mathrm{c}} - X_i, \lambda_\mathrm{c}) P_{i-m_\mathrm{c}}^z \\ & + \sum_{j=-m_\mathrm{c}+1}^{m_\mathrm{c}-1} \tfrac{1}{2}(X_{i+j+1} - X_{i+j-1}) s(X_{i+j} - X_i, \lambda_\mathrm{c}) P_{i+j}^z \\ & + \tfrac{1}{2}(X_{i+m_\mathrm{c}} - X_{i+m_\mathrm{c}-1}) s(X_{i+m_\mathrm{c}} - X_i, \lambda_\mathrm{c}) P_{i+m_\mathrm{c}}^z, \end{aligned} \tag{16}$$

and

$$\begin{aligned} R_i^x &= X_i, \\ R_i^z &= P_i^z - W_i^z. \end{aligned} \tag{17}$$

### 2.3 Evaluation of the surface texture parameter

The example of a surface texture parameter considered here is the root mean square value of the evaluated profile, denoted by $P_q$, $W_q$ and $R_q$ according to whether the evaluated profile is the primary, waviness or roughness profile [14]. A (generic) definition of this amplitude parameter is

$$A_q = \frac{1}{n_s} \sum_{k=1}^{n_s} A_{q,k}, \tag{18a}$$

$$A_{q,k}^2 = \frac{1}{l} \int_{L_k} [f(x)]^2 \, \mathrm{d}x, \tag{18b}$$

with $A_q \equiv P_q,\ W_q,\ R_q$ corresponding to the cases $f(x) \equiv p(x),\ w(x),\ r(x)$. The quantity $A_q$ is the average of quantities $A_{q,k}$ representing the surface texture parameter for each of $n_s$ contiguous segments $x \in L_k$ of length $l$, called the *sampling length*, of the evaluated profile. For the primary profile, $n_s = 1$ and $l = x_{n-m_\mathrm{s}} - x_{1+m_\mathrm{s}}$ is the horizontal length of the profile. For the waviness and roughness profiles, $n_s \leq 5$ and $l = \lambda_\mathrm{c}$, the cut-off wavelength of the Gaussian filter (see section 2.2).[7] In practice, the value for $n_s$ is chosen to be the number, not exceeding five, of complete sampling lengths of the waviness and roughness profiles.

#### 2.3.1 Measurement functions for the case of uncertainties associated with the ordinate values only

As in section 2.2, knowledge of $f(x)$ over the segment $L_k$ of the evaluated profile takes the form of set of points with coordinate valuess $(x_{k,i}, f_{k,i}),\ i = 1, \ldots, n_l$, with the $x$-coordinate values uniformly spaced with spacing interval $h$. Applying the trapezoidal quadrature rule to the definitions (18), the calculation of the amplitude parameter is implemented as

$$t_q = \frac{1}{n_s} \sum_{k=1}^{n_s} t_{q,k}, \tag{19a}$$

$$t_{q,k}^2 = \frac{h}{l} {\sum_{i=1}^{n_l}}'' f_{k,i}^2, \tag{19b}$$

where, as before, the first and last terms in the summation are multiplied by one half.

In the case that there is no uncertainty associated with the values $x_{k,i},\ i = 1, \ldots, n_l$, the

[7] In fact, the sampling length for the waviness profile is defined in specification standards as $l = \lambda_\mathrm{f}$, but, as the $\lambda_\mathrm{f}$-filter is not generally applied to obtain the waviness profile, it is usual practice to take $l = \lambda_\mathrm{c}$.

formulae (19) suggest the measurement functions

$$T_q = \frac{1}{n_s} \sum_{k=1}^{n_s} T_{q,k}, \tag{20a}$$

$$T_{q,k}^2 = \frac{h}{l} \sum_{i=1}^{n_l}{}'' \, F_{k,i}^2. \tag{20b}$$

In these measurement functions, $T_q$ and $T_{q,k}$ are approximations to the quantities $A_q$ and $A_{q,k}$ given by the definition (18). The values $t_q$ and $t_{q,k}$ are estimates of $T_q$ and $T_{q,k}$ calculated using the measurement functions (20) for the estimates $f_{k,i}$ of $F_{k,i}$, quantities representing the ordinates of the points defining the $k$th segment of the evaluated profile, the (known) sampling length $l$, and the (known) value $h$ of the spacing interval.[8]

### 2.3.2 Measurement functions for the case of uncertainties associated with both coordinates

Proceeding as in section 2.2, a generalization of the formula (19b) to the case that the $x$-coordinate values are not uniformly spaced is

$$t_{q,k}^2 = \frac{1}{2l}(x_{k,2} - x_{k,1}) f_{k,1}^2 + \frac{1}{2l} \sum_{i=2}^{n_l - 1} (x_{k,i+1} - x_{k,i-1}) f_{k,i}^2 + \frac{1}{2l}(x_{k,n_l} - x_{k,n_l - 1}) f_{k,n_l}^2. \tag{21}$$

In the case that there are uncertainties associated with the values $x_{k,i}$ and $f_{k,i}$, $i = 1, \ldots, n_l$, the formula (21) suggests the measurement functions

$$T_q = \frac{1}{n_s} \sum_{k=1}^{n_s} T_{q,k}, \tag{22a}$$

$$T_{q,k}^2 = \frac{1}{2l}(X_{k,2} - X_{k,1}) F_{k,1}^2 + \frac{1}{2l} \sum_{i=2}^{n_l - 1} (X_{k,i+1} - X_{k,i-1}) F_{k,i}^2 + \frac{1}{2l}(X_{k,n_l} - X_{k,n_l - 1}) F_{k,n_l}^2. \tag{22b}$$

[8]The choice of the particular implementation scheme described here, based on the use of a quadrature rule, is consistent with the decisions taken in the work [4] to prepare *softgauges* for surface texture parameters for the profile case. In that work, the evaluated profile $f(x)$ is represented by a cubic polynomial spline curve that interpolates the set of points defining the profile, and quadrature rules are chosen to evaluate *exactly* the integral in the definition (18) with $f(x)$ replaced by the interpolating spline curve. Some implementations of the calculation of $t_{q,k}$ use the formula $t_{q,k}^2 = \frac{h}{l} \sum_{i=1}^{n_l} f_{k,i}^2$, in which the first and last terms of the summation are *not* multiplied by one half. This implementation can be expected to provide an estimate of $T_q$ that is different from that provided by formulae (19) because it corresponds to a different measurement function, which cannot be interpreted as a quadrature rule applied to the definition (18). An advantage of using a measurement function motivated by the application of a quadrature rule is that its generalization to the case of non-uniformly $x$-coordinate values is straightforward.

The values $t_q$ and $t_{q,k}$ are estimates of $T_q$ and $T_{q,k}$ calculated using the measurement functions (22) for the estimates $x_{k,i}$ and $f_{k,i}$ of $X_{k,i}$ and $F_{k,i}$, quantities representing the coordinates of the points defining the $k$th segment of the evaluated profile, and the (known) sampling length $l$.

# 3 Measurement data

The measurement data consists of estimates $(x_i, z_i)$ of quantities $(X_i, Z_i),\ i = 1, \ldots, n$, representing the coordinates of points defining the measured profile. Two cases are considered.

## 3.1 Uncertainties associated with the ordinate values only

Consider the observation model

$$X_i = x_i, \quad Z_i = z_i + E_0 + E_i, \quad i = 1, \ldots, n, \tag{23}$$

in which $E_0$ and $E_i$ are independent random variables with expectations zero and variances

$$V(E_0) \equiv u_{\mathrm{s}}^2 = \rho_z u_z^2, \quad V(E_i) \equiv u_{\mathrm{r}}^2 = (1 - \rho_z) u_z^2, \quad i = 1, \ldots, n.$$

Here, $E_0$ can be considered as representing a ('systematic') error quantity common to the measured quantities $Z_i$ with standard deviation $u_{\mathrm{s}}$ and the $E_i$ as ('random') error quantities different for the $Z_i$ with standard deviations $u_{\mathrm{r}}$. The quantities $X_i$ take the values $x_i$ with no associated uncertainty.

It follows that $z_i$ are estimates of $Z_i,\ i = 1, \ldots, n$, with associated variances

$$u^2(z_i) = u_z^2, \quad i = 1, \ldots, n,$$

and covariances

$$\mathrm{cov}(z_i, z_j) = \rho_z u_z^2, \quad i, j = 1, \ldots, n, i \neq j,$$

i.e., $u_z$ is the standard uncertainty associated with each measured value $z_i$ and $\rho_z$ the correlation coefficient associated with each pair $(z_i, z_j)$ of values.

The covariance matrix $\boldsymbol{U_z}$ of dimension $n \times n$ associated with the vector $\boldsymbol{z} = (z_1, \ldots, z_n)^\top$ of dimension $n \times 1$ is given by

$$\boldsymbol{U_z} = \rho_z u_z^2 \mathbf{1}_n \mathbf{1}_n^\top + (1 - \rho_z) u_z^2 \boldsymbol{I}_n, \tag{24}$$

where $\mathbf{1}_n$ is the vector of dimension $n \times 1$ with all elements equal to unity and $\boldsymbol{I}_n$ is the identity matrix of dimension $n \times n$. If $\boldsymbol{z}$ and $\boldsymbol{U_z}$ are the only information available about the vector quantity $\boldsymbol{Z} = (Z_1, \ldots, Z_n)^\top$, then $\boldsymbol{Z}$ is characterized by the multivariate Gaussian distribution $\mathrm{N}(\boldsymbol{z}, \boldsymbol{U_z})$. The covariance matrix is completely described by the autocovariance function

$$\mathrm{acv}_z(k) = \mathrm{cov}(z_i, z_{i+k}) = \rho_z u_z^2 + (1-\rho_z)u_z^2\delta_{0k}, \quad k = 0, 1, \ldots,$$

a function that only depends on the 'lag' $k$ between $z_i$ and $z_{i+k}$, where $\delta_{ij}$ denotes the Kronecker delta function.

The observation model (23) can be used as the basis for making random draws from the probability distribution used to characterize $\boldsymbol{Z}$. For example, if $e_0$ and $e_i$, $i = 1, \ldots, n$, are random draws made independently from the Gaussian distributions $\mathrm{N}(0, u_\mathrm{s}^2)$ and $\mathrm{N}(0, u_\mathrm{r}^2)$ used to characterize, respectively, $E_0$ and $E_i$, $i = 1, \ldots, n$, then $\mathbf{z}_k$ given by

$$\boldsymbol{z}_k = \boldsymbol{z} + e_0\mathbf{1}_n + \boldsymbol{e}, \quad \boldsymbol{e} = (e_1, \ldots, e_n)^\top,$$

is a random draw from $\mathrm{N}(\boldsymbol{z}, \boldsymbol{U_z})$.

Other distributions may be appropriate to characterize $E_0$ and $E_i$, and doing so will change the distribution for $\boldsymbol{Z}$. For example, if the information available about $E_0$ takes the form of lower and upper bounds $\pm a$ (which might be the case for a systematic error quantity), then $E_0$ is characterized by the rectangular distribution $\mathrm{R}(-a, a)$ with semi-width $a = \sqrt{3}u_\mathrm{s}$.

### 3.2 Uncertainties associated with both coordinates

Consider the observation model

$$X_i = x_i + D_0 + D_i + F_i, \quad Z_i = z_i + E_0 + E_i + F_i, \quad i = 1, \ldots, n, \tag{25}$$

in which $F_i$ can be considered as representing an error quantity common to the measured quantities $X_i$ and $Z_i$, $D_0$ and $E_0$ as error quantities common to the $X_i$ and to the $Z_i$, respectively, and the $D_i$ and $E_i$ as error quantities different for the $X_i$ and for the $Z_i$. $D_0$, $D_i$, $E_0$, $E_i$ and $F_i$ are independent random variables with expectations zero and variances

$$\begin{aligned} V(D_0) &= \rho_x u_x^2, \\ V(D_i) &= (1-\rho_x)u_x^2 - \rho_{xz}u_x u_z, \\ V(E_0) &= \rho_z u_z^2, \\ V(E_i) &= (1-\rho_z)u_z^2 - \rho_{xz}u_x u_z, \\ V(F_i) &= \rho_{xz}u_x u_z. \end{aligned}$$

The standard uncertainties $u_x$ and $u_z$ and the correletion coefficients $\rho_x$, $\rho_z$ and $\rho_{xz}$ cannot be set independently, but must satisfy a set of conditions that ensure the variances defined by the above expressions are non-negative. For example, $V(D_i) \geq 0$ implies the condition $(1-\rho_x)u_x \geq \rho_{xz}u_z$.

It follows that, for $i, j = 1, \ldots, n, i \neq j$,

$$\begin{aligned} u^2(x_i) &= u_x^2, \\ \mathrm{cov}(x_i, x_j) &= \rho_x u_x^2, \\ u^2(z_i) &= u_z^2, \\ \mathrm{cov}(z_i, z_j) &= \rho_z u_z^2, \\ \mathrm{cov}(x_i, z_i) &= \rho_{xz} u_x u_z, \\ \mathrm{cov}(x_i, z_j) &= 0. \end{aligned}$$

The covariance matrix $\boldsymbol{U_b}$ of dimension $2n \times 2n$ associated with the vector

$$\boldsymbol{b} = (\boldsymbol{x}^\top, \boldsymbol{z}^\top)^\top = (x_1, \ldots, x_n, z_1, \ldots, z_n)^\top$$

of dimension $2n \times 1$ is given by

$$\boldsymbol{U_b} = \begin{pmatrix} \boldsymbol{U_x} & \boldsymbol{U_{xz}} \\ \boldsymbol{U_{zx}} & \boldsymbol{U_z} \end{pmatrix},$$

where

$$\begin{aligned} \boldsymbol{U_x} &= \rho_x u_x^2 \mathbf{1}_n \mathbf{1}_n^\top + (1 - \rho_x) u_x^2 \boldsymbol{I}_n, \\ \boldsymbol{U_z} &= \rho_z u_z^2 \mathbf{1}_n \mathbf{1}_n^\top + (1 - \rho_z) u_z^2 \boldsymbol{I}_n, \end{aligned}$$

and

$$\boldsymbol{U_{xz}} = \boldsymbol{U_{zx}} = \rho_{xz} u_x u_z \boldsymbol{I}_n.$$

The covariance matrices are completely described by the autocovariance functions, for $k = 0, 1, \ldots$,

$$\begin{aligned} \mathrm{acv}_z(k) &= \mathrm{cov}(z_i, z_{i+k}) = \rho_z u_z^2 + (1 - \rho_z) u_z^2 \delta_{0k}, \\ \mathrm{acv}_x(k) &= \mathrm{cov}(x_i, x_{i+k}) = \rho_x u_x^2 + (1 - \rho_x) u_x^2 \delta_{0k}, \end{aligned}$$

and

$$\mathrm{acv}_{xz}(k) = \mathrm{cov}(x_i, z_{i+k}) = \rho_{xz} u_x u_z \delta_{0k}.$$

In the same way as in section 3.1, the observation model (25) can be used as the basis for making random draws from the (joint) probability distribution used to characterize $\boldsymbol{B} = (\boldsymbol{X}^\top, \boldsymbol{Z}^\top)^\top$.

### 3.3 NanoSurf IV

NanoSurf IV is a stylus instrument designed at the National Physical Laboratory (NPL) to provide traceability in the measurement of surface texture [17]. The object to be measured is placed on a specimen table that in turn sits on a horizontal ($x$) slideway. A vertical ($z$) slideway is used to bring the stylus into contact with the surface of the object. A motor drive pushes or pulls the $x$ slideway via a coupling rod and the stylus follows the surface as it moves. The displacements in the $x$ and $z$ directions are measured using two non-polarising Michelson interferometers to provide measured $x$ and $z$ values for points on a profile of the surface.

There are four dominant sources of uncertainty [18] corresponding to

1. the metrology frame, including detector electronics,
2. imperfections in the optics, including stray light,
3. deadpath length, and
4. Abbe error.

All other sources of uncertainty, such as arising from diffraction effects, misalignment, the calculation of the refractive index of air, etc., are small compared with the above sources [18].

Abbe error only applies to the measured $x$ values since the design of the instrument ensures the error is negligible in the $z$ direction, and it is the dominant source of uncertainty for these values. The error is common to all the measured $x$ values and is, therefore, a source of correlation associated with pairs of these values. Corrections for errors in the deadpath length are common to the measured $x$ and $z$ values for the same point on the profile, but different for different points and are, therefore, a source of correlation associated with the measured $x$ and $z$ values for the same point. Errors due to imperfect optics are different for the $x$ and $z$ directions but common to the measured $x$ values and to the measured $z$ values. These errors are another source of correlation associated with the measured values. Finally, the errors associated with the metrology frame, including its thermal and mechanical stability, are considered to be random and so are different for each measured $x$ and $z$ value.

Indicative values for the standard uncertainties associated with the four effects are given in table 1. It follows that values of the standard deviations and correlation coefficients for the quantities in an observation model (25) for the measured quantities are as follows:

$$u_x = 0.65\,\mathrm{nm}, u_z = 0.28\,\mathrm{nm}, \rho_x = 0.94, \rho_z = 0.68, \rho_{xz} = 0.08.$$

The values suggest that the uncertainties associated with the measured $x$ values are appreciable compared with those associated with the measured $z$ values, the measured $x$ values are strongly correlated, whereas the measued $x$ and $z$ values are only weakly correlated.

| Source of uncertainty | Standard uncertainty/$\mathrm{nm}$ |
|---|---|
| Metrology frame | $0.10$ |
| Imperfect optics | $0.23$ |
| Deadpath length | $0.12$ |
| Abbe error | $0.59$ |

Table 1: Sources of uncertainty for measurements made using the NanoSurf IV instrument.

# 4 Measurement uncertainty evaluation

The basis for the evaluation of measurement uncertainty is the propagation of probability distributions. In order to apply the propagation of distributions, a measurement function of the generic form $Y = f(\boldsymbol{X})$ relating input quantities $\boldsymbol{X} = (X_1, \ldots, X_N)^\top$, about which information is available, and the output quantity $Y$, about which information is required, is formulated. Additionally, information concerning the input quantities is encoded as probability distributions for those quantities, such as rectangular (uniform), Gaussian (normal), etc. The information can take a variety of forms, including a series of indication values, data on a calibration certificate, and the expert knowledge of the metrologist. An implementation of the propagation of distributions provides a probability distribution for $Y$, from which can be obtained an estimate of $Y$, the standard uncertainty associated with the estimate, and a coverage interval for $Y$ corresponding to a stipulated coverage probability. Particular implementations of the approach are the GUM uncertainty framework [2, 9] and a Monte Carlo method [3, 7, 9].

The primary guide in metrology on uncertainty evaluation is the 'Guide to the expression of uncertainty in measurement' (GUM) [2, 1]. The GUM presents a framework for uncertainty evaluation based on the use of the law of propagation of uncertainty and the central limit theorem. The law of propagation of uncertainty provides a means for 'propagating uncertainties' through the measurement function, i.e., for evaluating the standard uncertainty $u(y)$ associated with the estimate $y = f(x_1, \ldots, x_N)$ of $Y$ given the standard uncertainties $u(x_i)$ associated with the estimates $x_i$ of $X_i$ (and, when they are non-zero, the covariances $u(x_i, x_j)$ associated with pairs of estimates $x_i$ and $x_j$). The central limit theorem is applied to characterize $Y$ by a Gaussian distribution (or a $t$-distribution with an effective degrees of freedom), which is used as the basis of providing a coverage interval for $Y$.

A Monte Carlo method for uncertainty evaluation provides an implementation of the propagation of distributions that is free from the limitations and approximations inherent in the GUM uncertainty framework. Such approximations include linearization of the measurement function in the application of the law of propagation of uncertainty and the use of the Welch-Satterthwaite formula for calculating effective degrees of freedom. The approach is based on the following consideration [7, 8]. The estimate $y$ of $Y$ is conventionally obtained by evaluating the measurement function for the estimates $x_i$ of $X_i$. However, since each $X_i$ is described by a probability distribution, a value as legitimate as $x_i$ can be obtained by drawing a value at random from the distribution. The method operates, therefore, in the following manner. A random draw is made from the probability distribution for each $X_i$ and the corresponding value of $Y$ is formed by evaluating the measurement function for these values. Many Monte Carlo trials are performed, i.e., the process is repeated many times, to obtain $M$, say, values $y_k,\ k = 1, \ldots, M$, of $Y$. An estimate of $Y$ is given by the (sample) average of the values $y_k$, and the standard uncertainty associated with the estimate by the (sample) standard deviation of those values. Finally, the values are used to provide an approximation to the probability distribution for $Y$, and hence a coverage interval for $Y$ corresponding to a stipulated coverage probability.

Multivariate measurement functions, which take the generic form $\boldsymbol{Y} = \boldsymbol{f}(\boldsymbol{X})$ relating input quantities $\boldsymbol{X} = (X_1, \ldots, X_N)^\top$ and output quantities $\boldsymbol{Y} = (Y_1, \ldots, Y_m)^\top$, are an important class of measurement model. The output quantities are generally mutually correlated because they depend on common input quantities. Generalizations of the GUM uncertainty framework and a Monte Carlo method for uncertainty evaluation apply to such multivariate measurement functions [8, 9].

A generalization of the law of propagation of uncertainty gives the covariance matrix $\boldsymbol{U_y}$ of dimension $m \times m$ associated with the estimate $\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x})$ of $\boldsymbol{Y}$ as

$$\boldsymbol{U_y} = \boldsymbol{C}\boldsymbol{U_x}\boldsymbol{C}^\top,$$

where $\boldsymbol{U_x}$ is the covariance matrix associated with the estimate $\boldsymbol{x}$ of $\boldsymbol{X}$ and $\boldsymbol{C}$ is a sensitivity matrix of dimension $m \times N$ containing the values of the first order partial derivatives $\partial f_i/\partial X_j,\ i = 1, \ldots, m, j = 1, \ldots, N$, evaluated at $\boldsymbol{x}$.

Application of a Monte Carlo method as described above gives the $M$ vector values $\boldsymbol{y}_k$, $k = 1, \ldots, M$, of $\boldsymbol{Y}$. An estimate of $\boldsymbol{Y}$ is given by the vector (sample) average of the values $\boldsymbol{y}_k$, and the covariance matrix associated with the estimate by the (sample) covariance matrix for those values. Finally, the values are used to provide an approximation to the joint probability distribution for $\boldsymbol{Y}$, and hence a coverage region for $\boldsymbol{Y}$ corresponding to a stipulated coverage probability.

In this work, the concern is with both (scalar) univariate and multivariate measurement functions. The measurement functions (2), (9), (11) and (15) to (17) for obtaining the mean centred, primary, waviness and roughness profiles from the measured profile are examples of multivariate measurement functions. The output quantities in these functions, which represent the coordinates of the points defining the mean centred, primary, waviness and roughness profiles, can be expected to be correlated because they depend on common input quantities, which represent the coordinates of the points defining the measured profile. The calculations of the amplitude parameters $T_{q,k}$ in the expressions (20b) and (22b) are also examples of multivariate measurement functions. The output quantities in these functions can also be expected to be correlated because they depend on input quantities representing the coordinates of the evaluated profile that are themselves correlated due to the mean centering and filtering process(es) used to obtain the profiles. The calculations of the amplitude parameter $T_q$ in terms of the quantities $T_{q,k}$ in the expressions (20a) and (22a) are examples of univariate measurement functions.

The calculation of a surface texture parameter in terms of the coordinates of the points defining the measured profile is described by a multi-stage measurement function in which the output quantities from one measurement function, e.g., describing the filtering of the mean centred and primary profiles, are used as input quantities to the measurement function in a further stage.

# 5 GUM uncertainty framework

## 5.1 Uncertainties associated with the ordinate values only

For the evaluation of the mean centred profile, the measurement function (2) is expressed as

$$\boldsymbol{Y} = \boldsymbol{C}_{\mathrm{m}}\boldsymbol{Z},$$

with $\boldsymbol{Z} = (Z_1, \ldots, Z_n)^\top$ and $\boldsymbol{Y} = (Y_1, \ldots, Y_n)^\top$. The sensitivity matrix $\boldsymbol{C}_{\mathrm{m}}$ of dimension $n \times n$ is given by

$$\boldsymbol{C}_{\mathrm{m}} = \boldsymbol{I}_n - \tfrac{1}{n}\boldsymbol{1}_n\boldsymbol{1}_n^\top.$$

The estimate $\boldsymbol{y}$ of $\boldsymbol{Y}$ is obtained by evaluating the measurement function for the estimate $\boldsymbol{z}$ of $\boldsymbol{Z}$, i.e.,

$$\boldsymbol{y} = \boldsymbol{C}_{\mathrm{m}}\boldsymbol{z}.$$

The covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ associated with $\boldsymbol{y}$ is given, by an application of the law of propagation of uncertainty, with no approximation, by

$$\boldsymbol{U}_{\boldsymbol{y}} = \boldsymbol{C}_{\mathrm{m}}\boldsymbol{U}_{\boldsymbol{z}}\boldsymbol{C}_{\mathrm{m}}^\top.$$

Substituting expression (24) for $\boldsymbol{U}_{\boldsymbol{z}}$,

$$\boldsymbol{U}_{\boldsymbol{y}} = \boldsymbol{C}_{\mathrm{m}}\left(\rho_z u_z^2\boldsymbol{1}_n\boldsymbol{1}_n^\top + (1-\rho_z)u_z^2\boldsymbol{I}_n\right)\boldsymbol{C}_{\mathrm{m}}^\top = (1-\rho_z)u_z^2\left(\boldsymbol{I}_n - \tfrac{1}{n}\boldsymbol{1}_n\boldsymbol{1}_n^\top\right). \qquad (26)$$

It follows that, for large $n$, $\boldsymbol{U}_{\boldsymbol{y}} \approx (1-\rho_z)u_z^2\boldsymbol{I}_n$, and the covariance matrix associated with the ordinate values of the mean centred profile is (approximately) that associated with the random error values for the measured profile, i.e., the contribution to the covariance matrix arising from correlated (systematic) error quantities is minimal.

For the evaluation of the primary profile, the measurement function (9) is expressed as

$$\boldsymbol{P} = \boldsymbol{S}_{\mathrm{s}}\boldsymbol{Y},$$

with $\boldsymbol{P} = (P_{1+m_\text{s}}, \ldots, P_{n-m_\text{s}})^\top$. The sensitivity matrix $\boldsymbol{S}_\text{s}$ of dimension $(n - 2m_\text{s}) \times n$ takes the form a band matrix, typified by the instance

$$\boldsymbol{S}_\text{s} = \begin{pmatrix} \times & \times & \times & 0 & 0 \\ 0 & \times & \times & \times & 0 \\ 0 & 0 & \times & \times & \times \end{pmatrix}$$

corresponding to $m_\text{s} = 1$ and $n = 5$ in which $\times$ denotes a (generally) non-zero element. The non-zero elements in each row are, in general,

$$\boldsymbol{s}_\text{s} = (hs_{\text{s},-m_\text{s}}, hs_{\text{s},-m_\text{s}+1}, \ldots, hs_{\text{s},0}, \ldots, hs_{\text{s},m_\text{s}-1}, hs_{\text{s},m_\text{s}})^\top.$$

The estimate $\boldsymbol{p}$ of $\boldsymbol{P}$ is obtained by evaluating the measurement function for the estimate $\boldsymbol{y}$ of $\boldsymbol{Y}$, i.e.,

$$\boldsymbol{p} = \boldsymbol{S}_\text{s}\boldsymbol{y}.$$

The covariance matrix $\boldsymbol{U}_{\boldsymbol{p}}$ associated with $\boldsymbol{p}$ is given, by an application of the law of propagation of uncertainty, with no approximation, by

$$\boldsymbol{U}_{\boldsymbol{p}} = \boldsymbol{S}_\text{s}\boldsymbol{U}_{\boldsymbol{y}}\boldsymbol{S}_\text{s}^\top. \tag{27}$$

Substituting expression (26) for $\boldsymbol{U}_{\boldsymbol{y}}$, and making use of expression (8),

$$\boldsymbol{U}_{\boldsymbol{p}} = \boldsymbol{S}_\text{s}\left[(1-\rho_z)u_z^2\left(\boldsymbol{I}_n - \tfrac{1}{n}\boldsymbol{1}_n\boldsymbol{1}_n^\top\right)\right]\boldsymbol{S}_\text{s}^\top = (1-\rho_z)u_z^2\left(\boldsymbol{S}_\text{s}\boldsymbol{S}_\text{s}^\top - \tfrac{1}{n}\boldsymbol{1}_{n-2m_s}\boldsymbol{1}_{n-2m_s}^\top\right). \tag{28}$$

It follows that, for large $n$, $\boldsymbol{U}_{\boldsymbol{p}} \approx (1-\rho_z)u_z^2\boldsymbol{S}_\text{s}\boldsymbol{S}_\text{s}^\top$, which is a symmetric band matrix with constant diagonals. The structure of the matrix reflects the limited support of the weighting function for the Gaussian filter.

Similar considerations apply to the evaluations of the waviness and roughness profiles. The measurement functions (11) are expressed as

$$\boldsymbol{W} = \boldsymbol{S}_\text{c}\boldsymbol{P}, \quad \boldsymbol{R} = \boldsymbol{P} - \boldsymbol{W} = \boldsymbol{G}_\text{c}\boldsymbol{P},$$

with $\boldsymbol{W} = (W_{1+m_\text{s}+m_\text{c}}, \ldots, W_{n-m_\text{s}-m_\text{c}})^\top$ and $\boldsymbol{R} = (R_{1+m_\text{s}+m_\text{c}}, \ldots, R_{n-m_\text{s}-m_\text{c}})^\top$. The sensitivity matrices $\boldsymbol{S}_\text{c}$ and $\boldsymbol{G}_\text{c}$ of dimension $(n - 2m_\text{s} - 2m_\text{c}) \times (n - 2m_\text{s})$ are band matrices. The non-zero elements in each row of the matrices are, respectively,

$$\boldsymbol{s}_\text{c} = (hs_{\text{c},-m_\text{c}}, hs_{\text{c},-m_\text{c}+1}, \ldots, hs_{\text{c},0}, \ldots, hs_{\text{c},m_\text{c}-1}, hs_{\text{c},m_\text{c}})^\top,$$

and

$$\boldsymbol{g}_\text{c} = (-hs_{\text{c},-m_\text{c}}, -hs_{\text{c},-m_\text{c}+1}, \ldots, (1 - hs_{\text{c},0}), \ldots, -hs_{\text{c},m_\text{c}-1}, -hs_{\text{c},m_\text{c}})^\top.$$

The covariance matrices $\boldsymbol{U}_{\boldsymbol{w}}$ and $\boldsymbol{U}_{\boldsymbol{r}}$ associated with estimates $\boldsymbol{w}$ and $\boldsymbol{r}$ of $\boldsymbol{W}$ and $\boldsymbol{R}$ are given, by applications of the law of propagation of uncertainty, with no approximation, by

$$\boldsymbol{U}_{\boldsymbol{w}} = \boldsymbol{S}_\text{c}\boldsymbol{U}_{\boldsymbol{p}}\boldsymbol{S}_\text{c}^\top \tag{29}$$

and

$$U_r = G_c U_p G_c^\top . \tag{30}$$

Substituting expression (28) for $U_p$, it follows that

$$\begin{aligned} U_w &= S_c \left[ (1-\rho_z) u_z^2 \left( S_s S_s^\top - \tfrac{1}{n} \mathbf{1}_{n-2m_s} \mathbf{1}_{n-2m_s}^\top \right) \right] S_c^\top \\ &= (1-\rho_z) u_z^2 \left( S_c S_s S_s^\top S_c^\top - \tfrac{1}{n} \mathbf{1}_{n-2m_s-2m_c} \mathbf{1}_{n-2m_s-2m_c}^\top \right), \end{aligned} \tag{31}$$

and

$$\begin{aligned} U_r &= G_c \left[ (1-\rho_z) u_z^2 \left( S_s S_s^\top - \tfrac{1}{n} \mathbf{1}_{n-2m_s} \mathbf{1}_{n-2m_s}^\top \right) \right] G_c^\top \\ &= (1-\rho_z) u_z^2 G_c S_s S_s^\top G_c^\top . \end{aligned} \tag{32}$$

The above analysis indicates that the influence of the mean centering step in the calculation, effectively to remove the contribution from a common (systematic) error quantity affecting the ordinates of the measured profile, is appreciable. The evaluation of the covariance matrices $U_p$, $U_w$ and $U_r$ arising from the filtering operations, in the case that the step of mean centering is not applied, is given in appendix A.

For the evaluation of the surface texture parameters $T_{q,k}$, the measurement function (20b) is used to obtain the sensitivity matrix $Q$ of dimension $n_s \times n_s n_l$ containing the values of the first order partial derivatives $\partial T_{q,k}/\partial F_{j,i}$ evaluated at the estimates $f_{j,i}$ of $F_{j,i}$, quantities representing the ordinates of the points defining the $j$th segment of the evaluated profile. For $j = k$,

$$\frac{\partial T_{q,k}}{\partial F_{j,i}} = \begin{cases} \dfrac{h f_{j,i}}{2 t_{q,k} l}, & i = 1, n_l, \\[2ex] \dfrac{h f_{j,i}}{t_{q,k} l}, & i = 2, \ldots, n_l - 1, \end{cases}$$

and, for $j \neq k$,

$$\frac{\partial T_{q,k}}{\partial F_{j,i}} = 0, \quad i = 1, \ldots, n_l.$$

For the calculations of $t_{q,k}$ for the waviness and roughness profiles, $Q$ is a block-diagonal matrix with diagonal blocks given by $q_k^\top$, $k = 1, \ldots, n_s$, with

$$q_k^\top = \frac{h}{t_{q,k} l} \left( \tfrac{1}{2} f_{k,1}, f_{k,2}, \ldots, f_{k,n_l-1}, \tfrac{1}{2} f_{k,n_l} \right).$$

For the (special) case of the primary profile, $Q$ is the (row) vector $q_1^\top$ of dimension $1 \times n$. Applying the law of propagation of uncertainty, the covariance matrix $U_t$ associated with the estimate $\boldsymbol{t_q} = (t_{q,1}, \ldots, t_{q,n_s})^\top$ of $\boldsymbol{T_q} = (T_{q,1}, \ldots, T_{q,n_s})^\top$ is given, based on a linearization of the measurement function (20b), by

$$\boldsymbol{U_t} = \boldsymbol{Q}\boldsymbol{U_f}\boldsymbol{Q}^\top,$$

where $\boldsymbol{U_f}$ is the covariance matrix associated with the estimates $f_{j,i}$ of $F_{j,i}$. In practice, $\boldsymbol{U_f}$ will be $\boldsymbol{U_p}$ or (a part of) $\boldsymbol{U_w}$ or $\boldsymbol{U_r}$ according to whether the evaluated profile is the primary, waviness or roughness profile.

Finally, for the evaluation of the surface texture parameter $T_q$, the measurement function (20a) is expressed as[9]

$$T_q = \frac{1}{n_s}\boldsymbol{1}_{n_s}^\top \boldsymbol{T_q},$$

and so the standard uncertainty $u(t_q)$ associated with the estimate $t_q$ of $T_q$ is given, by an application of the law of propagation of uncertainty, with no approximation, by

$$u^2(t_q) = \frac{1}{n_s^2}\boldsymbol{1}_{n_s}^\top \boldsymbol{U_t}\boldsymbol{1}_{n_s}.$$

## 5.2 Uncertainties associated with both coordinates

For the evaluation of the primary profile, the measurement functions (15) define a (non-linear) relationship between input quantities

$$\boldsymbol{M} = \begin{pmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{pmatrix}$$

representing the coordinates $\boldsymbol{X} = (X_1, \ldots, X_n)^\top$ and $\boldsymbol{Y} = (Y_1, \ldots, Y_n)^\top$ of the (mean centred) measured profile and output quantities

$$\boldsymbol{P} = \begin{pmatrix} \boldsymbol{P}^x \\ \boldsymbol{P}^z \end{pmatrix}$$

representing the coordinates $\boldsymbol{P}^x = (P^x_{1+m_\mathrm{s}}, \ldots, P^x_{n-m_\mathrm{s}})^\top$ and $\boldsymbol{P}^z = (P^z_{1+m_\mathrm{s}}, \ldots, P^z_{n-m_\mathrm{s}})^\top$ of the primary profile. The measurement functions are used to obtain the sensitivity matrix

$$\boldsymbol{S}_\mathrm{s} = \begin{pmatrix} \boldsymbol{S}_\mathrm{s}^{xx} & \boldsymbol{S}_\mathrm{s}^{xz} \\ \boldsymbol{S}_\mathrm{s}^{zx} & \boldsymbol{S}_\mathrm{s}^{zz} \end{pmatrix},$$

[9] In the following expression, $T_q$, a *scalar* quantity representing the surface texture parameter for the evaluated profile, is not to be confused with $\boldsymbol{T_q}$, a *vector* quantity with elements $T_{q,k}$ representing the surface texture parameter for the contiguous segments of the evaluated profile.

in which the $ij$th elements of each sub-matrix of dimension $(n - 2m_s) \times n$, are given by the first order partial derivatives

$$(\boldsymbol{S}_s^{xx})_{ij} = \frac{\partial P_i^x}{\partial X_j},$$
$$(\boldsymbol{S}_s^{xz})_{ij} = \frac{\partial P_i^x}{\partial Y_j},$$
$$(\boldsymbol{S}_s^{zx})_{ij} = \frac{\partial P_i^z}{\partial X_j},$$
$$(\boldsymbol{S}_s^{zz})_{ij} = \frac{\partial P_i^z}{\partial Y_j},$$

evaluated at the estimates $x_i$ and $y_i$, $i = 1, \ldots, n$, of the (input) quantities $X_i$ and $Y_i$. Applying the law of propagation of uncertainty, the covariance matrix associated with estimates $\boldsymbol{p}$ of $\boldsymbol{P}$ is given by

$$\boldsymbol{U_p} = \boldsymbol{S}_s \boldsymbol{U_m} \boldsymbol{S}_s^\top,$$

where $\boldsymbol{U_m}$ is the covariance matrix associated with estimates $\boldsymbol{m}$ of $\boldsymbol{M}$.

The elements of the sub-matrices $\boldsymbol{S}_{s,xx}$ and $\boldsymbol{S}_{s,xz}$ are straightforwad to evaluate, as they take the values zero or one. However, the partial derivatives $\partial P_i^z/\partial X_j$ and $\partial P_i^z/\partial Z_j$ can be algebraically complicated and are not presented here. The use of numerical differentiation tools, including finite-difference methods [12, 21] and the complex-step method [20, 22], are valuable for checking the values of derivatives obtained analytically. In this regard, the complex-step method can deliver considerably greater accuracy than conventional finite-difference methods, and may generally be used in its own right to provide the elements of sensitivity matrices for the purposes of uncertainty evaluation.

Similar considerations apply to the evaluations of the waviness and roughness profiles, and the surface texture parameter. The measurement functions (16), (17), and (22) are used as the basis for obtaining sensitivity matrices and the law of propagation of uncertainty, expressed in terms of these sensitivity matrices, for propagating covariance matrices through linearized versions of the measurement functions.

Finally, for problems, such as those considered here, for which the numbers of input and quantities in a measurement function are large, it can be helpful to express the covariance matrices associated with the estimates of the quantities in terms of sub-matrices (cf. $\boldsymbol{S}_s$ above), e.g.,

$$\boldsymbol{U_m} = \begin{pmatrix} \boldsymbol{U_m}^{xx} & \boldsymbol{U_m}^{xz} \\ \boldsymbol{U_m}^{zx} & \boldsymbol{U_m}^{zz} \end{pmatrix}.$$

Since $\boldsymbol{U_m}$ is a symmetric matrix, it is only necessary to store the $\boldsymbol{U_m}^{xx}$, $\boldsymbol{U_m}^{zz}$ and $\boldsymbol{U_m}^{xz} = (\boldsymbol{U_m}^{zx})^\top$, and the law of propagation of uncertainty can be implemented in terms of the sub-matrices of $\boldsymbol{U_m}$ and $\boldsymbol{S}_s$.

# 6 Monte Carlo method

For the $\ell$th trial, $\ell = 1, \dots, M$, where $M$ is the total number of trials, the following steps are undertaken in an implementation of a Monte Carlo method for uncertainty evaluation:

1. Use the coordinate values $(x_i, z_i),\ i = 1, \dots, n$, of the points defining the measured profile and the observation model (23) or (25) to generate a 'candidate' measured profile defined by points with coordinate values $(x_{\ell,i}, z_{\ell,i}),\ i = 1, \dots, n$;

2. Apply mean centering to the candidate measured profile to obtain the corresponsing mean centred profile;

3. Apply a Gaussian filter with cut-off wavelength $\lambda_{\mathrm{s}}$ to the mean centred profile to obtain the corresponding primary profile;

4. Apply a Gaussian filter with cut-off wavelength $\lambda_{\mathrm{c}}$ to the primary profile to obtain the corresponding waviness and roughness profiles;

5. Evaluate the surface texture parameter for each of the primary, waviness and roughness profiles to obtain values $p_{q,\ell}$, $w_{q,\ell}$ and $r_{q,\ell}$, respectively.

The average and standard deviation of the values $p_{q,\ell},\ \ell = 1, \dots, M$, provide an estimate of $P_q$ and the associated standard uncertainty, and similarly for the parameters $W_q$ and $R_q$. Information about intermediate quantities is also available. For example, the vector average and covariance matrix of the vector values $\boldsymbol{z}_\ell,\ \ell = 1, \dots, M$, where $\boldsymbol{z}_\ell = (z_{\ell,1}, \dots, z_{\ell,n})^\top$, provide estimates of the ordinates $\boldsymbol{Z}$ of the measured profile and the associated covariance matrix, which would be expected to correspond to the prescribed vector $\boldsymbol{z}$ and covariance matrix $\boldsymbol{U}_{\boldsymbol{z}}$.

The two cases of measurement data (sections 3.1 and 3.2) are treated through the choice of observation model in step 1 of the above procedure. Alternative observation models can straightforwardly be considered by modifying this step accordingly. Different surface texture parameters are treated by modifying step 4 of the procedure: the only requirement is to be able to evaluate the surface texture parameter for a profile determined from the candidate measured profile constructed in step 1. In particular, parameters for which it is difficult to apply the GUM uncertainty framework can be considered straightforwardly. Examples include the amplitude parameter *Pa*, which is not everywhere a differentiable function of its input quantities, and the spacing parameter *PSm*, which is defined by a numerical procedure. Consequently, the described Monte Carlo method provides a very general approach to the evaluation of uncertainties in the calculation of surface texture parameters.

# 7 Results

## 7.1 Case 1

The measured profile, defined by data $(x_i, z_i),\ i = 1, \ldots, n$, is simulated to have the following characteristics:

- The spacing interval is $h = 0.5\,\mu\text{m}$;
- The number of measured points is $n = 2m_\text{s} + 7m_\text{c}$, where $m_\text{s} = \lambda_\text{s}/h$ and $m_\text{c} = \lambda_\text{c}/h$;[10]
- The measured $x$-coordinate values, in micrometres, are

$$x_i = ih, \quad i = 1, \ldots, n;$$

- The measured $z$-coordinate values, in micrometres, are

$$z_i = a_1 \sin\left(\frac{2\pi x_i}{L_1}\right) + a_2 \sin\left(\frac{2\pi x_i}{L_2}\right) + e_0 + e_i, \quad i = 1, \ldots, n,$$

  where $L_1 = 400\,\mu\text{m}$, $L_2 = 30\,\mu\text{m}$, and $e_0$ and $e_i$ are random draws made independently from, respectively, $\text{N}(0, \rho_z u_z^2)$ and $\text{N}(0, (1 - \rho_z)u_z^2)$.

The measured profile is simulated by sampling a (continuous) profile, which is defined as the sum of two sinusoidal components with amplitudes $a_1$ and $a_2$ and wavelengths $L_1$ and $L_2$, and adding a (common) systematic error $e_0$ and random errors $e_i$. Gaussian filters with cut-off wavelengths $\lambda_\text{s} = 2.5\,\mu\text{m}$ and $\lambda_\text{c} = 80\,\mu\text{m}$ are applied to obtain the primary, waviness and roughness profiles.

Different 'test problems' are considered by choosing different values for $a_1$, $a_2$ and $u_z$ as follows:

**A** $a_1 = 100\,\text{nm},\ a_2 = 100\,\text{nm},\ u_z = 1\,\text{nm}$;

**B** $a_1 = 10\,\text{nm},\ a_2 = 10\,\text{nm},\ u_z = 1\,\text{nm}$;

**C** $a_1 = 10\,\text{nm},\ a_2 = 10\,\text{nm},\ u_z = 5\,\text{nm}$;

**D** $a_1 = 10\,\text{nm},\ a_2 = 10\,\text{nm},\ u_z = 10\,\text{nm}$.

[10] The choice of $n$ is such that the primary profile is defined by $7m_\text{c}$ measured points, and the waviness and roughness profiles by $5m_\text{c}$ points, which corresponds to (exactly) $n_s = 5$ sampling lengths.

For each of these problems, values of $0$ and $0.9$ are set for the correlation coefficient $\rho_z$ associated with pairs of measured values $z_i$, corresponding to measurements for which the measured values are uncorrelated and strongly correlated.

Appendix B.1 contains graphs to illustrate the results obtained for problem A with $\rho_z = 0$.

Figure 1 illustrates the simulated measured profile and the result of mean centering and filtering that profile to obtain the primary profile. For the latter, the figure shows the differences between the measured and primary profiles, which are seen to correspond to a combination of a vertical offset (related to the effect of mean centering), random errors and a sinusoidal component at the (shorter) wavelength $L_2$ but with a much reduced amplitude (compared to the amplitude $a_1$ of the component with that wavelength in the measured profile).

Figure 2 illustrates the waviness and roughness profiles obtained by filtering the primary profile. The waviness and roughness profiles correspond closely to the sinusoidal components of, respectively, the longer wavelength $L_1$ and shorter wavelength $L_2$ in the measured profile, although the waviness profile is subject to a small vertical offset related to the effect of mean centering the measured profile.

Figures 3 and 4 show the variances associated with the ordinate values defining the measured, primary, waviness and roughness profiles. For the primary profile, the horizontal line marks the values (all equal to $u_z^2$) of the diagonal elements of $\boldsymbol{U_z}$, the covariance matrix associated with the ordinate values $\boldsymbol{z}$ defining the profile. The crosses in the figure mark the variances of the components of the vectors $\boldsymbol{z}_\ell, \ell = 1, \ldots, M$, obtained by 'simulating' $M$ measured profiles $\boldsymbol{z}_\ell$ according to the observation model (23). For the primary, waviness and roughness profiles, the horizontal lines mark the values of the diagonals of the matrices $\boldsymbol{U_p}$, $\boldsymbol{U_w}$ and $\boldsymbol{U_r}$ obtained by appplying the law of propagation of uncertainty. The crosses in the figures mark the variances of the components of the vectors $\boldsymbol{p}_\ell, \boldsymbol{w}_\ell, \boldsymbol{r}_\ell, \ell = 1, \ldots, M$, obtained by mean centering and filtering the 'simulated' measured profiles, i.e., by applying a Monte Carlo method.

Figures 5 to 8 show the correlation coefficients, as a function of lag $k$, associated with the ordinate values defining the different profiles. For each covariance matrix ($\boldsymbol{U_z}$, $\boldsymbol{U_p}$, etc.), the corresponding correlation matrix ($\boldsymbol{C_z}$, $\boldsymbol{C_p}$, etc.) is evaluated[11] and the $(i, j)$th element of the correlation matrix is plotted against the lag $k = |j - i|$.

Finally, figure 9 illustrates the approximations to the probability density functions (PDFs) for the surface texture parameters $P_q$, $W_q$ and $R_q$ obtained using the GUM uncertainty framework and a Monte Carlo method. For the former, the approximation takes the form of a Gaussian PDF with expectation and standard deviation obtained using the law of propagation of uncertainty. For the latter, the approximation takes the form of a scaled frequency distribution (histogram). In each case, the origin (zero value of the quantity) corresponds to the estimate provided by the law of propagation of uncertainty.

[11] For example, $\boldsymbol{U_z}$ and $\boldsymbol{C_z}$ are related by $\boldsymbol{U_z} = \boldsymbol{D_z C_z D_z}$, where $\boldsymbol{D_z}$ is a diagonal matrix with diagonal elements $u(z_1), \ldots, u(z_n)$.

| | | Primary, $P_q$ | | Waviness, $W_q$ | | Roughness, $R_q$ | |
|---|---|---|---|---|---|---|---|
| | | $p_q$/nm | $u(p_q)$/nm | $w_q$/nm | $u(w_q)$/nm | $r_q$/nm | $u(r_q)$/nm |
| A | GUF | 99.047 | 0.030 | 67.441 | 0.032 | 69.397 | 0.035 |
| | MCM | 99.048 | 0.030 | 67.440 | 0.032 | 69.399 | 0.035 |
| B | GUF | 9.939 | 0.030 | 6.773 | 0.032 | 6.966 | 0.035 |
| | MCM | 9.954 | 0.030 | 6.774 | 0.032 | 6.985 | 0.035 |
| C | GUF | 10.12 | 0.15 | 6.59 | 0.16 | 7.31 | 0.17 |
| | MCM | 10.48 | 0.14 | 6.60 | 0.16 | 7.77 | 0.16 |
| D | GUF | 11.23 | 0.29 | 6.63 | 0.31 | 8.73 | 0.33 |
| | MCM | 12.50 | 0.27 | 6.69 | 0.31 | 10.20 | 0.30 |

Table 2: Results for case 1 when $\rho_z = 0$. ‘GUF’ denotes the GUM uncertainty framework, and ’MCM’ a Monte Carlo method.

| | | Primary, $P_q$ | | Waviness, $W_q$ | | Roughness, $R_q$ | |
|---|---|---|---|---|---|---|---|
| | | $p_q$/nm | $u(p_q)$/nm | $w_q$/nm | $u(w_q)$/nm | $r_q$/nm | $u(r_q)$/nm |
| A | GUF | 99.050 2 | 0.009 4 | 67.426 | 0.010 | 69.429 | 0.011 |
| | MCM | 99.050 5 | 0.009 4 | 67.426 | 0.010 | 69.430 | 0.011 |
| B | GUF | 9.920 2 | 0.009 4 | 6.750 | 0.010 | 6.960 | 0.011 |
| | MCM | 9.922 0 | 0.009 5 | 6.751 | 0.010 | 6.962 | 0.011 |
| C | GUF | 9.957 | 0.047 | 6.794 | 0.051 | 6.977 | 0.055 |
| | MCM | 9.995 | 0.047 | 6.795 | 0.050 | 7.027 | 0.055 |
| D | GUF | 10.043 | 0.094 | 6.70 | 0.10 | 7.08 | 0.11 |
| | MCM | 10.191 | 0.093 | 6.70 | 0.10 | 7.28 | 0.11 |

Table 3: As figure 2, but when $\rho_z = 0.9$.

Figures 10 to 13 show a selection of graphs to illustrate the results obtained for problem A with $\rho_z = 0.9$. Appendices B.2 to B.4 contains graphs to illustrate the results obtained for problems B to D.

Table 2 summarises the results for each problem when $\rho_z = 0$. Given are the estimates $p_q$, $w_q$ and $r_q$ of the amplitude parameters $P_q$, $W_q$ and $R_q$, and the associated standard uncertainties $u(p_q)$, $u(w_q)$ and $u(r_q)$, obtained using the GUM uncertainty framework (GUF) and a Monte Carlo method (MCM). In the application of a Monte Carlo method, $M = 10\,000$ trials are undertaken. Table 3 summarises the results when $\rho_z = 0.9$.

A number of observations are made about the results:

1. The variances associated with the ordinate values defining the different profiles obtained using a Monte Carlo method appear to be scattered about those obtained using the law of propagation of uncertainty (figures 3 and 4), except for the case of the waviness profile for which they appear serially correlated. The observed behaviour

for the waviness profile arises because the variances are calculated in terms of ordinate values that exhibit a correlation that is stronger (in this case) than for the other profiles (figures 5 and 7). The variances associated with the ordinate values defining the waviness profile are appreciably smaller than those for the primary and roughness profiles, which is a consequence of the effect of the Gaussian filters to remove short-wavelength (high frequency) components of the measured profile to give the waviness profile.

2. The correlation coefficients associated with the ordinate values defining the primary, waviness and roughness profiles are unaffected by the value of $\rho_z$ (figures 5 and 7 when $\rho_z = 0$ and figures 12 and 13 when $\rho_z = 0.9$). For example, the ordinate values of the primary profile are uncorrelated for lags $k$ greater than $\lambda_\mathrm{s}/h = 5$ for both cases considered (figure 5 and 12). The observed behaviour is a consequence of the step of mean centering, which removes the contribution made by common (systematic) error quantities influencing the measured profile. The ordinate values defining the roughness profile are generally uncorrelated, except for small lags, irrespective of the value of $\rho_z$ (figures 7 and 13), which is a consequence of the effect of the Gaussian filters to remove long-wavelength (low frequency) components of the measured profile to give the roughness profile. There is good agreement between the results returned by the GUM uncertainty framework and a Monte Carlo method (figures 6 and 8).

3. Since the measurement functions defining the operations of mean centering and Gaussian filtering are linear, the results (variances, correlation coefficients, etc.) returned by the law of propagation of uncertainty are exact.

4. When $\rho_z = 0$, the standard uncertainties associated with the estimates $p_q$, $w_q$ and $r_q$ are comparable for each problem, and increase in proportion to the standard uncertainty $u_z$ associated with the ordinate values defining the measured profile (table 2). For all problems, the standard uncertainty $u(r_q)$ is (marginally) greater than $u(w_q)$, which is (marginally) greater than $u(p_q)$. There is good agreement between the standard uncertainties returned by the GUM uncertainty framework and a Monte Carlo method. However, as $u_z$ increases relative to the estimates $p_q$, $w_q$ and $r_q$ (problems B, C and D), so the estimates of $P_q$ (and $R_q$) returned by the two approaches become increasingly different, whereas those of $W_q$ remain essentially the same. The described effect is clearly indicated in figures 14, 16 and 18.

5. When $\rho_z = 0.9$, the results are qualitatively the same as when $\rho_z = 0$, i.e., the standard uncertainties increase in proportion to $u_z$, the GUM uncertainty framework and a Monte Carlo method return standard uncertainties that are in good agreement, and the approaches return estimates for $P_q$ and $R_q$ that are increasingly different as $u_z$ increases (figures 15, 17 and 19). Quantitatively, the standard uncertainties are smaller for the case $\rho_z = 0.9$ compared with those for the case $\rho_z = 0$ (tables 2 and 3).

### 7.2 Case 2

The measured profile is defined by data $(x_i, z_i),\ i = 1, \ldots, n$, simulated to have the following characteristics (cf. section 7.1):

- The spacing interval is $h = 0.5\,\mu\mathrm{m}$;
- The number of measured points is $n = 2m_\mathrm{s} + 7m_\mathrm{c}$, where $m_\mathrm{s} = \lambda_\mathrm{s}/h$ and $m_\mathrm{c} = \lambda_\mathrm{c}/h$;
- The measured $x$-coordinate values, in micrometres, are

$$x_i = ih + d_0 + d_i + f_i, \quad i = 1, \ldots, n,$$

  where $d_0$, $d_i$ and $f_i$ are random draws made independently from, respectively, the Gaussian distributions $\mathrm{N}(0, \rho_x u_x^2)$, $\mathrm{N}(0, (1-\rho_x)u_x^2 - \rho_{xz}u_x u_z)$ and $\mathrm{N}(0, \rho_{xz}u_x u_z)$;
- The measured $z$-coordinate values, in micrometres, are

$$z_i = a_1 \sin\left(\frac{2\pi x_i}{L_1}\right) + a_2 \sin\left(\frac{2\pi x_i}{L_2}\right) + e_0 + e_i + f_i, \quad i = 1, \ldots, n,$$

  where $a_1 = a_2 = 0.01\,\mu\mathrm{m}$, $L_1 = 400\,\mu\mathrm{m}$, $L_2 = 30\,\mu\mathrm{m}$, and $e_0$ and $e_i$ are random draws made independently from, respectively, from the Gaussian distributions $\mathrm{N}(0, \rho_z u_z^2)$ and $\mathrm{N}(0, (1-\rho_z)u_z^2 - \rho_{xz}u_x u_z)$.

Gaussian filters with cut-off wavelengths $\lambda_\mathrm{s} = 2.5\,\mu\mathrm{m}$ and $\lambda_\mathrm{c} = 80\,\mu\mathrm{m}$ are applied to obtain the primary, waviness and roughness profiles.

Different 'test problems' are considered by choosing different values for $\rho_x$, $\rho_z$ and $\rho_{xz}$ as follows:

**E** $\rho_x = 0,\ \rho_z = 0,\ \rho_{xz} = 0;$

**F** $\rho_x = 0,\ \rho_z = 0.9,\ \rho_{xz} = 0;$

**G** $\rho_x = 0.9,\ \rho_z = 0,\ \rho_{xz} = 0;$

**H** $\rho_x = 0,\ \rho_z = 0,\ \rho_{xz} = 0.9;$

**I** $\rho_x = 0.3,\ \rho_z = 0.3,\ \rho_{xz} = 0.3.$

For each test problem, the standard uncertainties $u_x$ and $u_z$ are set equal to $1\,\mathrm{nm}$.

Figures 20 to 23 in appendix C.1 illustrate the results obtained for problems E to H. For each problem is provided a graph illustrating the approximations to the PDFs for the surface

| | | Primary, $P_q$ | | Waviness, $W_q$ | | Roughness, $R_q$ | |
|---|---|---|---|---|---|---|---|
| | | $p_q$/nm | $u(p_q)$/nm | $w_q$/nm | $u(w_q)$/nm | $r_q$/nm | $u(r_q)$/nm |
| E | GUF | 9.908 | 0.030 | 6.723 | 0.032 | 6.944 | 0.035 |
| | MCM | 9.923 | 0.030 | 6.723 | 0.032 | 6.963 | 0.035 |
| F | GUF | 9.894 1 | 0.009 4 | 6.729 | 0.010 | 6.951 | 0.011 |
| | MCM | 9.895 6 | 0.009 5 | 6.729 | 0.010 | 6.953 | 0.011 |
| G | GUF | 9.935 | 0.030 | 6.790 | 0.032 | 6.939 | 0.035 |
| | MCM | 9.950 | 0.030 | 6.790 | 0.032 | 6.958 | 0.035 |
| H | GUF | 9.901 | 0.030 | 6.754 | 0.032 | 6.906 | 0.035 |
| | MCM | 9.917 | 0.030 | 6.755 | 0.032 | 6.926 | 0.035 |
| I | GUF | 9.925 | 0.025 | 6.731 | 0.027 | 6.969 | 0.029 |
| | MCM | 9.936 | 0.025 | 6.731 | 0.027 | 6.983 | 0.029 |

Table 4: Results for case 2.

texture parameters $P_q$, $W_q$ and $R_q$ obtained using the GUM uncertainty framework and a Monte Carlo method.[12]

Appendix C.2 contains graphs to illustrate the results obtained for problem I.

Figure 24 shows the variances associated with the $x$- and $z$-coordinates defining the measured profile. The horizontal lines mark the values of $u_x^2$ and $u_z^2$, respectively. The crosses mark the variances of the components of the vectors $\boldsymbol{x}_\ell, \ell = 1, \ldots, M$, and $\boldsymbol{z}_\ell, \ell = 1, \ldots, M$, obtained by 'simulating' $M$ measured profiles $(\boldsymbol{x}_\ell, \boldsymbol{z}_\ell)$ according to the observation model (25).

Figures 25 to 27 show the variances associated with the $x$- and $z$-coordinates defining the primary, waviness and roughness profiles obtained from the GUM uncertainty framework and a Monte Carlo method.

Figures 28 to 31 show the correlation coefficients, as a function of lag $k$, associated with the x-coordinates $x_i$ and $x_{i+k}$, the z-coordinates $z_i$ and $z_{i+k}$, and the $x$- and $z$-coordinates $x_i$ and $z_{i+k}$ for each profile obtained using the GUM uncertainty framework.[13]

Finally, figure 32 shows the approximations to the PDFs for the surface texture parameters $P_q$, $W_q$ and $R_q$ obtained using the GUM uncertainty framework and a Monte Carlo method.

Table 4 summarises the results for each problem.

A number of observations are made about the results (see also section 7.1):

[12]As before, the origin (zero value of the quantity) corresponds to the estimate provided by the law of propagation of uncertainty.

[13]There are no discernable differences from those obtained using a Monte Carlo method, which are consequently not shown.

1. For all five problems and all three types of profile, there is excellent agreement between the standard uncertainties returned by the GUM uncertainty framework and a Monte Carlo method.

2. For problems E, G and H, the standard uncertainties associated with the estimates $p_q$ are in good agreement (and similarly for the estimates $w_q$ and $r_q$). The standard uncertainties also agree well with those obtained for problem B and $\rho_z = 0$ (section 7.1). The results suggest that uncertainty associated with the measured $x$-coordinates, and correlation associated with pairs of measured $x$-coordinates or pairs of measured $x$- and $z$-coordinates, has little influence on the uncertainty associated with estimates of these *particular* surface texture parameters.

3. For problems F and I, for which there is correlation associated with pairs of measured $z$-coordinates, the standard uncertainties associated with the estimates are smaller than those for problems E, F and G, for which there is no such correlation.

4. For problem I, the correlation coefficients associated with pairs of $x$-coordinates in the primary, waviness and roughness profiles (figures 29, 30 and 31) are identical to those for the measured profile (figure 28). The correlation coefficients associated with pairs of $z$-coordinates are the same as those for the problems in case 1. The effect of the applied Gaussian filters is to introduce correlation associated with the $x$- and $z$-coordinates of neighbouring points (for which the lag $k$ is small).

### 7.3 Case 3

The measured profile is defined as in section 7.2. Two 'test problems' are considered to mimic measurements made by NPL's instrument NanoSurf IV (see section 3.3):

**J** $u_x = 0\,\mathrm{nm},\ u_z = 0.28\,\mathrm{nm},\ \rho_x = 0,\ \rho_z = 0,\ \rho_{xz} = 0;$

**K** $u_x = 0.65\,\mathrm{nm},\ u_z = 0.28\,\mathrm{nm},\ \rho_x = 0.94,\ \rho_z = 0.68,\ \rho_{xz} = 0.08.$

For the first test problem, it is assumed that there are uncertainties associated with the measured ordinate values only. The second problem corresponds to the indicative values for the standard uncertainties associated with the four main effects described in section 3.3. Figures 33 and 34 in appendix D and table 5 summarizes the results obtained for problems J and K.

Similarly to the problems of cases 1 and 2 (sections 7.1 and 7.2), the results suggest that identifying a component of the uncertainties associated with the measured $z$-coordinates with a common (systemetic) error quantity, leading to correlation associated with the measured coordinates, gives estimates of the surface texture parameters with smaller associated standard uncertainties. The results for problem K give indicative values for the standard uncertainties associated with estimates of the surface texture parameters $P_q$, $W_q$ and $R_q$ that may be obtained using NPL's NanoSurf IV surface texture measuring instrument.

| | | Primary, $P_q$ | | Waviness, $W_q$ | | Roughness, $R_q$ | |
|---|---|---|---|---|---|---|---|
| | | $p_q$/nm | $u(p_q)$/nm | $w_q$/nm | $u(w_q)$/nm | $r_q$/nm | $u(r_q)$/nm |
| J | GUF | 9.992 2 | 0.008 3 | 6.754 2 | 0.009 0 | 6.965 6 | 0.009 7 |
| | MCM | 9.992 3 | 0.008 4 | 6.754 1 | 0.008 9 | 6.967 2 | 0.009 7 |
| K | GUF | 9.902 7 | 0.004 7 | 6.739 4 | 0.005 1 | 6.942 6 | 0.005 5 |
| | MCM | 9.903 0 | 0.004 8 | 6.739 4 | 0.005 1 | 6.943 1 | 0.005 6 |

Table 5: Results for case 3.

# 8 Conclusions

Surface texture parameters defined in ISO specification standards are widely used to associate numerical values to the topography of a surface. However, if the values of a parameter are to be used for the comparison of different surfaces and for the interpretation of surface texture tolerances on engineering drawings, it is essential that the values are accompanied by statements of uncertainty. Furthermore, it is important that those statements are reliable and convey meaningful information about the parameter. Consideration has been given in this report to the problem of uncertainty evaluation for a particular (amplitude) surface texture parameter, viz., the root mean square value ($P_q$, $W_q$ or $R_q$) of an evaluated (primary, waviness or roughness) surface profile. A formulation of the problem has been given in terms of a multi-stage measurement model that defines the mathematical relationship between all quantities involved in the measurement and the available information about those quantities. The applications of the conventional approach of 'uncertainty propagation' (the GUM uncertainty framework) and a Monte Carlo method that provides a more generally-applicable approach, have been described, and the results obtained from the two approaches for simulated measurement data compared.

The conclusions of the work are summarized as follows:

1. For the particular surface texture parameter considered, there is good agreement between the standard uncertainties provided by the GUM uncertainty framework and those provided by a Monte Carlo method. However, there are cases when the estimates of the parameter for the primary and roughness profiles returned by the two approaches can be appreciably different, notably when the uncertainties associated with the measured coordinates are large compared with the amplitude of the profile.

2. For the particular surface texture parameter considered, uncertainty associated with the measured $x$-coordinates, and correlation associated with pairs of measured $x$-coordinates or pairs of measured $x$- and $z$-coordinates, has little influence on the uncertainty associated with estimates of the parameter. However, the uncertainty is strongly influenced by the (component of) uncertainty associated with the measured $z$-coordinates that quantifies (independent) random errors. The operation of mean centering the measured profile (and, to a lesser extent, of filtering the profile) has the

effect of removing contributions made by (common) systematic error quantities to the measured coordinates.

3. Since the measurement functions defining the steps of mean centering and Gaussian filtering are linear, the results returned by the law of propagation of uncertainty of the GUM uncertainty framework are exact for these steps. However, the step of evaluating the surface texture parameter considered in terms of the evaluated (filtered) profiles is non-linear, for which the law of propagation of uncertainty can be expected to be approximate. The degree of approximation can depend on properties of the evaluated profile, such as the magnitude of the uncertainties associated with the measured coordinates.

4. Software implementation of the law of propagation uncertainty requires storing and manipulating large matrices of data. For the simulations considered, the number of measured points is $n = 1\,130$. The covariance matrix associated with the coordinates defining the measured profile is a matrix of dimension $1\,130 \times 1\,130$ (for the case of uncertainties associated with the $z$-coordinates) and dimension $4\,520 \times 4\,520$ (for the case of uncertainties associated with both coordinates). Consideration should be given to exploiting the structure of covariance and sensitivity matrices involved in the calculations. For example, covariance matrices are symmetric, and those encountered in this work can often by summarized (perhaps approximately) by an autocovariance function.

5. In contrast, a Monte Carlo method, which is a generally-applicable procedure, requires only to undertake (albeit many times for different realizations of the measured data) the evaluation of the surface texture parameter. Furthermore, 'updating procedures' are available [9], which avoid the need to store the complete set of values of the surface texture parameter (the number of which can be large).

## Acknowledgements

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# A Uncertainty evaluation when no mean centering is applied

Consideration is given to the evaluation of the covariance matrices $\boldsymbol{U_p}$, $\boldsymbol{U_w}$ and $\boldsymbol{U_r}$ in the case that there is uncertainty associated with the ordinate values of the measured profile only and the step of mean centering is not applied (cf. section 5.1).

Substituting expression (24) for $\boldsymbol{U_z} \equiv \boldsymbol{U_y}$ in expression 27), and making use of expression (8),

$$\boldsymbol{U_p} = \boldsymbol{S}_\mathrm{s}\left(\rho_z u_z^2 \mathbf{1}_n \mathbf{1}_n^\top + (1-\rho_z) u_z^2 \boldsymbol{I}_n\right)\boldsymbol{S}_\mathrm{s}^\top = \rho_z u_z^2 \mathbf{1}_{n-2m_\mathrm{s}} \mathbf{1}_{n-2m_\mathrm{s}}^\top + (1-\rho_z) u_z^2 \boldsymbol{S}_\mathrm{s} \boldsymbol{S}_\mathrm{s}^\top . \tag{33}$$

If follows that as the correlation associated with the ordinate values of the measured profile increases, i.e., $\rho_z \to 1$ and $\boldsymbol{U_z} \to u_z^2 \mathbf{1}_n \mathbf{1}_n^\top$, that associated with the estimates of the primary profile also increases, because $\boldsymbol{U_p} \to u_z^2 \mathbf{1}_{n-2m_\mathrm{s}} \mathbf{1}_{n-2m_\mathrm{s}}^\top$.

Substituting expression (33) for $\boldsymbol{U_p}$ in expressions (29) and (30),

$$\begin{aligned}\boldsymbol{U_w} &= \boldsymbol{S}_\mathrm{c}\left(\rho_z u_z^2 \mathbf{1}_{n-2m_\mathrm{s}} \mathbf{1}_{n-2m_\mathrm{s}}^\top + (1-\rho_z) u_z^2 \boldsymbol{S}_\mathrm{s} \boldsymbol{S}_\mathrm{s}^\top\right)\boldsymbol{S}_\mathrm{c}^\top \\ &= \rho_z u_z^2 \mathbf{1}_{n-2m_\mathrm{s}-2m_\mathrm{c}} \mathbf{1}_{n-2m_\mathrm{s}-2m_\mathrm{c}}^\top + (1-\rho_z) u_z^2 \boldsymbol{S}_\mathrm{c} \boldsymbol{S}_\mathrm{s} \boldsymbol{S}_\mathrm{s}^\top \boldsymbol{S}_\mathrm{c}^\top ,\end{aligned}$$

and

$$\begin{aligned}\boldsymbol{U_r} &= \boldsymbol{G}_\mathrm{c}\left(\rho_z u_z^2 \mathbf{1}_{n-2m_\mathrm{s}} \mathbf{1}_{n-2m_\mathrm{s}}^\top + (1-\rho_z) u_z^2 \boldsymbol{S}_\mathrm{s} \boldsymbol{S}_\mathrm{s}^\top\right)\boldsymbol{G}_\mathrm{c}^\top \\ &= (1-\rho_z) u_z^2 \boldsymbol{G}_\mathrm{c} \boldsymbol{S}_\mathrm{s} \boldsymbol{S}_\mathrm{s}^\top \boldsymbol{G}_\mathrm{c}^\top .\end{aligned}$$

If follows that as the correlation associated with the ordinate values of the measured profile increases, that associated with the estimates of the waviness profile also increases, because $\boldsymbol{U_w} \to u_z^2 \mathbf{1}_{n-2m_\mathrm{s}-2m_\mathrm{c}} \mathbf{1}_{n-2m_\mathrm{s}-2m_\mathrm{c}}^\top$, but that associated with the estimates of the roughness profile decreases, because $\boldsymbol{U_r} \to \mathbf{0}_{n-2m_\mathrm{s}-2m_\mathrm{c}}$.

These results are (perhaps) intuitive if the source of the correlation is an error common to the ordinate values of the measured profile and is considered as a 'long-wavelength' component of the profile. Then, by virtue of the filtering operation, the error persists in the primary and waviness profiles but is removed when determining the roughness profile.

# B Results for Case 1

## B.1 Problem A

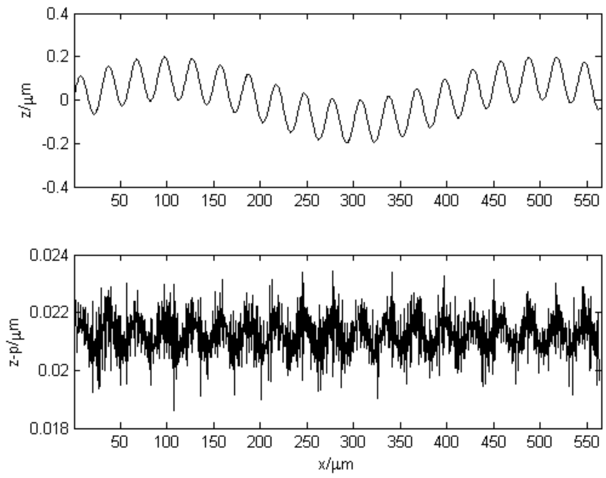


Figure 1: Simulated measured profile (top) and the differences between the measured and primary profiles (bottom) after mean centering and application of a $\lambda_s$ filter to the measured profile when $\rho_z = 0$.

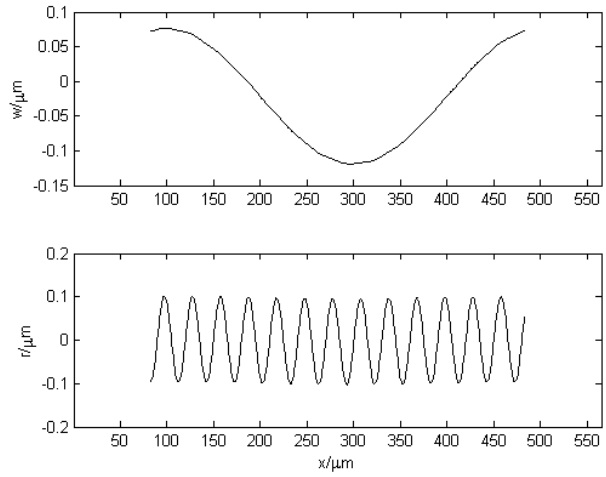


Figure 2: Waviness profile (top) and roughness profile (bottom) after application of a $\lambda_c$ filter to the primary profile.

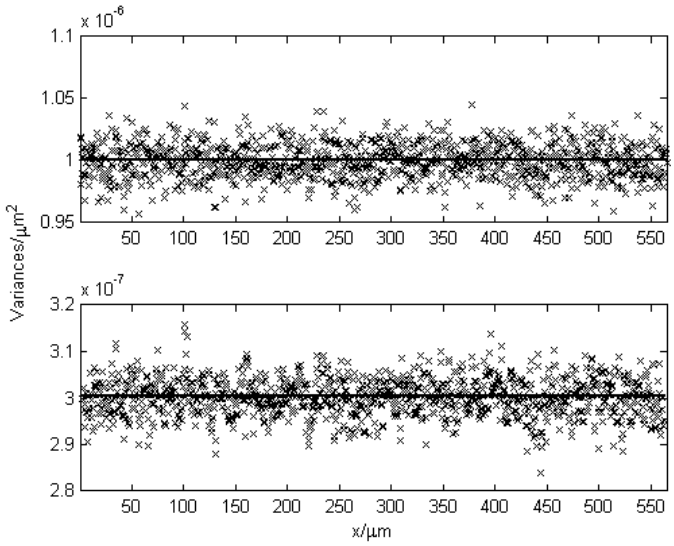


Figure 3: Variances associated with the ordinate values defining the measured (top) and primary (bottom) profiles. The variances determined using the GUM uncertainty framework, which are the same for each ordinate value, are shown as the horizontal line; those determined using a Monte Carlo method are shown as crosses.

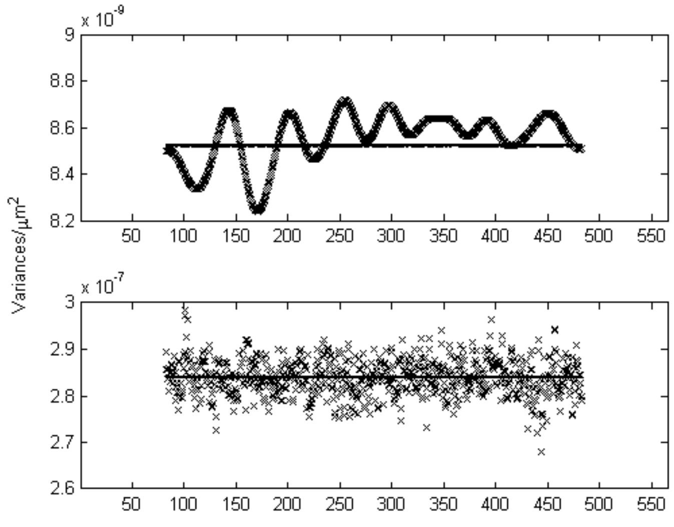


Figure 4: As figure 3, but for the waviness (top) and roughness (bottom) profiles.

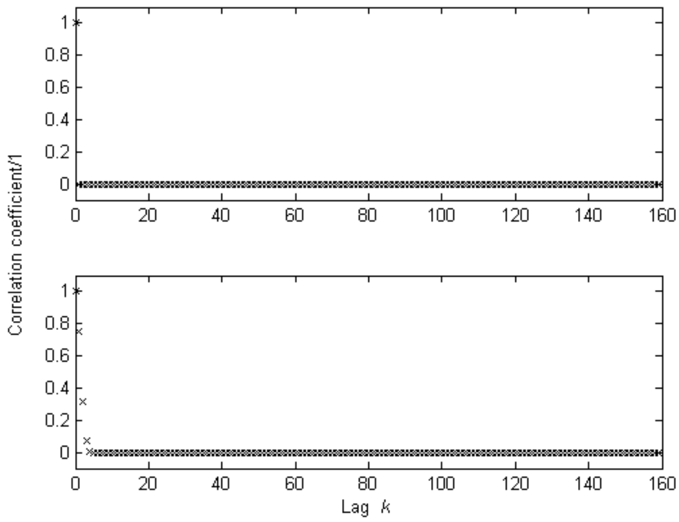


Figure 5: Correlation coefficients, as a function of lag $k$, associated with the ordinate values defining the measured (top) and primary (bottom) profiles. For the measured profile the correlation coefficients are defined by the observation model for the ordinates. For the primary profile they are determined using the GUM uncertainty framework.

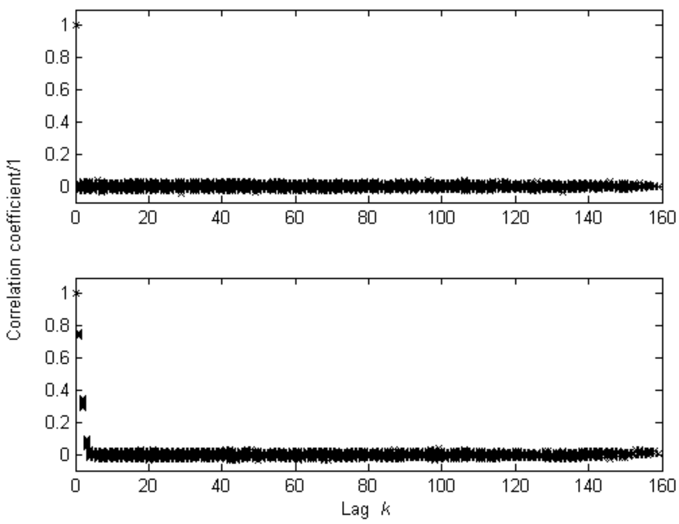


Figure 6: As figure 5, but determined using a Monte Carlo method.

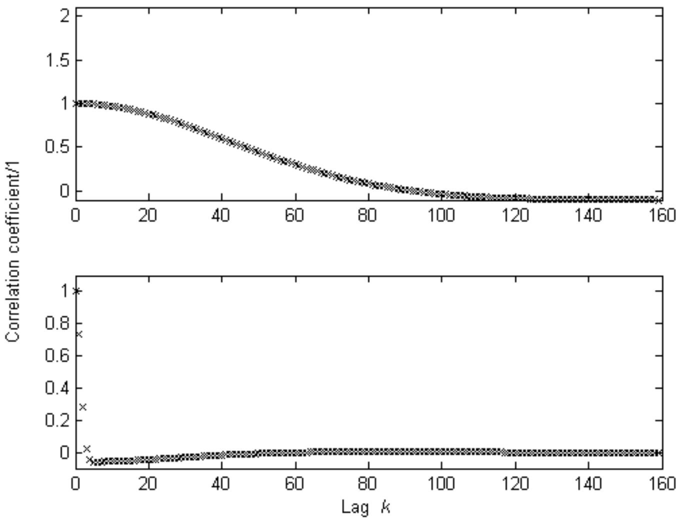


Figure 7: Correlation coefficients, as a function of lag $k$, associated with the ordinate values defining the waviness (top) and roughness (bottom) profiles, determined using the GUM uncertainty framework.

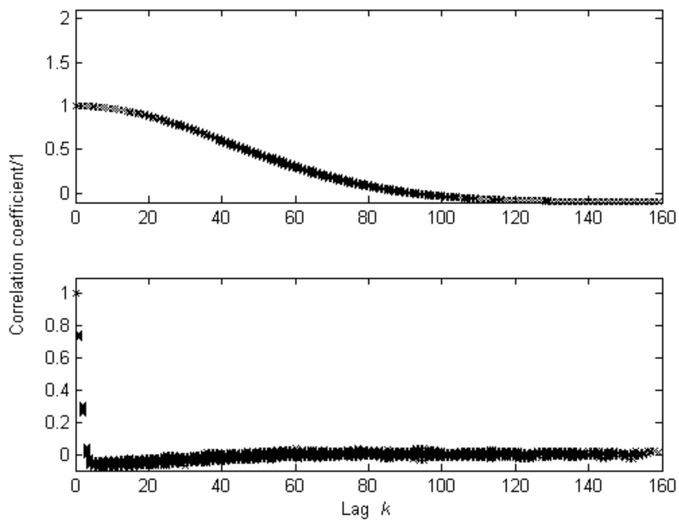


Figure 8: As figure 7, but determined using a Monte Carlo method.

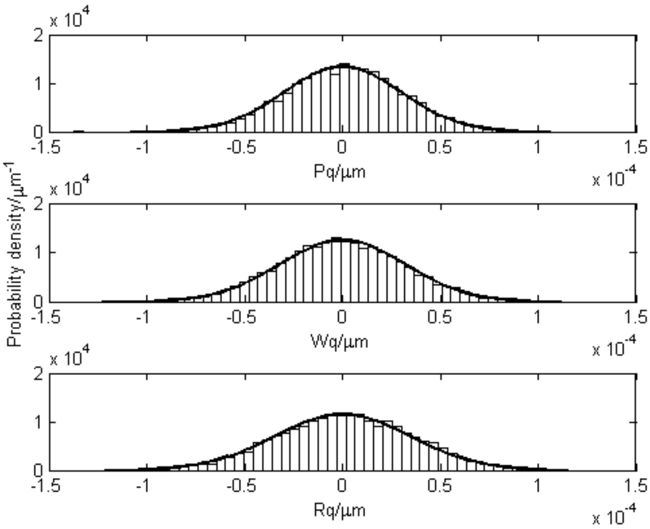


Figure 9: Approximations to the PDFs for the quantities $P_q - p_q$ (top), $W_q - w_q$ (middle) and $R_q - r_q$ (bottom), where $p_q$, $w_q$ and $r_q$ are the estimates of, respectively, $P_q$, $W_q$ and $R_q$ obtained using the GUM uncertainty framework. The results provided by the GUM uncertainty framework are shown as continuous Gaussian PDFs, and those provided by a Monte Carlo method as scaled frequency distributions (histograms).

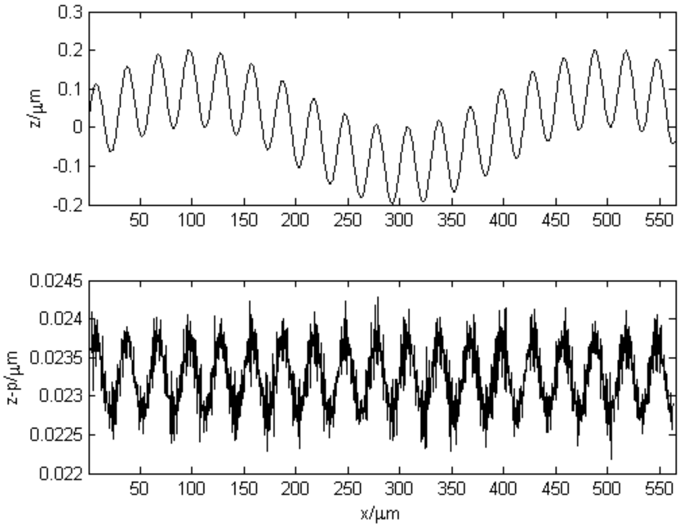


Figure 10: As figure 1, but when $\rho_z = 0.9$.

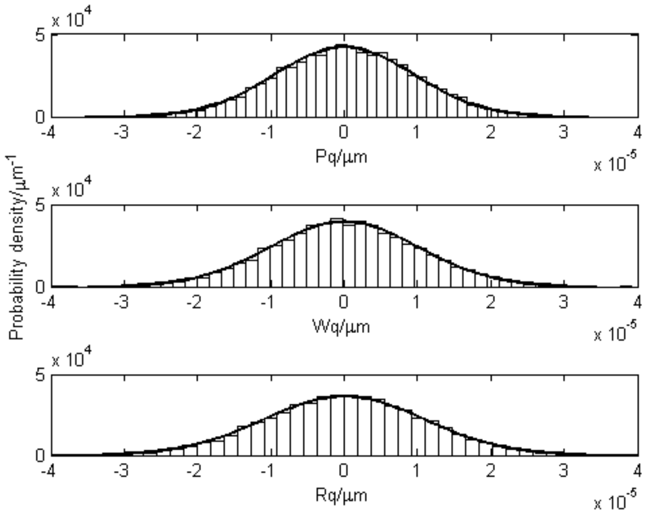


Figure 11: As figure 9, but when $\rho_z = 0.9$.

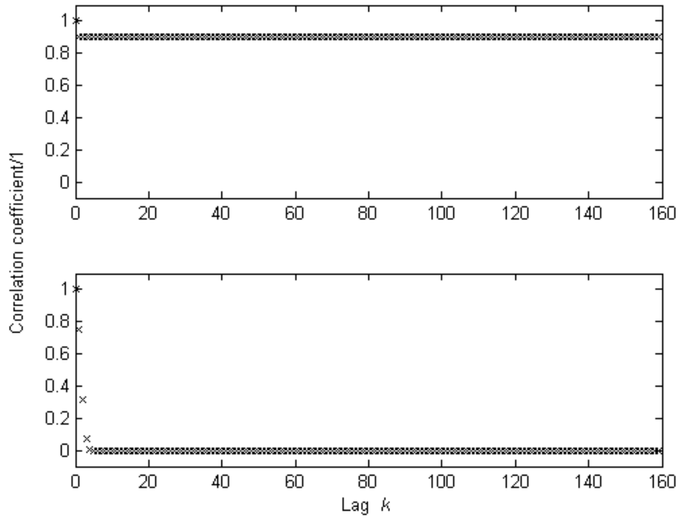


Figure 12: As figure 5, but when $\rho_z = 0.9$.

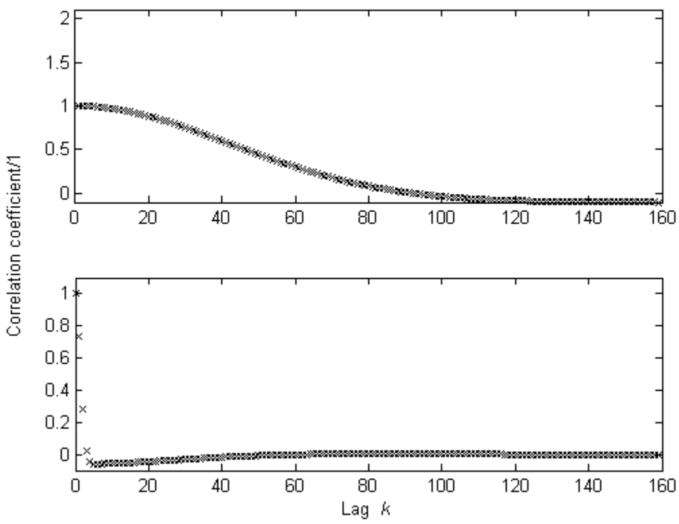


Figure 13: As figure 7, but when $\rho_z = 0.9$.

## B.2 Problem B

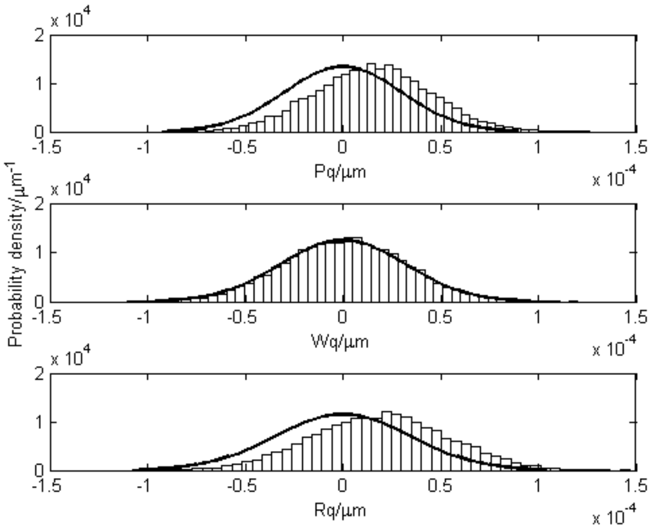


Figure 14: As figure 9, but for case 1, problem B when $\rho_z = 0$.

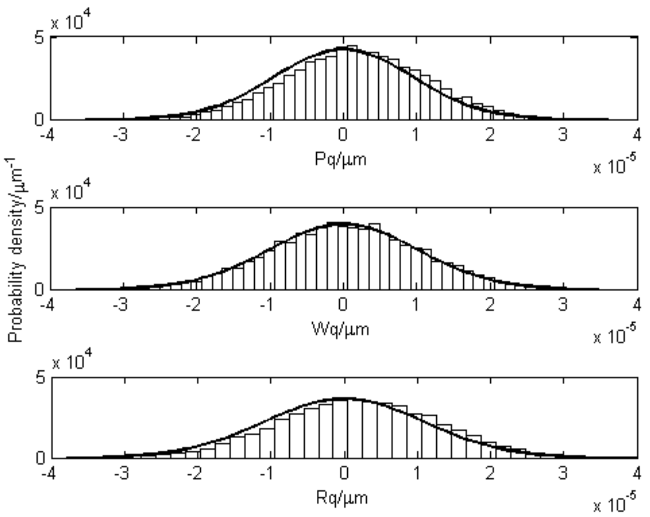


Figure 15: As figure 9, but for case 1, problem B when $\rho_z = 0.9$.

## B.3 Problem C

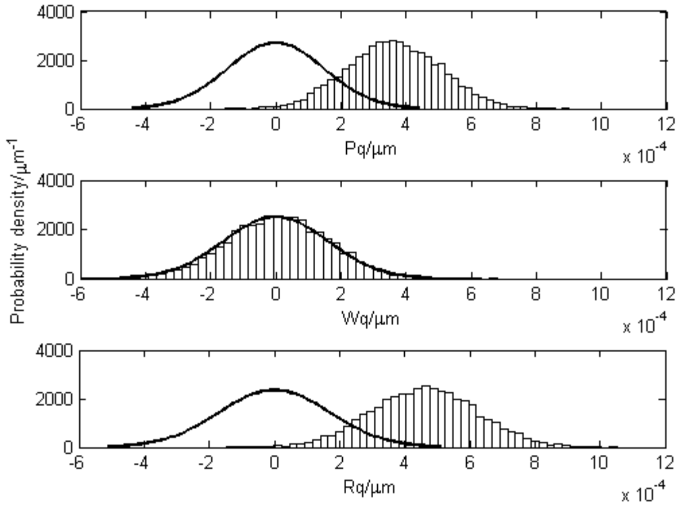


Figure 16: As figure 9, but for case 1, problem C when $\rho_z = 0$.

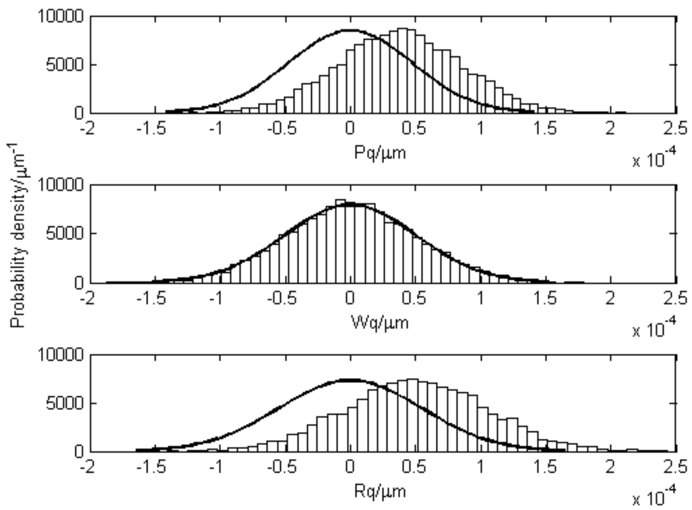


Figure 17: As figure 9, but for case 1, problem C when $\rho_z = 0.9$.

## B.4 Problem D

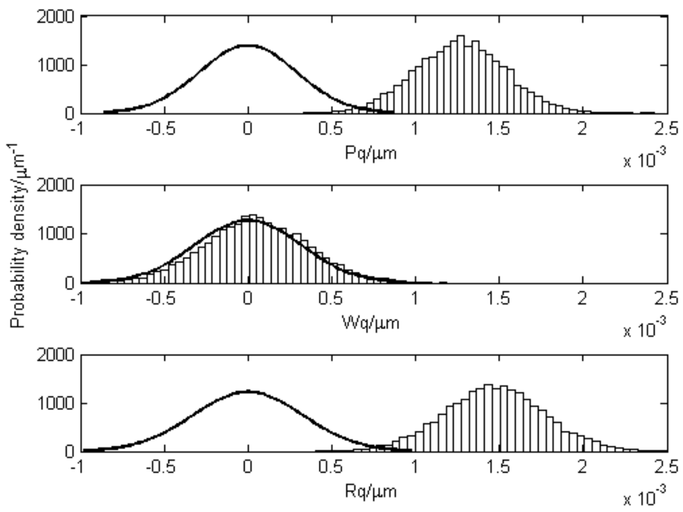


Figure 18: As figure 9, but for case 1, problem D when $\rho_z = 0$.

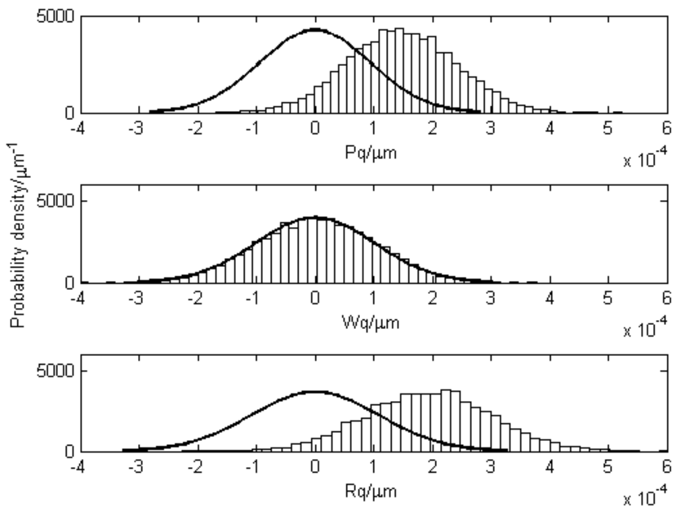


Figure 19: As figure 9, but for case 1, problem D when $\rho_z = 0.9$.

# C Results for Case 2

## C.1 Problems E to H

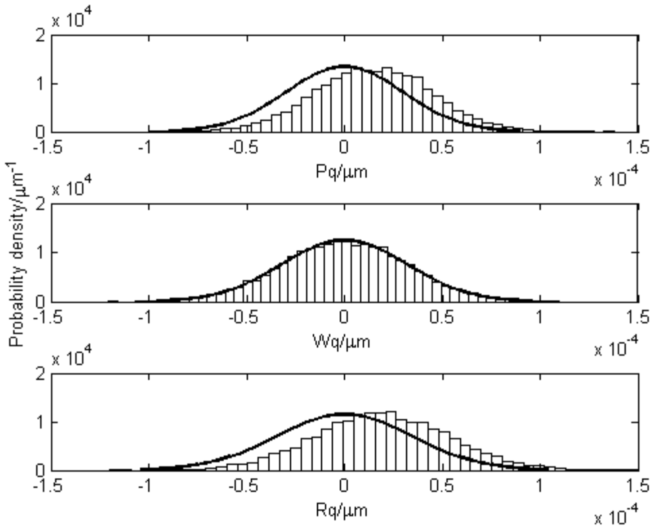


Figure 20: As figure 9, but for case 2, problem E.

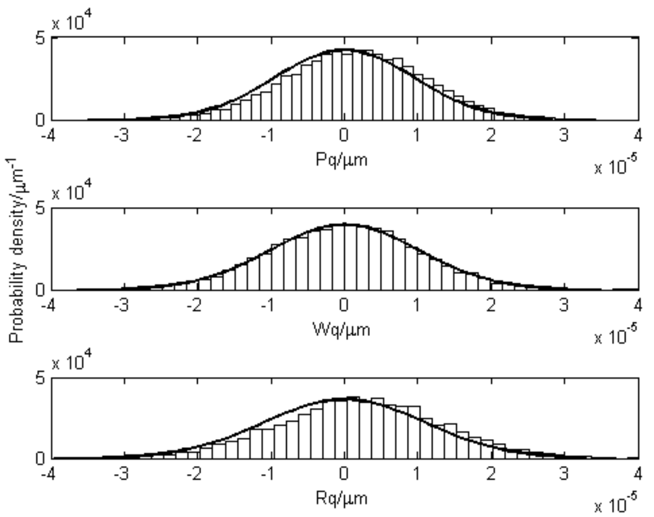


Figure 21: As figure 9, but for case 2, problem F.

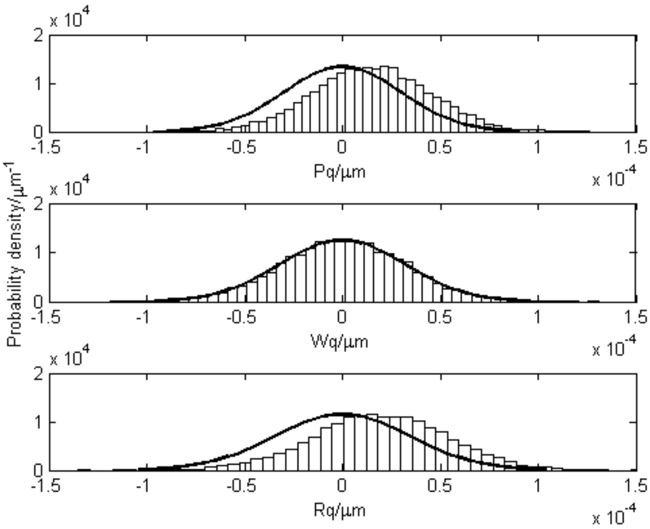


Figure 22: As figure 9, but for case 2, problem G.

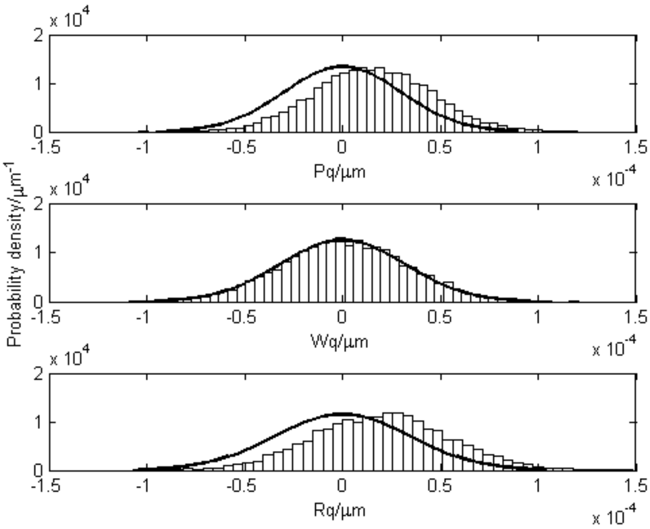


Figure 23: As figure 9, but for case 2, problem H.

## C.2 Problem I

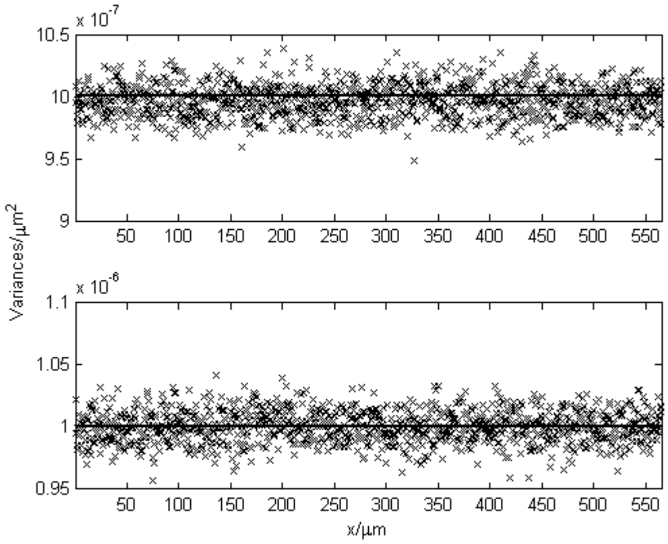


Figure 24: Variances associated with the $x$-coordinates (top) and $z$-coordinates defining the measured profile.

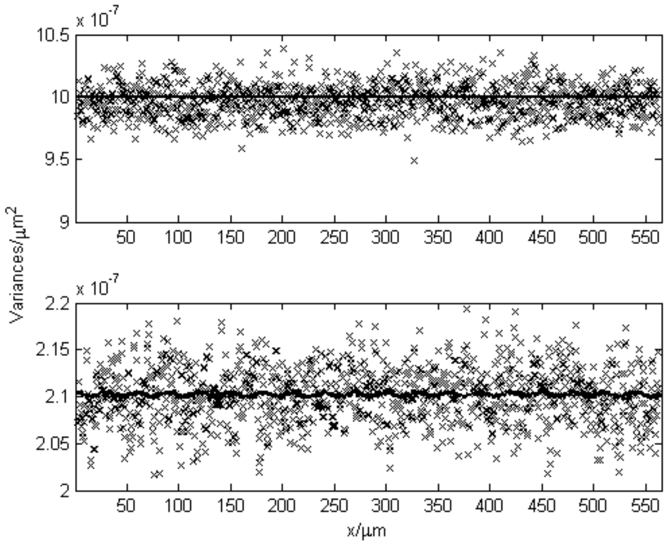


Figure 25: Variances associated with the $x$-coordinates (top) and $z$-coordinates defining the primary profile. The variances determined using the GUM uncertainty framework are shown as the black continuous line; those determined using a Monte Carlo method are shown as crosses.

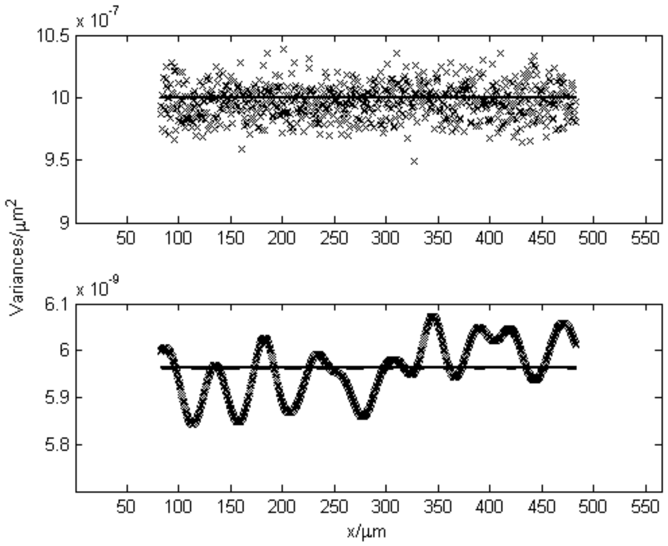


Figure 26: As figure 25, but for the waviness profile.

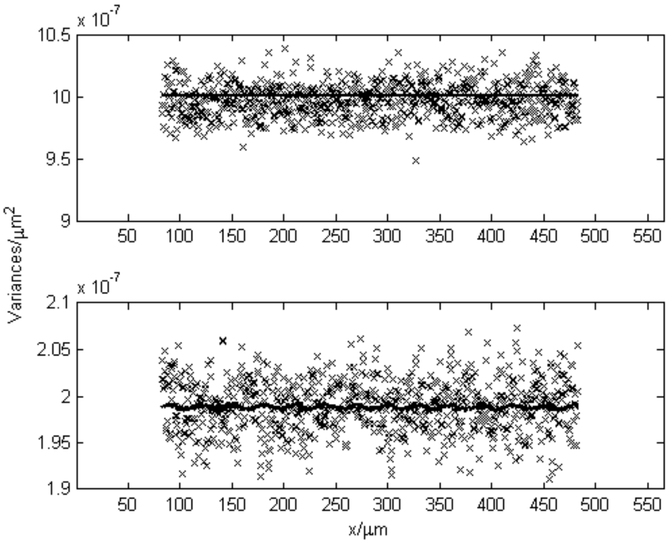


Figure 27: As figure 25, but for the roughness profile.

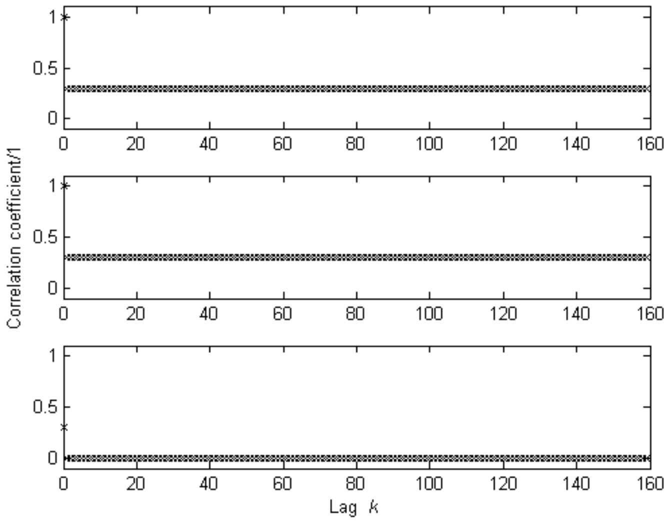


Figure 28: Correlation coefficients determined using the GUM uncertainty framework, as a function of lag $k$, associated with the $x$-coordinates $x_i$ and $x_{i+k}$ (top), the $z$-coordinates $z_i$ and $z_{i+k}$ (middle), and the $x$- and $z$-coordinates $x_i$ and $z_{i+k}$ for the measured profile.

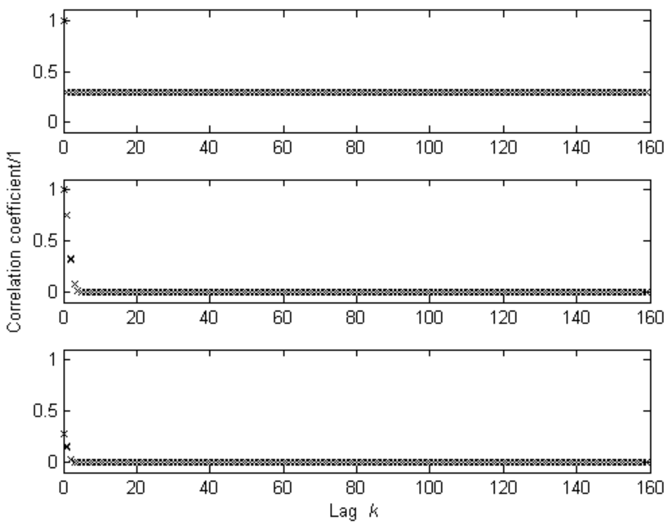


Figure 29: As figure 28, but for the primary profile.

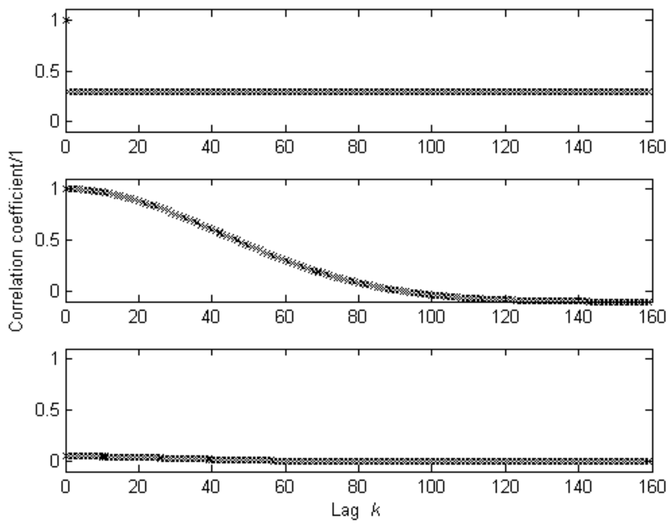


Figure 30: As figure 28, but for the waviness profile.

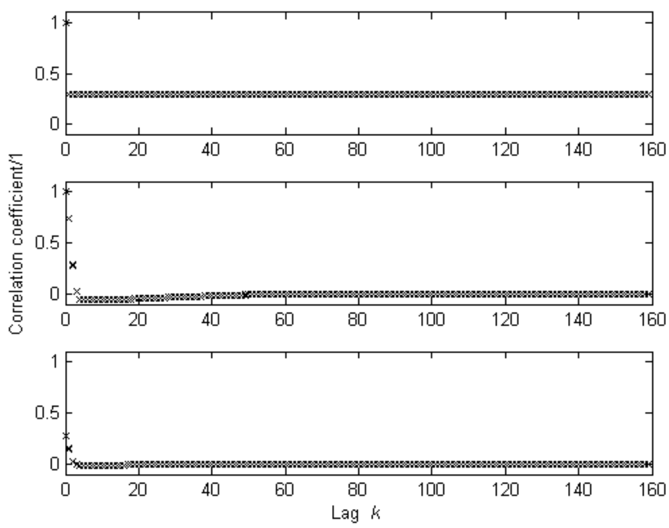


Figure 31: As figure 28, but for the roughness profile.

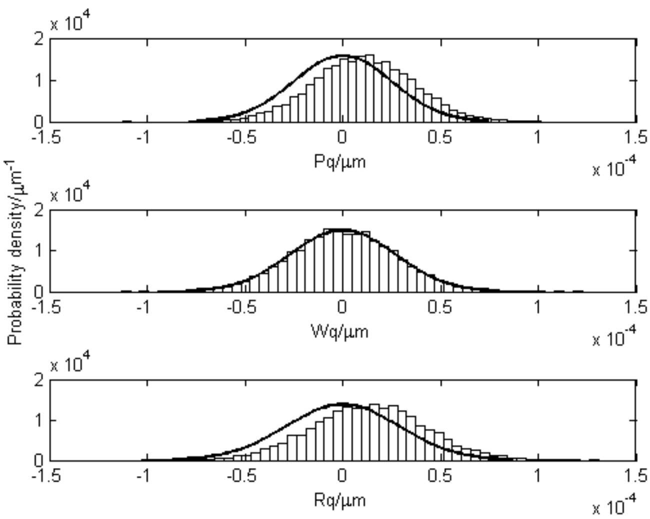


Figure 32: As figure 9, but for case 2, problem I.

# D Results for Case 3

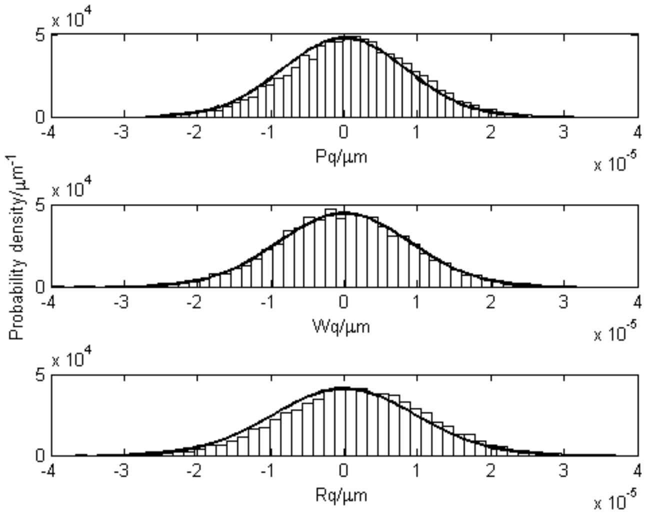


Figure 33: As figure 9, but for case 3, problem J.

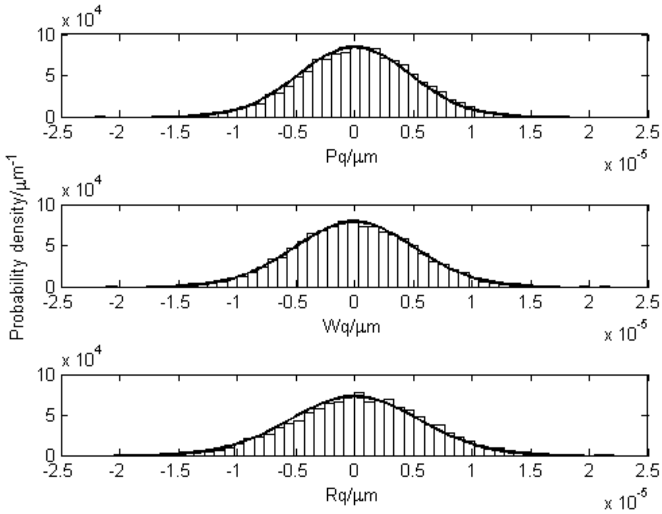


Figure 34: As figure 9, but for case 3, problem K.