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Algorithms for Surface Texture Profiles and Parameters

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A thesis submitted to the University of Huddersfield
in partial fulfilment of the requirements for
the degree of Doctor of Philosophy

The University of Huddersfield in collaboration with the
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This thesis is concerned with the development of algorithms for the reliable calculation of surface texture profile parameters published by the International Organisation for Standardisation (ISO). Some of these parameters are impossible to compute exactly given a discrete set of measured profile points. A need to represent the profile as a continuous function therefore arises, a need that occurs in many metrological applications. By reconstructing surface profiles accurately, with elements of numerical safety, we can provide a mathematically sound basis on which to compute surface texture profile parameters. As an important direct benefit, parameters involving the integrals of profiles can be calculated exactly from the interpolant introduced. Another advantage of a continuous representation is that it allows measured surface profile data, that is shown to be inherently non-uniform in the $x$-axis spacing, to be re-sampled at uniform intervals as it has been discovered that standard filtering techniques are apparently ineffective with non-uniform spacing. A novel method for data fitting discretely sampled surface profiles is presented with the advantages clearly stated. This provides a solid basis for profile parameters to be calculated upon and also intelligent functions for the evaluation of measurement uncertainty to be appended, which is equally important for the evolution of algorithms designed to be the complete evaluation of a parameter with a traceable measure of uncertainty.
I would like to thank everybody who has supported my work and wellbeing in the duration of this project.

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1.1 Metrology

Metrology is the science of measurement. Derived from Greek *metron*, meaning 'a measure', and *ology*, 'the study of'. The International Bureau of Weights and Measures (BIPM) adds to this definition ”...embracing both experimental and theoretical determinations at any level of uncertainty in any field of science and technology”. It is something that is of vital importance to us all.

Measurement is a language that extends across all others, used when we wish to convey something about quantity, size, speed and time. It is probably best explained in the following quote:

’When you can measure what you are speaking about, and express it in numbers, you know something about it; but when you cannot express it in numbers, your knowledge is of a meagre and unsatisfactory kind. It may be the beginning of knowledge, but you have scarcely, in your thoughts, advanced to the stage of science.’

Lord Kelvin (1824-1907)
Our world is full of measurement. We use it everyday and it provides us with functional information about things. Its presence alone has become essential in modern life. It seems that when we obtain one or more measurements of something then we automatically achieve an elementary understanding of it. Even though this information may not be important to us it may give us a strange reassurance. Maybe due to the fact that we are usually afraid of things we do not understand, whereas once something is measured we now know something about it and this fear can be removed. Nevertheless, measurement is everywhere and always will be. We use it every day and it is extremely important that we all speak the same language. Units of measurement are universal and not dependent on one’s native tongue, almost like a version of *esperanto* that did catch on.

Our confidence in metrology enters almost every aspect of our lives. We put trust in the transfer of millions of gallons of oil from oil well to petrol pump is correctly measured so that we pay for the amount we use and no more. The same applies to high-volume services such as gas, electricity and telecommunications but also mundane items such as milk, bread and sugar. The efficient production of the tools we use everyday rely heavily on accurate measurements, from the internal combustion engine to the latest microprocessor. In these cases and others the reliability and life time of products depend upon manufacturing tolerances of micrometres, maybe less.

Since early man began measuring things for his own purpose there have been many acts to try and standardise and specify ways of measuring length, from cubits to barleycorns, and today we have the metre from the SI derived units (*Le Système International d’unités*) [4]. With very few exceptions the SI system is used in every country in the world today. The lack of a standardised system of measurements, in days gone by, was a source of error and fraud in commercial and social transactions. This in turn slowed international commerce and it was only the great expansion of
industry and trade that forced the adoption of measurement standards.

1.1.1 Precision metrology

Industries such as aerospace, automotive and computing are worth hundreds of billions of pounds. The performance and perceived quality of most products manufactured by these industries has a direct influence on their commercial success. These factors are controlled by how well they are made and there is a constant awareness to improve both and hence increase commercial success. This competition has forced the decline of engineering tolerances by a factor of three every decade since 1960 for form measurement. Consistent evolution in precision metrology together with the advent of new measurement technologies, ironically only possible due to the former, have allowed these tolerances to continually fall.

It is now common knowledge that the performance of many manufactured components continues to improve even when the errors in manufacturing are reduced far beyond what is first thought to be required. A superb example of how precision metrology is linked to quality and commercial success can be found in the forces required to open car doors manufactured in the US and Japanese markets [65]. In the 1980s the forces required to open the doors of US and Japanese cars differed by a factor of three. The origin of the difference was that Japanese car doors had a tolerance of 1mm on their door and door assemblies and easier to open than their American counterpart who used an equivalent tolerance of 2mm. The ease of opening of the door is an important aspect in the perceived quality of the product as a whole, which is directly related to the precision of manufacture. This had large economic consequences for the US motor industry.

In 1989, United Airlines flight 232 crash landed at Sioux City airport, Iowa, with
the loss of 110 of its 285 passengers aboard [10]. The Douglas DC-10 aircraft had suffered an uncontained failure of its number two engine which destroyed all three hydraulic systems. With no controls working except thrust levers for the two remaining engines, the aircraft broke up when attempting an emergency landing. The catastrophic failure of the engine was a result of a surface imperfection in the turbine fan disk that was judged to be smaller than a grain of sand. This imperfection was the result of an error in manufacturing and overlooked by quality control measures.

1.1.2 Measurement, what’s that got to do with the price of eggs?

Measurement is an almost magical ability to assign a number to different aspects and features and thereby making them instantly comparable with other measurements. If this feature happens to be the size of eggs, then ultimately this will affect the price. On a more serious tone, it is measurement that is the root of the research contained in these pages and it is the act of standardisation that is the cause for it to be conducted. The topic concerned is surface texture, specifically the unambiguous quantification of the features in surface texture with software to calculate surface texture parameters. Traditionally, surface metrology has seen as important owing to its strong association with other disciplines such as control of machine tools and manufacturing processes [24].

1.2 Surface Texture

1.2.1 What causes surface texture?

Every surface, even though it may appear smooth to the human eye, has some form of texture structure that takes the form of a series of peaks and valleys. Examination under a magnifying instrument will reveal this complex structure of peaks and valleys that vary in height and spacing and make up a surfaces texture. Examining this tex-
ture has a very practical significance. Surface texture has properties that are a result of the way the surface was produced (e.g. cutting tools produce uniform spacing with defined directions whilst grinding produces random spacing) as well as other factors such as crystal structure and paint on the surface.

These factors combined make up the characteristics of a surfaces profile and often affect the performance, quality and service life of the product. If we could control surface texture then we could control these aspects of a product but in order to attempt this we must quantify it by measuring it. Measuring the surface texture during the production cycle allows the product to be improved by controlling and optimising the manufacturing processes. This control of surface texture, for example, has been utilised in the automotive industry for many years [33] and has allowed reduced running-in times for engines with increased fuel efficiency and lower emissions. Of course, this has not just benefited the automotive industry, everything from prosthetic hip joints [6] to hard disk drives and even dentistry [74] have seen improved performance from the control of surface texture. Measuring at the end of the cycle will reveal a guide to the performance capability of the product, thus in some cases contribute to its perceived quality.

1.2.2 Measuring the surface

The first step in quantifying the texture of a surface is to measure it. The earliest documented interest in understanding surface texture by paying attention to the process that creates it dates back to the 1920s [48]. Around this time there was a feeling among engineers that smooth surfaces were what was needed and rough surfaces were far from ideal. And so Bentley in the UK began to manufacture their engines with very smooth cylinder bores. The result was that in the Le Mans 24 hour race their car engines seized, demonstrating conclusively that smoothness did not necessarily im-
Figure 1.1: An example of the Abbot-Firestone curve [1] (right) representing a surface profile.

ply good performance [21]. This incident and similar ones alerted the manufacturing community to the importance of the surface finish and stimulated the development of instruments.

Once this interest had started measurement instruments built specifically for this purpose soon arose. A dedicated stylus instrument was described in the early 1930s using an optical lever arrangement to record on photographic paper [11]. For this instrument the workpiece was traversed by a wedge shaped steel stylus while a skid traversed a reference surface of the same nominal curvature. Then these machines were built to present some kind of graphical feedback, with one of the first by Abbot and Firestone [1] representing the surface as a simple curve, see Figure 1.1, from which realistic numbers could be determined depending upon the surface application. This simple curve linked performance to contact and showed a plot of the material to air ratio of the surface as a function of depth.

After this emergence in instrumentation some very important literature in the field was published, most notably by the pioneer R. E. Reason et al. [51] and Schesinger [57].
amongst others [43], [58]. These works helped bring together the subject as a more formal discipline. With surface metrology becoming somewhat of a subject of interest types of surface roughness standard specimens were made commercially available [7]. The demonstration of digital computing in both theory [72] and practice [75] boosted the subject of surface metrology to an extent never envisaged. Advances in electronics and computing saw big advancements in post-measurement processing of data such as filtration [50], [26] and simulation of surface performance [66]. The digital age had been embraced and computers were increasingly used as part of the instrument [68], [9] in addition to being an invaluable tool for running surface analysis techniques [71].

1.2.3 Measurement Instruments

Stylus contact measurement instruments are still being used today, although they produce more than just a simple graphical output showing the peak and valley height information. They have advanced somewhat from these early examples and can now measure at the \( \text{nm} \) level that is traceable to national measurement standards [29]. The action of these instruments are quite similar whereby the stylus, usually diamond tipped, sends the trace of the traversed profile to a transducer to convert this vertical movement into an electrical signal. The co-ordinate values come from this signal. A stylus measurement instrument is a very sensitive piece of equipment and needs careful calibration [73].

Today a range of instruments are available for surface texture measurement, not just stylus orientated machines. A range of non-contact instruments exist that mainly consist of, but not limited to, one of the following kind:

- Laser Triangulation. This is one of the simplest non-contact measurement systems. It is relatively low cost, but offers poor resolution. It works by focusing a laser beam onto a surface and that illuminated point is imaged onto a position sensitive
device. This device is calibrated in terms of the surface height.

- Atomic Force Microscope (AFM). Strictly speaking this is a contact measurement instrument but due to the very low stylus force involved they are usually considered non-contact for practical purposes. The stylus for these instruments is made out of silicon and can be as small as 1nm in diameter. When the stylus tip is brought into proximity of a sample surface, forces between the tip and the surface lead to a deflection of the cantilever. It is important to note that it is these atomic forces that are being measured and not the vertical displacement of the stylus. Therefore, distortions are possible due to interactions between the surface and the probe. AFMs offer a high resolution but are notoriously difficult to calibrate.

- Scanning Interferometer. This uses conventional white light as its light source. A piezo drive system is used to scan the objective lens about a focal point. As the imaging system is traversed through its range the focal point is noted for each pixel in a charge coupled device (CCD) image sensor. The major benefit of this type of system is a lot of points can be measured with high resolution very quickly. However, the interaction of light with the sample can cause measurement errors can occur, especially for roughness measurement [17].

Currently only stylus contact instruments are included in international standards for surface texture measurement [14]. Even though limitations of the stylus instrument were documented as research progressed in this field [69], they are at present the most reliable and repeatable source of surface measurement data whilst recent studies have shown optical instruments to differ in their results by as much as 109% [52]. All real data used in this study is sourced from stylus instruments although the software developed is not specific for any type of instrument.
The surface profile results from the intersection of the real surface (see Appendix B) by a specified plane. A surface texture measuring instrument records the co-ordinates \((x, z)\) of points that represent the profile as it traces the stylus tip across the surface (see Figure 1.2), and applies software to filter the data (e.g. to separate the measured primary profile into waviness and roughness profiles) and compute various surface texture parameters that aim to describe properties of the surface. A typical profile consists of thousands of co-ordinate values.

The most common surface texture parameters in use today have been published as an ISO specification standard for surface texture profiles [15], which are the concern of this study, and are also being developed for areal surfaces [63] [64]. The standard for surface texture profile parameters, ISO 4287: 1997 [15] provides eleven different parameters for the quantification of different surface profile characteristics, of which nine are calculated from profile height measurements \((z\) data), one from profile spacing measurements \((x\) data) and one is a hybrid of both. ISO 4287 and the parameters published therein will be the focus of the next chapter.

Figure 1.2: Surface profile measurement by stylus instruments
1.2.4 Roughness, Waviness and Form

There are three main elements to the measured profile we get from a surface: roughness, waviness and form. These elements are rarely found in isolation and most surfaces are a combination of all three. Figure 1.3 illustrates how when these components are put together they make up the traced profile. It is usual to assess them separately. Roughness, waviness and form are defined as follows [49]:

- **Roughness**: This is the irregularities which are inherent in the production process.
Roughness is superimposed on the waviness.

- **Waviness**: This is usually produced by instabilities in the machining process, such as an imbalance in a grinding wheel, or by deliberate actions in the machining process. Waviness has a longer wavelength than roughness.

- **Form**: The overall shape of the surface, ignoring the variations that are contributed from roughness and waviness.

Surface texture can be considered to be what remains after the removal of the form element by best fit optimisations of the nominal form. This can be thought of as the dominating shape or angle of the profile, for example when measuring a spherical object it is favourable to ignore the curvature and only examine the surface as though it were flat. After form is removed from the measured profile we are left with the primary profile. The primary profile contains the roughness and waviness elements.

Each component is separated from one another by what is known as a profile filter with differing cut-off values (e.g. $\lambda_s$ and $\lambda_c$, see Appendix B.1.6). The filter suppresses certain wavelengths whilst retaining others. The roughness component is probably the most important as it is produced only by the method of manufacture resulting from the process rather than the machine. The roughness profile is the what we are concerned with in this document, however, the parameters and software discussed are generic to all profiles.

1.2.5 **Surface Texture Profile Parameters**

The use of a parameter to associate a numerical value to the measured topography of a surface was proposed many years ago (Hume [18] gives a brief history). A single numerical value allows different surfaces to be readily compared and facilitates the in-
interpretation of surface-texture tolerances on engineering drawings. During the period when parameters were being proliferated into the field the accuracy of the determination of these surface roughness parameters was bought into question as quick as they were being presented [55]. In time the strongest set of parameters were recruited into an international standard, in order to create a common group of parameters that everyone can share. The international standard previously mentioned is ISO 4287:1997, Geometrical Product Specifications (GPS) - Surface Texture: Profile method - Terms, definitions and surface texture parameters [15]. This means that this is the standard that specifies the terms, definitions and parameters to be used in the determination of surface texture profiles by stylus measurement instruments. Most of these are included in the Appendix for further reference.

1.3 Project Aims

There is an unmistakable trend towards miniaturisation in both the consumer market and for industrial applications. The advantages to the consumer are clear. Smaller means lighter weight for better portability, with less energy consumption, more functionality in the same space, and so on. In the industrial world, smaller means that systems are more robust, measurements can be made with little disturbance to the region of interest and generally small sensors are intrinsically safer than their conventional counterparts. The UK Government recently commissioned the Royal Society and the Royal Academy of Engineering to produce a report entitled Nanoscience and nanotechnologies: opportunities and uncertainties [62]. This report highlighted metrology as one of the key enabling technologies for the commercial and societal success of micro and nanotechnology. Therefore the reliance on qualitative measurement characteristics such as accuracy, correctness and reproducibility is becoming greater than ever.

The study described in this report is timely because a number of recent compar-
isons of surface texture measurements [32], [67] have shown some alarming spreads in the results, some differing by up 75%. It is difficult to say whether such variations are due to the instrument performance, the variation over the surface or the software employed to calculate the parameters. The consolidation and development of algorithms and software to compute surface texture parameters accurately with elements of numerical safety is the immediate focus of this study and will help to ensure that the uncertainty contribution caused by the software is minimised and well quantified.

To determine a numerical value for a surface texture parameter involves a number of stages including definition and interpretation of the parameter, measurement and analysis of the measurement data, as well as evaluating measurement uncertainty [36]. The use of a single numerical value to describe a certain property of a surface profile allows different surfaces to be readily compared, an example of this immediate comparability is given in Figure 1.4. The asymmetry of the amplitude distribution curves shown in the right of the figure can readily be seen, this difference is a measure of the skewness of the profile. The information conveyed by surface texture parameters is legitimate only if those parameters are based upon mathematically unambiguous definitions. In the absence of such a requirement it may be possible that these definitions could be understood in different ways. This will lead to different interpretations in the way the parameters should be calculated, and as a consequence, different software developers will implement mathematically different algorithms to compute the same surface parameter. Leach and Harris [31] have discussed one particular surface texture parameter, the two-dimensional spacing parameter, $RSm$, in order to illustrate the difficulties of interpreting such parameters unambiguously. It is shown that the ISO definition of the parameter is ambiguous and its evaluation open to interpretation. Such ambiguities in the definitions of surface texture parameters can lead to serious problems in ensuring traceability of surface texture measurement to national and international standards as well as in interpreting the functionality of a surface.
Results from this study [31] show that the $RSm$ parameter value can vary by nearly 10% simply by reversing the order of the data under examination.

However, this quantitative comparison between surfaces of one or many profile parameters are only meaningful if these values are accompanied by a statement of measurement uncertainty. Without this, the comparative property of parameters is essentially invalidated and differences between values cannot be regarded as significant. Ability to provide reliable statements of uncertainty are crucial in order to provide traceability of measurement to national and international standards.

This project was formulated under an Engineering and Physical Sciences Research Council (EPSRC) CASE Studentship supported by the National Physical Laboratory (NPL). This will feed into NPL’s programme in industrial metrology and surface
1.3.1 Parameter Definitions

The importance of mathematically unambiguous definitions for surface roughness parameters has already been introduced, most noticeably by Leach and Harris [31], and the current ISO standard was found to be guilty of possessing ambiguities in their definitions. Although the terms within the standard are explicitly described, ambiguity lies within the terms of their parameter definition. These terms, stated in section 3 of ISO 4287, are required for the evaluation of nearly all parameters in the standard, and in order to understand the functionality of the parameters it is necessary to evaluate these terms. The Appendix of this document includes the description of the terms, which include 'sampling length', 'profile element' and 'discrimination level'. In the process of translating the set of roughness parameters to software functions terms such as these described can be thought of as auxiliary or 'helper' functions and run the risk of being regarded as having a lower importance level than the main parameter functions. The evaluation of these functions in a mathematically unambiguous way are vital in striving for a reliable calculation for each parameter.

The standard defines the length of the profile being assessed as the 'evaluation length' and this may contain one or more 'sampling lengths'. A sampling length is a profile whose length in the x-axis is numerically equal to the characteristic wavelength of the profile filter $\lambda c$ (see Appendix B.1.8). This may seem very straightforward. However, what happens if the length of the profile that has been measured is not wholly divisible by a multiple of $\lambda c$? How should the evaluation and sampling lengths be determined when the measured profile is five and a half times the numerical value of $\lambda c$? It is obvious that some of the measurement needs to be discarded in this case in order to satisfy the standard definition, but what part of the profile should be discarded? The software developed for this study has been instructed to calculate the
maximum number of sampling lengths that are possible in the given roughness profile and extract them consecutively from the centre of the profile to ensure that an equal amount of data is discarded from each end of the measured profile. The difference in the values of the roughness parameters will probably be negligible no matter what part of the profile is disregarded, however, other terms are not as stable with respect to differing evaluations.

The research mentioned by Leach and Harris [31] concerning the value of the parameter $RSm$ showed that this parameter is heavily influenced by the process used to evaluate the term 'profile element'. A profile element is defined to be a profile peak and the adjacent profile valley, see Appendix B.2.3 for full description. In order to be acknowledged as a 'profile element' a profile peak and an adjacent profile valley must pass the height and spacing discrimination levels. The default value of these discrimination levels are that a profile element must be greater in width than 1% of
the sampling length and must be greater in height than 10% of the parameter \( R_z \). These discrimination levels are designed to eliminate 'insignificant' profile elements such as those highlighted in Figure 1.5, these are therefore not recognised in the division of profile elements \( X_{s1} \) to \( X_{s6} \). The standard does not, however, state the course of action when a detected profile element does not satisfy the discrimination levels. In Figure 1.5 it appears that they are merged into profile elements that are deemed significant rather than simply discarded, but what process should be followed when this occurs? Should such elements be merged into the next detected valid profile element or the previous? Results from [31] show substantial differences in results by implementing various approaches.

To complete the reference software library so that it is free from ambiguities for all functions, it may be necessary to implement formal methods such as those discussed in Scott [59] in order to solve the more complicated ambiguities contained in the 'profile element' term.

Commercial software packages for surface texture are very specialised products and tend to be developed independently of national institutions. The specific details of the algorithms used in these proprietary software packages are not made public and so any steps, if any, taken to avoid ambiguous definitions or other obstacles encountered in development are not known outside of the company. Despite the high price tag for such software the results from these commercial packages are usually far from being in agreement with software developed by national measurement institutions, even in current comparisons [35].
1.3.2 Softgauges

ISO 5436-2 [16] introduced into international standardisation the concept of the software measurement standard or softgauge in the context of the measurement of surface texture. The standard defines Type F1 softgauges (reference data) and Type F2 software measurement standards (reference software), and it is the latter definition that describes the product of this study.

Type F2 software measurement standards are reference software, that should be traceable computer software against which software in a measuring instrument can be compared. Type F2 software measurement standards are used to test the numerical correctness of software by inputting a common data set into both the software under test and the reference software and comparing the results delivered by the software under test with those obtained from the reference software.

1.3.3 Summary

To summarise, we can define the main aims of this study as:

• Highlight inadequacies and ambiguity in existing surface textures parameter definitions from the international standard, ISO 4287 [15].

• Develop and present suggestions to overcome highlighted deficiencies in the standard definitions.

• Establish a software library of sufficient quality that satisfies the requirements to become a Type F2 software measurement standard outlined in ISO 5436-2 [16] with the aim being encompassed into the softgauges project for the national measurement
Incorporate and propagate the uncertainty of measurement through the calculation of each parameter so a complete result with a statement of uncertainty can be given. (E.g. $10 \pm 2\mu m$ at a confidence level of 95%)

1.4 Structure of Thesis

In the first chapter we introduce metrology in general, outlining its importance in the world today. We give a brief description of the evolution of precision metrology up to the present day. We then introduce surface texture and what it is and how it occurs, with emphasis on the components that comprise surface texture (roughness, waviness and form). The need to measure surface texture is explained and why there is a need to measure it accurately. The measurement process using a stylus measurement instrument is described and the data that is gained through this process is presented. Finally the aim of this project is defined and why there is such a need for this work.

In chapter 2 we detail the published International Standardisation Organisation (ISO) standard associated with surface texture profile parameters, ISO 4287: 1997 [15]. Initial implementations utilising objects in MatLab are laid out and we discuss points noted about each parameter that concern the character of the parameter. In the final section of the chapter we analyse all aspects that affect the translation of the parameters into software. These include the ambiguity of definition for some parameters and also algorithms that are implied by ISO 4287 in the calculation of parameter but are not actually defined. This concludes with some remarks on the improvement of initial implementations.

In chapter 3 we develop a new algorithm for the interpolation of surface texture profiles. The purpose of this method is to improve upon the initial implementation of
the Amplitude Parameters (average of ordinates) and bring it closer to the definitions stated within the pages of ISO 4287. The need for this new method is presented along with the concept of natural cubic spline interpolants and the advantages of these constrained functions with respect to surface profiles are presented. We show that using a quadrature rule to calculate the definite integral of the absolute profile is an advantage over a simple summation. However, now that the profile is fitted with a continuous function we can calculate this integral exactly and dispose of such quadrature methods.

The work concerning surface profile data fitting is extended in chapter 4 as we detail the advantages of using such a technique. Some refinements to the data fitting method are described and the full process explained. It is also shown that using such a method can virtually eliminate the deficiency of the Gaussian filter with non-uniformly spaced points. A testing scheme is outlined and results presented.

For chapter 5 the surface texture parameters are given with respect to using the new interpolation routine that has been implemented.

Chapter 6 gives an outline of the evaluation of uncertainty in measurement. We show the analytical method that the Guide to the Uncertainty in Measurement provides for the evaluation of a standard combined uncertainty and why in some cases this method is not appropriate because its requirements are not always met by surface texture parameters. The use of Monte-Carlo simulation is presented as a numerical alternative to mainstream GUM.

Chapter 7 recites the aims of research and provides a summary for each section together with an explanation of the evolution of research and aims fulfilled. The software developed is outlined and why the research has produced many advantages
for the field of software development for surface texture metrology. The possibilities of further work that extend upon the study in this document are described.
2 Surface Texture Profile Parameters

2.1 Parameters

Since an interest in surface measurement began there have been methods to quantify certain aspects of a surface. It would be ideal if every surface could be assigned a number that completely characterises its roughness component, thus removing the need for a subjective assessment. However, no single value can convey the complexities of a surface and, therefore, a series of descriptors, or parameters, are needed.

A surface parameter can be thought of as a function of the surface profile (in the case of two-dimensional measurement). A set of parameters can give us a readily comparable group of values that quantify certain aspects of the surface. Surfaces that are manufactured can be produced in a large number of ways, with surface roughness parameters historically developed nationally to fulfill specific needs in specialist industries. The introduction of computers and the continual advancement of technology gave engineers and academics the chance to develop numerous parameters during the 1980s. The outbreak of these parameters, many poorly defined and of limited use, was appropriately called a 'parameter rash' by Whitehouse [70].
2.1.1 Reference Software Library

In this chapter we detail the most common surface texture parameters in use today, namely those that have been published by the International Organization for Standardization (ISO) for use with two-dimensional profiles. This standard, ISO 4287: 1997 [15] provides eleven different parameters for the quantification of different surface profile characteristics, of which nine are calculated from profile height measurements ($z$ data), one from profile spacing measurements ($x$ data) and one is a hybrid combination of both. Initial implementations, utilising objects in MatLab, are described and we discuss points noted about each parameter that concern the character of the parameter. With an object-oriented approach, a set of properties and functions associated with each other, in this case a roughness profile’s $x$ and $z$ coordinate and parameter values, are referenced through a single entity, the roughness profile object. For such a purpose the $RProfile$ object class was created to encapsulate the parameter functions, profile co-ordinates and other attributes of a roughness profile. The purpose of these initial implementations is to familiarise ourselves with these international standard parameters which are the focus of subsequent chapters. A glossary of terms used in this chapter is included in Appendix B.

This code library has been specifically designed so that it can be extended throughout the course of future research to include such advancements as uncertainty evaluation, which is beyond the scope of the software produced in this study. Utilising an object-oriented approach, a set of properties and functions associated with each other, in this case a roughness profile’s $x$ and $z$ coordinate and parameter values, are referenced through a single entity, the roughness profile class. For such a purpose the $RProfile$ object class was created to encapsulate the parameter functions, profile coordinates and other attributes of a roughness profile.
In the process of developing this software library issues concerning numerical stability in calculation were observed. For example, many of the parameters involve a summation of profile ordinate values, these are usually very high (but finite) in precision and very large in number, and as a consequence when summing a set of such numbers a certain amount of rounding error can occur. This error is introduced when the partial sum becomes a certain order of magnitude larger than the next number in the addition procedure due to the limitation that a computer can only store values to a certain number of significant figures. For instances where this occurs Kahan’s method for accurate computer addition [23] has been introduced. Although the process increases computation by a factor of four, it yields more accurate results when adding very large and very small numbers together.

2.1.2 RProfile Object Constructor

The interface for the RProfile class constructor is presented in Appendix A.1. It can be seen that the return variable r is of type RProfile. This format is shown here as the descriptions for all profile parameters in this chapter are defined as methods of the RProfile class. This class is instantiated by a pair of vectors, the x and z coordinate values defining the roughness profile. In addition to the coordinate vectors there is the option to create an instance of an RProfile object with the numerical value of the \( \lambda_c \) profile filter that was used to derive the given profile. To create an instance of the RProfile class, \( r \), the following command should be invoked at the MatLab command line:

\[
\text{r} = \text{RProfile}(x,z,L_c)
\]

The last argument, \( L_c \), relating to the \( \lambda_c \) value is optional. The other two arguments correspond to the coordinate vectors and are compulsory.

The roughness parameter values can then be accessed by invoking the respective
parameter function of the object. The functions for roughness parameter all have a get prefix with the parameter name that is stated in ISO 4287:1997. For example, to retrieve the value(s) for the mean deviation of the assessed profile parameter $Ra$ then the command will be:

$$Ra = \text{getRa}(r)$$

where $r$ is an $RProfile$ object, this is always the first argument of a 'get' function. Some parameters have other arguments, compulsory or optional, that may have to be submitted to the function such as discrimination levels.

### 2.2 Parameter Definitions and Algorithms

#### 2.2.1 Amplitude Parameters (Peak to Valley)

All of the following parameter functions except for $Rt$ return a row vector of values, one value for the parameter function in each sampling length and the last index being the mean of all those values.

**Maximum profile peak height, $Rp$**

This parameter is the largest profile peak height $Zp$ within the sampling length, this being the height of the highest point or peak of the profile from the mean line. So in a given data set of $x$ and $z$ points $Rp$ would return the highest value achieved in the $z$ data set, see Figure 2.1. This value is especially sensitive to sharp spikes in the profile data (e.g. poor material processing).

**Minimum profile valley depth, $Rv$**

This parameter is the largest profile valley depth $Zv$ within the sampling length, this being the distance between the lowest point or valley of the profile from the
mean line. In a given data set of $x$ and $z$ points $Rv$ would return the absolute of the lowest value achieved in the $z$ data set ($Rv = |\min(z)|$). This value, as with $Rp$, is especially sensitive to extreme values in the profile data (e.g. scratches, cracks).

Given the same data set as featured in figure 2.1, the value of $Rv$ would return the value as $Rp$. ($Rv = Rp = 1$ for the given data set).

Maximum height of profile, $Rz$

This is the sum of the largest profile peak height $Zp$ and the largest profile valley depth $Zv$ within the sampling length, being the distance between the largest and lowest points of the profile. In the data set of $x$ and $z$ the value of $Rz$ would be the sum of the highest and the lowest points achieved in the $z$ data set which is also the sum of the parameters $Rp$ and $Rv$ ($Rz = \max(z) + |\min(z)| = Rp + Rv$).

![Figure 2.1: The points where $z = Rp$ on the sample data set are highlighted ($Rp = 1$).](image)
Mean height of profile elements, $R_c$

The ISO standard defines $R_c$ to be the mean value of the profile element heights $Z_t$ within a sampling length. Expressed mathematically,

$$R_c = \frac{1}{m} \sum_{i=1}^{m} Z_{t_i},$$

where $m$ is the number of profile elements in a sampling length. This implementation of $R_c$ invokes the height and spacing discrimination levels described in the standard which is controlled within the private function called within $R_c$, profileElements. If no tolerance levels are passed to the function the default height discrimination used shall be 10% of $R_z$ and the default spacing discrimination shall be 1% of the sampling length. Both of these arguments are optional, but if the spacing discrimination is to be set then so must the height discrimination. However, the height discrimination can be given without the spacing discrimination, in this case the spacing level will be set to the default (1% of sampling length).

Total height of profile, $R_t$

This is the sum of the largest profile peak height $Z_p$ and the largest profile valley $Z_v$ within the evaluation length. This parameter does not yield the same result as $R_z$. For $R_z$ is concerned with the sampling length and $R_t$ is the result over the evaluation length. Because of this $R_t \geq \max(R_z)$ will always be true for any profile.

This parameter returns a single value and not a vector and is not necessarily equivalent to the maximum value from the output of $R_z$, but is equivalent to $\max(R_p) + \max(R_v)$. 
2.2.2 Amplitude Parameters (Average of Ordinates)

All of the following parameter functions return a row vector of values, one value for the parameter function in each sampling length and the last index being the mean of all those values.

Arithmetical mean deviation of the assessed profile, \( Ra \)

This is the arithmetical mean of the absolute ordinate values \( Z(x) \) within the sampling length. Expressed mathematically,

\[
Ra = \frac{1}{l} \int_{0}^{l} |Z(x)| \, dx,
\]

where \( l \) is the sampling length. The result of this function is shown in Figure 2.2.

The \( Ra \) value does not provide any information as to the shape of the irregularities on the surface and it is possible to obtain similar values for surfaces having very different profiles.

Root mean square deviation of the assessed profile, \( Rq \)

\( Rq \) is the root mean square of the ordinate values \( Z(x) \) within the sampling length. Expressed mathematically,

\[
Rq = \sqrt{\frac{1}{l} \int_{0}^{l} Z(x)^2 \, dx},
\]

where \( l \) is the sampling length. This is the root mean square of the departures from the mean line of the profile.

When compared to the arithmetic average \( Ra \), as shown in Figure 2.2, the root mean square parameter has the effect of giving [28] extra weight to the numerically higher values of surface height. The \( Ra \) parameter is widely used in machining specifications.
Figure 2.2: Graphical deviation of $Ra$ and $Rq$ using the MatLab function on the sample data. ($Ra = 0.6236$, $Rq = 0.7027$).

since the current implementation is a very simple calculation. $Rq$ is more robust and is widely used in optical applications where it is more directly related to the optical quality of a surface.

*Skewness of the assessed profile, $Rsk$*

This is the quotient of the mean cube value of the ordinate values $Z(x)$ and the cube of $Rq$ within the sampling length, $l$. Expressed mathematically

$$ Rsk = \frac{1}{Rq^3} \left[ \frac{1}{l} \int_0^l Z(x)^3 dx \right]. $$  \hspace{1cm} (2.4)

The skewness is derived from the amplitude distribution curve; it is the measure of the profile symmetry about the mean line. This parameter represents the degree of bias in either the upward or the downward direction of an amplitude distribution.
Figure 2.3: Test data profile with the amplitude distribution curve showing the positive skew in $Rsk$ value of the data introduced by the addition of noise. (Compared with original test data profile in Figure 2.1)

The direction of skew is dependent on whether the bulk of the material is above or below the mean line and will result in negative or positive skew respectively. This parameter is strongly influenced by isolated peaks or valleys and can distinguish between two profiles having the same $Ra$ value.

Using the function on the test data gave a result which was equivalent to zero to sixteen decimal places as the data used was almost identical on both sides of the mean line. However when noise was added to the data this value became equal to 0.1 (to 2 decimal places) therefore a small amount of skewness was added with the noise, as shown in Figure 2.3.

**Kurtosis of the assessed profile, $Rku$**

This is the quotient of the mean quartic value of the ordinate values $Z(x)$ and the fourth power of $Rq$ within the sampling length, $l$. Expressed mathematically

$$Rku = \frac{1}{Rq^4} \left[ \frac{1}{l} \int_0^l Z(x)^4 dx \right]. \quad (2.5)$$

This parameter can not only detect whether the profile spikes are evenly distributed but also provides the measure of the sharpness of the profile. A spiky surface will have
a high kurtosis value and a bumpy surface will have a low kurtosis value, however this parameter cannot tell the difference between a peak or a valley.

The difference between the two sets of test data was almost 0.5. The addition of noise increased the kurtosis value and this can easily be seen in the comparison of the two data sets (Figure 2.4), with the noise added data being the more spiky profile.

2.2.3 Spacing Parameters

Mean width of the profile elements, RSm

This is the mean value of the profile element widths Xs within a sampling length. Expressed mathematically,

\[ RSm = \frac{1}{m} \sum_{i=1}^{m} Xs_i \]  \hspace{1cm} (2.6)

where \( m \) is the number of profile elements in the sampling length. This implementation of \( RSm \) invokes the height and spacing discrimination levels described in the standard. This is controlled within the private function called within \( RSm \), profileElements. If no tolerance levels are passed to the function, the default height discrimination used is 10% of \( Rz \) and the default spacing discrimination is 1% of the sampling length. Both of these arguments are optional, but if the spacing discrimination is to be set then so must the height discrimination. However, the height discrimination can be given without the spacing discrimination, in this case the spacing level will be set to the default (1% of sampling length).

The value of the \( RSm \) parameter for the original data set was calculated as 6.2832. This is correct, as one wavelength for the sine function is \( 2\pi \), and no elements fell below the discriminations levels. When an element is found not to meet the discrimination levels there is a 'grey' area in the standard, as it does not state how to proceed.
Figure 2.4: The two test data sets with detected profile elements highlighted. The $RSm$ parameter would be the mean value of the sum of the width of these elements.

Should this element be eliminated from the profile, or should it be merged into the other elements, and if so then into which one? The way that this is implemented will have an effect on the outcome of the $RSm$. Additionally the standard does not state whether the peak and valley events have to pass the discrimination levels separately or together. This function for $RSm$ tests for the discrimination level on the combined peak and valley events, namely the profile element as a whole. When an element is found not to pass the test for the discrimination level then will keep looking until it does and merges the failed element into the next element that passes, see profileElements for additional ambiguities.
2.2.4 Hybrid Parameters

Root mean square slope of the assessed profile, $R\Delta q$

This is the root mean square value of the ordinate slopes $dZ/dX$ within the sampling length. ISO 4287 does not provide us with a formula for $R\Delta q$, however, taking the ordinate slopes as the tangent between each measured point we could express it mathematically as

$$R\Delta q = \sqrt{\frac{1}{m} \sum_{i=1}^{m-1} \left( \frac{Z_{i+1} - Z_i}{X_{i+1} - X_i} \right)^2},$$

where $m$ is the number of measured points in a sampling length. However, this formula is not presented in ISO 4287 and the subsequent calculation of this parameter can differ depending on the method used to compute the 'ordinate slopes $dZ/dX$'. This method could be one of many difference formulae [3] available for such a problem and equation (2.7) shows a simple point to point interpolation method to compute the slopes in question. The parameter depends on both amplitude and spacing and is therefore a hybrid parameter. The slope of the profile is the angle it makes with a line parallel to the mean line.

This function produced the largest difference between the values given for each data set. The values were 0.6998 and 1.5644 for the original and noise added data, respectively. The noise produces a more varying surface with many outliers than before and so the gradients at many points will be greater in contrast to the smoother curve of the sine function.
2.3 Problems with ISO Definitions

2.3.1 Implied Functions

The ISO standard defines the eleven parameters that have been presented previously. However, these are not the only functions that need to be implemented if we wish to develop even the most basic software for surface profile parameters. Here we present three auxiliary algorithms needed to accompany the set of parameter algorithms.

Sampling Length Dissection Algorithm

This function splits the given evaluation length $x$ with its respective profile values $z$ into five sampling lengths equal to the numerical value of the wavelength of the profile filter $Lc$. Alternatively, if five equal sampling lengths cannot be made, then it splits the profile into as many equal samples of length $Lc$ as possible. If not all of the data values in the vectors $x$ and $z$ are used in the process of splitting them into sampling lengths, then the data values used for the sampling lengths will be taken from the middle of the $x$ and $z$ vectors (an equal number of points are discarded from each end of the vectors).

Profile Element Detection Algorithm

Given a set of sampling length data points as two column vectors this 'helper' function returns a two column matrix that contains the start and end points of each profile element in the sampling length. A profile element is determined when the profile crosses the mean line ($z = 0$) and subsequently crosses it again in the same direction. Each element is represented by a separate column in the returned matrix with $x$ ordinate starting point in the first column and $x$ ordinate finishing point of each profile element in the second column.

Each profile element detected must meet both height and spacing discrimination lev-
els. Any element found not to be of the given percentage of $R_z$ (default 10%) in total height or found not to be of a given percentage of the sampling length (default 1%) in width shall be rejected and merged into the subsequent profile element found that passes the discrimination bands.

Profile Element Extraction Algorithm

Given a set of sampling length data points as two column vectors this 'helper' function returns a two column matrix that contains the start and end points of each profile element in the sampling length. A profile element is determined when the profile crosses the mean line ($z = 0$) and subsequently crosses it again in the same direction. Each element is represented by a separate column in the returned matrix with $x$ ordinate values in the first column and $z$ ordinate values in the second.

2.3.2 Ambiguity of Definition

The information conveyed by surface texture parameters is legitimate only if those parameters are based upon mathematically unambiguous definitions. In the absence of such a requirement it may be possible that these definitions could be understood in different ways. This will lead to different interpretations in the way the parameters should be calculated, and as a consequence, different software developers may implement mathematically different algorithms to compute the same surface parameter. As previously mentioned for the case of $RS_m$ the study carried out by Leach and Harris [31] highlights that it is not only the parameter definition where ambiguities arise but also in the aforementioned implied functions. Many parameters rely considerably on the safe calculation of these functions that are not outlined for an accurate result.

In Section 4.2 of ISO 4287: 1997 [15], four amplitude parameters are defined and all require the evaluation of a definite integral over the sampling length (a length of
the measured surface profile). Surface profiles are measured discretely and, therefore, these parameters can only be evaluated approximately, by methods not stated in the ISO literature. This point in particular is the direct focus of the next chapter.

2.3.3 Measurement Uncertainty

A measurement is only complete if it is accompanied by a statement of uncertainty in the measurement. It is no different when providing the value for a calculated surface texture parameter, without which it is difficult to assess whether the difference in the results obtained from two interpretations of the same parameter is critical to understanding the surface being measured. A number of recent comparisons of surface texture measurements have shown some alarming spreads in the results [32] and it is difficult to say whether such variations are due to the instrument performance, software employed to calculate the parameters or whether it could have been explained if the parameter values were coupled with a statement of uncertainty. The authoritative document published by ISO that addresses the fundamental principles of the problem of uncertainty evaluation is the Guide to the Expression of Uncertainty in Measurement [19], affectionately known as the 'GUM'. However, the methodology that is covered in this guide is not sufficient to apply to the complex nature of surface texture measurement. The aspect of the uncertainty in measurement is a complex topic in itself and will be re-visited later in this document.

2.4 Summary

The standard definitions for surface texture profile parameters have been presented and annotated. The main flaws associated with definitions have been highlighted in order to show areas where they can be improved. It has become obvious that the main deficiency is caused by using a definite integral in the definition of a function for discrete data. Therefore this is the focus of the next chapter.
3.1 Amplitude Parameters (Average of Ordinates)

In this chapter the focus is upon one section of the international standard, ISO 4287:1997 [15], that was discussed in the previous chapter. In Section 4.2 entitled Amplitude parameters (average of ordinates) of this standard four parameters are defined, all of which were introduced in the previous chapter. These parameters $Ra$, $Rq$, $Rsk$ and $Rku$ all require the evaluation of the definite integral of profile elements in their formulae which follow the format

$$Ra_{(k=1)}, Rq_{(k=2)} = \left( \frac{1}{l} \left( \int_{0}^{l} |z(x)|^k \, dx \right) \right)^{1/k},$$

(3.1)

and

$$Rsk_{(k=3)}, Rku_{(k=4)} = \frac{1}{Rq^k} \left( \frac{1}{l} \left( \int_{0}^{l} |z(x)|^k \, dx \right) \right)^{1/k},$$

(3.2)

where $l$ is the profile sampling length. As previously stated surface profiles are measured discretely and, therefore, the way these parameters are declared mean they can only be evaluated approximately. The approximation as a discrete sum of one parameter, $Ra$, from definite integral to discrete function is given by
This process of numerical quadrature introduces a certain amount of discretisation error [39]. The total error from this approximation (3.3) is made up of truncation and rounding errors. Truncation error arises from reducing the real surface profile into a number of discrete points and then approximating the definite integral at these intervals. This area does not fit exactly to the definite integral of the real surface profile. Introducing a sum and division into the calculation causes rounding errors when computed as the results are taken to a certain number of significant figures at each step in these procedures. This has been reduced by using Kahan’s famous summation algorithm for computer addition [23] in the function where needed. This algorithm significantly reduces the numerical error in the total obtained by adding a sequence of finite precision floating point numbers, compared to the obvious approach of plain addition. This is done by keeping a separate running compensation as a variable to accumulate small errors. Kahan was the primary architect behind the IEEE standard for binary floating-point arithmetic, IEEE 754-1985 [42].

The $Ra$ value is defined to be the arithmetical mean deviation of the assessed profile, graphically represented in Figure 3.1. The surface texture parameters are designed to assign a value to a specific property of the surface profile, not assign a value to a specific property of the measured (digitised) surface profile. However, in the world we live in all we have to work with is this discrete measured profile. As a result the best that can be done is provide an approximation to this value. However, this is not what is wanted by these parameters and so it is important to estimate the underlying real surface profile and its integral, and subsequently the error bounds associated with this approximation.
3.1.1 The Current Implementation

Currently the function used for $Ra$ (also $Rq$, $Rsk$ and $Rku$) follows the discrete function given in equation (3.3) for approximating the definite integral. The value returned by this function is illustrated in Figure 3.2 as the sum of the area of the coloured bars.

This function seems rather crude although it appears to be the most common implementation in use today [60] and is defined using this method in leading guides to surface texture measurement [28], [37]. It appears obvious that this implementation must be improved in order to be closer to the format stated in the standard (3.1), this can be achieved by providing a better approximation to the definite integral. All parameters in this section of the standard are based upon this discrete summation formula and, therefore, all of the implementations for these parameters can be im-
proved.

One of the major flaws with this function is that it completely ignores the relationship between the measured profile points. If this surface from which the profile was measured is thought of as the underlying function, $f$, to the set of $n$ measured profile points then we could say that this set is $f(x)$ where $0 \leq x \leq l$ sampled at $n$ points. If the cosine function is the underlying surface profile and we measure at every interval of $\pi$, and apply our function of $Ra$ to the measured points this would
give an incorrect result of 1, see Figure 3.3. The true result should be $2/\pi$, however, making the most of the data points that we have in our profile to produce the absolute profile (Figure 3.3, bottom graph) a closer result of 0.5238 could be achieved.

The current function does not take into account the points where the profile crosses the mean line, or more accurately (because the data is discrete) it does not take into account the points where it is implied that the profile crosses the mean line. To maximise the reliability of these amplitude parameter values it is essential that the greatest amount of information is extracted from the profile points given in order to
create, to the best of our knowledge, a solid platform on which to evaluate surface texture parameters. Due to the fact that surface profile data is discrete, a reliable and accurate method of quadrature needs to be applied in order to provide a reliable and accurate estimate of the integral. It is obvious that this is a primitive computation and can be improved by looking into other methods of quadrature.

### 3.2 Quadrature Algorithms

Three of the numerical techniques that exist to help solve this problem of quadrature are the Trapezoidal rule, Simpson’s rule and Romberg integration. The aim here is to provide a brief introduction of these concepts and an implementation of them for determining surface texture parameters. The following definitions and equations for this sections are well established and can be found in many texts on the subject such as that by Mason.\textsuperscript{83}

#### 3.2.1 The Trapezoidal Rule

The function $f(x)$ is approximated between $a$ and $b$ by a straight line. The integral is approximated by the area of the trapezium under the line. Therefore the approximate value of the integral is given by:

$$I \approx \frac{1}{2} \left( f(a) + f(b) \right) (b - a).$$

\textit{Truncation Error}

To obtain an estimate of the error for this rule, it is shown that the trapezoidal rule effectively approximates $f(x)$ by its Lagrange interpolating polynomial of degree 1. The error in approximating a function $f$ by a Lagrange polynomial of degree $n$ (provided the first $n + 1$ derivatives are continuous) is given by the following equation
\[ e_n(x) = -\frac{f^{(n+1)}(\xi_x)}{(n+1)!} \prod_{i=0}^{n}(x-x_i), \]  

(3.5)

where \( x_i \) \((i = 1, \ldots, n)\) are the tabular points and \( \xi_x \) lies somewhere in \((a, b)\). It is assumed that \( f, \, f' \) and \( f'' \) are continuous on \([a, b]\) then for the case of fitting a polynomial of degree 1 between two tabular points \( a \) and \( b \) this is

\[ e_1(x) = -\frac{1}{2} f''(\xi_x)(x-a)(x-b), \]  

(3.6)

where \( \xi_x \) lies somewhere in \((a, b)\). (For \( x \in [a, b] \), \( x - a \geq 0 \) and \( x - b \leq 0 \), so if \( f'(\xi) \geq 0 \), then \( e_1(x) \geq 0 \).) The error in estimating \( \int_a^b f(x)dx \) by the integral of an interpolating polynomial of degree 1 is equal to the integral of the error function, \( E \).

\[ E = \int_a^b e_1(x)dx. \]  

(3.7)

Let \( m \) be the minimum value of \( |f''(x)| \) in \([a, b]\), and \( M \) the maximum value (i.e. \( m \leq |f''(x)| \leq M \) for \( x \in [a, b] \)). Therefore by equation (3.6)

\[ -\frac{1}{2} m(x-a)(x-b) \leq |e_1(x)| \leq -\frac{1}{2} M(x-a)(x-b) \quad x \in [a, b]. \]  

(3.8)

Integrating the previous inequality this gives

\[ \int_a^b -\frac{1}{2} m(x-a)(x-b)dx \leq |\int_a^b e_1(x)dx| \leq \int_a^b -\frac{1}{2} M(x-a)(x-b)dx. \]  

(3.9)

The result of evaluating the integrals is

\[ \frac{1}{12} m(b-a)^3 \leq |E| \leq \frac{1}{12} M(b-a)^3. \]  

(3.10)

Since \( f'' \) is continuous on \([a, b]\), \( |f''(x)| \) must take all values between \( m \) and \( M \). Therefore there is some \( \xi \in (a, b) \) such that
In general the value $\xi$ is unknown. However, an upper bound of $E$ can be found by substituting $\max_{a \leq x \leq b} |f''(x)|$ for $f''(\xi)$ in equation (3.11).

The Composite Trapezoidal Rule

For this rule, the interval $[a, b]$ is divided into $n$ subintervals, all of equal width. The width of each subinterval is

$$h = \frac{b - a}{n}. \quad (3.12)$$

The trapezoidal rule is then applied to each subinterval. This gives

$$\int_{a}^{b} f(x)dx = \frac{1}{2}(f_0 + f_1)h + \frac{1}{2}(f_1 + f_2)h + \ldots + \frac{1}{2}(f_{n-1} + f_n)h - E_n, \quad (3.13)$$

from which

$$\int_{a}^{b} f(x)dx = \frac{h}{2}(f_0 + 2f_1 + 2f_2 + 2f_{n-1} + f_n) - E_n, \quad (3.14)$$

where the truncation error $E_n$ is dependent on the number, $n$, of subintervals. By using equation (3.11) the total error in applying the trapezoidal rule to each subinterval $[x_{i-1}, x_i]$ is given by

$$E_n = \sum_{i=1}^{n} \frac{1}{12} f''(\xi_i)h^3, \quad (3.15)$$

where $\xi_i$ is in $[x_{i-1}, x_i]$ for each $i$. Since $f''$ is continuous then there must exist a number $\xi$ between $a$ and $b$ for which $f''(\xi)$ is equal to the average of the values of the $f''(\xi_i)$, i.e.

$$f''(\xi) = \frac{1}{n} \sum_{i=1}^{n} f''(\xi_i). \quad (3.16)$$
From this we have \( \sum_{i=1}^{n} f''(\xi_i) = nf''(\xi) \), and remembering (3.12) we can write (3.14) as

\[
E_n = \frac{h^3}{12} \sum_{i=1}^{n} f''(\xi_i) = \frac{h^3}{12} (nf''(\xi)) = \frac{1}{12} \left( \frac{(b-a)^3}{n^3} \right) (nf''(\xi)) \quad (3.17)
\]

\[
= \frac{1}{12} (b-a) \left( \frac{(b-a)^2}{n^2} \right) f''(\xi) \quad (3.18)
\]

\[
= \frac{1}{12} (b-a) h^2 f''(\xi). \quad (3.19)
\]

**Upper Error Bound on the Truncation Error**

If \( M \) is the maximum value of \(|f''(\xi)|\) for \( \xi \in [a, b] \), then an upper bound for the absolute value of the truncation error in using the composite trapezoidal rule can be given as

\[
|E_n| \leq \frac{1}{12} (b-a) M h^2 \quad \text{where} \quad M = \max_{a \leq \xi \leq b} |f''(\xi)|. \quad (3.20)
\]

This value can be used as the uncertainty boundary of the result from calculating the definite integral using the composite trapezoidal rule. It is an indication of amount of uncertainty introduced from applying this function to the profile values.

### 3.2.2 Simpson’s 1/3 Rule

Here, the underlying function \( f \) is approximated by the quadratic curve through the points \( a \) and \( b \) and the midpoint of the interval and usually provides greater accuracy over the trapezoidal rule.

\[
\int_{a}^{b} f(x) dx \approx \frac{(b-a)}{6} \left( f(a) + 4f \left( \frac{b-a}{2} \right) + f(b) \right). \quad (3.21)
\]

The composite version of Simpson’s 1/3 rule is obtained by dividing \([a, b]\) into an even number, \( n \), of equal subintervals each of width \( h \). Simpson’s rule is applied to the first pair of subintervals, then the next pair and so on, to give
\[ I = \int_{a}^{b} f(x)dx \approx \frac{h}{6} \left( f_0 + f_n + 4(f_1 + f_3 + \ldots + f_{n-1}) + 2(f_2 + f_4 + \ldots + f_{n-2}) \right). \quad (3.22) \]

**Upper Error Bound on the Truncation Error**

If \( M \) is the maximum value of \(|f^{(4)}(\xi)|\) for \( \xi \in [a, b] \), then an upper bound for the absolute value of the truncation error in using Simpson’s 1/3 rule can be given as

\[ |E_n| \leq \frac{1}{180} (b - a) M h^4 \quad \text{where} \quad M = \max_{a \leq \xi \leq b} |f^{(4)}(\xi)|. \quad (3.23) \]

However the need to evaluate the term \( f^4(\xi) \), the fourth derivative of the underlying function, cannot be fulfilled due to the nature of the underlying function being cubic. Simpson’s 1/3 rule is therefore here purely for completion sake and no more detail of the truncation error bound will be provided.

### 3.2.3 Romberg Integration

Whichever technique of quadrature is chosen, some method is required for determining what number \( n \), of subintervals, will give an estimate of the integral \( I \) to the required level of accuracy. The most straightforward method is to calculate an estimate using \( n \) subintervals, \( I_n \), then another using twice the number of subintervals (effectively halving the step size \( h \)), \( I_{2n} \). However, this method could be subject to a phenomenon called consistent inaccuracy whereby two successive estimates agree to within a specified accuracy and neither is close to the true value of the integral.

Romberg’s method [54] provides a more effective method is to exploit the nature of the truncation error in quadrature techniques in order to obtain better algorithms. This method generates a triangular formation of numerical estimates of the definite
Figure 3.4: Graphic comparison of quadrature methods. The top figure showing the Mid-point rule which is what the current implementation (3.3) uses. The middle figure illustrates the trapezoidal rule and the bottom figure Simpson’s rule.

integral by using Richardson extrapolation [53] repeatedly on the trapezium rule. A more specific form of the error in the trapezium rule may be shown to be

\[ I = T_n + c_1 h^2 + c_2 h^4 + c_3 h^6 + \ldots + c_k h^{2k}. \]  

(3.24)

Where before, the error, \( E_n \), associated with the Trapezoidal rule using \( n \) subintervals was expressed finitely, in (3.15) its negative, \(-E_n\), is now expressed as the infinite series \( c_1 h^2 + c_2 h^4 + c_3 h^6 + \ldots \). If the step size, \( h \), is small then in this series the largest contributor to the error is \( h^2 \), \( h^4 \) gives the next largest and so on. If the number of
subintervals, \( n \), is doubled then it follows that \( f(x) \) is a ‘sufficiently smooth’ function.

\[
I = T_{2n} + c_1 \left( \frac{h}{2} \right)^2 + c_2 \left( \frac{h}{2} \right)^4 + c_3 \left( \frac{h}{2} \right)^6 + \ldots + c_k \left( \frac{h}{2} \right)^{2k} \tag{3.25}
\]

\[
= T_{2n} + \frac{1}{4} c_1 h^2 + \frac{1}{16} c_2 h^4 + \frac{1}{64} c_3 h^6 + \ldots + \frac{1}{2^{2k}} c_k h^{2k}. \tag{3.26}
\]

By combining both of these estimates in a weighted average calculation by subtracting (3.24) from four times (3.25) the error term of \( h^2 \) can be eliminated

\[
3I = (4T_{2n} - T_n) + c_1 \frac{3}{4} h^4 + c_2 \frac{15}{16} h^6 + \ldots + c_k \frac{2^{2(k-1)} - 1}{2^{2(k-1)}} h^{2k}. \tag{3.27}
\]

Divide this by three and the estimate, \( I \approx (4T_{2n} - T_n)/3 \), is achieved with error \( O(h^4) \).

By combining two Trapezoidal results of \( O(h^2) \) accuracy, a new result is obtained of \( O(h^4) \) accuracy. Applying the Romberg method first eliminates the contribution to the error provided by the \( h^2 \), then the \( h^4 \) term and so on. Repeating this method again by labelling

\[
T^{(0)}_n = T_n, \quad T^{(1)}_n = 4T^{(0)}_{2n} - T^{(0)}_n, \tag{3.28}
\]

and in the same way as before combine the two results \( T^{(1)}_n \) and \( T^{(1)}_{2n} \) to eliminate the \( h^4 \) error term and produce a new estimate with error \( O(h^6) \)

\[
I \approx \frac{4^2 T^{(1)}_{2n} - T^{(1)}_n}{4^2 - 1} = \frac{16T^{(1)}_{2n} - T^{(1)}_n}{15}. \tag{3.29}
\]

This process may be repeated indefinitely where the general formula is as follows

\[
I \approx T^{(j)}_n = \frac{4^j T^{(j-1)}_{2n} - T^{(j-1)}_n}{4^j - 1} \quad (j = 1, 2, 3, \ldots), \tag{3.30}
\]

with error \( O(h^{2j+2}) \). This method is only valid when \( f(x) \) can be differentiated to an appropriately high degree. Also it is only really applicable for values of \( n \) that are ‘sufficiently large’, if a small value of \( n \) is used, say \( n = 1 \) or \( 2 \) then repeated Romberg steps may not improve the estimate significantly but they will not worsen it. The
value of \( n \) for surface profile will nearly always be in the ‘sufficiently large’ category because of the high number of measured profile points and therefore the number of intervals will also be.

### 3.2.4 Improving the Current Implementation

When implementing a technique of quadrature for a set of discrete data, it has been shown that a value for the error bound can be computed. This means that the ‘true’ value for the integral over the interval lies within the boundary of the calculated result plus, or minus, the absolute value given for the error bound, thus

\[
I^* - E \leq I \leq I^* + E, \tag{3.31}
\]

where \( I^* \) is the calculated result and \( E \) the error bound. This could be interpreted as a statement for algorithmic uncertainty when using this particular process of quadrature, i.e. the integral over the interval given by this process is \( I^* \pm E \) at confidence level of 100%. However, these error bounds are usually derived from knowledge of the underlying function and its derivatives. In the case of a surface profile there is no such function that dictates where the profile points lie.

If there is an underlying function to the measured profile then new possibilities would arise. For instance, we could resample the profile at much smaller intervals thereby achieving a much more accurate estimation by use of quadrature. By applying some method of data fitting to the profile that interpolates the points then this could be achieved, but only if the data fit is sensible for this purpose and reliable to compute. The remainder of this chapter details the process of these improvements.
3.3 Profile Data Fitting

In the previous section the possibility of interpolating the discrete measured profile point was introduced as the application of some method of data fitting to our measured profile points would provide new possibilities. This would effectively 'replace' our discrete set of points with a continuous representation of the measured profile.

It was also outlined that in order to fit an underlying function to a series of surface profile points then it must obey the following criteria:

- **Interpolate measured points** - The fitted function must pass through all of the measured points in order to preserve the characteristics of the profile. Not fulfilling this requirement will mean that some peaks, valleys or points where the profile intersects with the mean-line are lost. Where \( f \) is the fitted function and \( z \) the vector of \( n \) measured profile points the following interpolation conditions must be obeyed.

\[
f(x_i) = z_i \quad i = 1, 2, 3, \ldots, n. \tag{3.32}
\]

- **Be a 'sensible' fit** - The profile represents a real life surface profile and the fitted function must respect this. This means that the function must be continuous throughout the range and not contribute any outliers to the trend of the profile. The introduction of spurious points caused by this problem of 'overfitting' [5] may introduce unwanted features to the profile and therefore unstable parameter values.

- **Be reliable to compute** - When the fitted function is computed it must produce a stable and reliable output. Small changes in the input profile data points must only produce small changes in the output function. It must be able to accept the very small values that comprise a surface profile and not be susceptible to ill conditioning.

The easiest method of fitting an interpolating function to a set of data points is to fit a polynomial of degree \( n - 1 \) by solving a square system of linear equations. Figure
3.5 shows a small surface roughness profile segment comprising of one peak at the adjacent valley element. Added to this segment have been the two ‘end’ points that depict where this segment intersects with the mean-line. In total this segment is made up of eleven data points.

When attempting to solve the square system of equations for these mere eleven points it was found that ill conditioning prevented a stable solution from being found (lower degree polynomials were possible but they are not interpolants). Switching from the
monomial basis to the numerically stable Chebyshev basis [40] proved more successful, Figure 3.6 shows this interpolant. Although satisfying the first (interpolates points) and last (renowned Chebyshev stability) criteria for a sound data fit, it does not, however, satisfy the second. The second criterion is that it be a 'sensible' fit does not apply as it has the tendency to 'wobble' between data points, a feature known as Runge’s phenomenon [56] and especially apparent in polynomials of high degree. This property is particularly noticeable, as with all polynomials with equidistant spaced data points, at the beginning and end of the data series. This can be eliminated by reducing the polynomial’s degree which would in turn not ensure interpolation and,

Figure 3.6: Interpolating Chebyshev polynomial for 11 profile points, $T_{10}(z)$. 
therefore, fail to satisfy the interpolation equations (3.32).

What is needed is a function that can control or limit this energy in the bending of the data fit to an extent where it will not produce these notorious 'wobbles' that are associated with polynomials.

3.3.1 Natural Cubic Spline Interpolants

Natural cubic spline interpolants [45], [47] to functions of one variable, which in the case of a surface profile can be thought of as the $z$ ordinate values, are solutions of a variational calculation. Given the data, such as a vector of $z$ ordinate values, let \{s(x) : x \in \mathbb{R}\} be any function with a square integrable second derivative that satisfies the interpolation conditions given by equation (3.32). The equation

$$I(s) = \int_a^b [s''(x)]^2 dx,$$  \hspace{1cm} (3.33)

where $a$ and $b$ define the interval is least, subject to the condition given by (3.32) if and only if $s$ has the form

$$s(x) = \sum_{i=1}^n \phi_i |x - x_i|^3 + \phi_{n+1} + \phi_{n+2}x \quad x \in \mathbb{R},$$  \hspace{1cm} (3.34)

the parameters \{\phi_i : i = 1, 2, \ldots, n\}, $a$ and $b$ being restricted not only by the interpolation requirements but also by the constraints

$$\sum_{i=1}^n \phi_i = \sum_{i=1}^n \phi_i x_i = 0.$$  \hspace{1cm} (3.35)

This resulting spline bends in such a way, that its internal energy, due to bending is minimal, consistent with the interpolation constraints imposed on it [27]. These conditions determine the parameters uniquely when $n \geq 2$, which is the usual case. It can be seen that equation (3.34) is a linear combination of cubic radial basis functions (RBF) augmented by a linear polynomial and that equation (3.35) is equivalent to
the requirement that $|s(x)|$ is $O(|x|)$ for large $|x|$. 

Equation (3.34) is from the linear space of natural RBF cubic spline functions that have the general form

$$S(x) = \sum_{i=1}^{n} \phi_i |x - x_i|^{2k+1} + \sum_{j=0}^{k} c_j x^j \quad x \in \mathbb{R}, \quad (3.36)$$

where the coefficients ($\phi_i$, where $i = 1, 2, \ldots, n$) satisfy the conditions

$$\sum_{i=1}^{n} \phi_i x_i^j = 0 \quad j = 0, 1, \ldots, k. \quad (3.37)$$

The term ‘natural’ refers to the fact that a mechanical spline that interpolates but is not subject to torques at the data points, will flatten out to zero curvature at its extremities, corresponding to the zero second derivative end conditions given by equation (3.35). The natural cubic spline, equation (3.34), is optimal in the sense of minimising equation (3.33), if and only if $k = 1$ in (3.36). However, it should not be regarded as universally optimal as different conditions that dictate the optimality cause different optimal interpolants. The fitting of a weighted cubic spline that minimises a weighted sum of equation (3.33), where if the weights were constant a natural cubic spline would result, would reduce the phenomena of ‘wobble’ even further. This would allow the spline to fit closer to rapidly varying data such as the nature of a surface profile. Having this property would restrict the continuity of the derivatives of such a spline, due to it being subject to torques that are absent from natural splines, and therefore, not be suitable for calculating the error bounds described in the implementation of quadrature methods.

Figure 3.7 shows the natural cubic RBF spline solution to the eleven point data segment resampled over a one hundred point range. It can easily be seen that this fit satisfies the first two of the conditions outlined earlier. The fact that natural spline
interpolation has a unique solution [20] together with the interpolation constraints (given by equation (3.35)) imposed also contribute to satisfying the third condition. The solution for this natural cubic spline interpolant is found by setting up the following system of equations

$$Q\phi = z ,$$

(3.38)

where $z$ is an $n \times 1$ vector of profile points including implied mean line crossing points. Additionally
\[ Q = \begin{pmatrix} A & P \\ \frac{P}{P^T} & 0 \end{pmatrix}, \quad (3.39) \]

where 0 represents the 2 x 2 zero matrix and the elements of \( A \) are given by

\[ A_{ij} = |x_i - x_j|^3, \quad (3.40) \]

and the elements of \( P \) are given by

\[ P = \begin{pmatrix} x_0^1 & x_1^1 \\ \vdots & \vdots \\ x_n^0 & x_n^1 \end{pmatrix} = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}, \quad (3.41) \]

The values of the coefficients \( \phi_i : i = 1, 2, \ldots, n \) are then computed. The interpolated fit over the range \( x_1 \) to \( x_n \) can then be calculated by setting up the original set of equations (3.38) and substituting the following components that make up \( Q \) in equation (3.39) with their respective counterparts marked with a * as follows

\[ A^*_{ij} = |x_i - t_j|^3, \quad (3.42) \]

\[ P^* = \begin{pmatrix} t_0^1 & t_1^1 \\ \vdots & \vdots \\ t_m^0 & t_m^1 \end{pmatrix} = \begin{pmatrix} 1 & t_1 \\ \vdots & \vdots \\ 1 & t_m \end{pmatrix}, \quad (3.43) \]

where \( t \) is the \( m \) x 1 vector of resampled \( x \) values and \( t_i \in [a, b] \), using equal spacing distance even though the values of \( x \) are not (as a result of the addition of the implied mean line crossing points). In the case of Figure 3.7, \( m = 100 \). The function values over the range can then be found by using the \( \phi \) coefficients that were calculated in the previous step.

The use of natural cubic splines in data fitting with surface profile points is ideal
because they are a minimum variance interpolant, the bending energy is minimised. In the same way a balloon expands into the shape that requires the least amount of resistance, these splines naturally take the form that allows the minimal amount of bending to occur whilst still interpolating all of the points. In other words the spline forms the path of least resistance - the most natural route.

3.3.2 Integral Calculation

Now that we have a stable function interpolating the measured profile points we can resample over our sampling length in order to generate a denser set of points. This will give much smaller intervals between points and therefore a greater accuracy with any chosen method of quadrature. However, the underlying function is known and continuous over the length of the profile meaning that we can not only get closer to the integral value, we can calculate it exactly.

Using the RBF interpolant defined in (3.34), with $a$ and $b$ being the end points of the sampling length, the value we are interested in is the integral

$$\int_a^b s(x)dx = F(b) - F(a),$$  \hspace{1cm} (3.44)

where $F(x)$ is the antiderivative of $s(x)$,

$$F(b) = \int_0^b s(x)dx = F(b) - F(0).$$  \hspace{1cm} (3.45)

and

$$F(a) = \int_a^0 s(x)dx = F(0) - F(a)$$  \hspace{1cm} (3.46)

Evaluating the antiderivatives in (3.46) and (3.45) the integral in (3.44) resolves to

$$\int_a^b s(x)dx = \frac{\sum_{i=1}^n \phi_i \mid x - b \mid^4}{4} + \frac{\sum_{i=1}^n \phi_i \mid x - a \mid^4}{4}$$
Figure 3.8: Area calculated using the trapezoidal rule with measured profile points.

\[ + \left( \phi_{n+1}b + \frac{\phi_{n+2}b^2}{2} \right) - \left( \phi_{n+1}a + \frac{\phi_{n+2}a^2}{2} \right) \]  

which can be refactored and stated as

\[ \int_{a}^{b} s(x) dx = \sum_{i=1}^{n} \phi_i \left( |x - b|^4 + |x - a|^4 \right) + \phi_{n+1}(b - a) + \frac{\phi_{n+2}(b^2 - a^2)}{2}. \]  

Now that we have an equation that allows us to calculate the integral exactly over a profile length, see Figure 3.9, then we can calculate the value of the amplitude parameters exactly over this length. The difference between this and using the trapezoidal rule over the same length can be seen with Figure 3.8.
3.4 Summary

It has been shown that there are a number of techniques to improve upon the 'old' discretisation method of the averaging amplitude parameters $R_a$, $R_q$, $Rsk$ and $Rku$, mainly documenting the case for $R_a$ as it is visually easier to interpret when overlaid with the profile that it has been calculated from, but the principles apply to all parameters in the aforementioned Section 4.2 of the international standard, ISO 4287:1997. The following points have been proposed as improvements

- The need to include implied mean line crossing points simply by linearly inter-
polating the data where these occur and provide each profile peak or valley element with calculated boundary values.

- The conditions that need to be achieved when fitting a function to a series of surface profile points in order to preserve the desired characteristics of the profile from just the measured values.

- The implementation of a proven method of numerical quadrature to estimate the integral and deriving the upper error bound of the calculation for this method.

- As a suitable continuous function has been selected to represent the measured profile the integral over the profile length can be calculated exactly where there is a viable option.

A clear advantage of utilising the first two points can be seen in Figure 3.10. The top plot represents a forty-point test profile sampled from the sine function at equidistant intervals on the range \( x = 0, \ldots, 10\pi \) so that five full oscillations are included. The profile using the absolute values of this test profile is illustrated in the middle plot, which clearly over estimates the integral of the implied absolute profile, which in turn is pictured in the bottom plot using a natural cubic spline interpolant fitted to the profile with the implied mean line crossing points included.

The results in Table 3.1 show the advantage of using the third and fourth bullet points above. The results produced for each method of quadrature used an interpolated natural cubic spline fit over the data used for Figure 3.10. This function is then used, where applicable, to provide an upper error bound. These can be compared to the true value for \( Ra \) over the five sine waves and the previous discrete method given by equation (3.3). The Romberg method is the most flexible and more accurate re-
results can be obtained by increasing the number of steps \((n)\), however, this inevitably increases processing time. Although the output values from Romberg do not converge to the true answer, the method was not applied to the true profile. It was applied to a number of points sampled from the true profile which in turn were fitted with a natural cubic spline interpolant.

The natural cubic spline curve that has been demonstrated can be represented in many forms, not only by the equation in (3.34). There are many functions that can

![Figure 3.10: Illustrating the importance of including the implied mean line crossing points of the measured profile.](image-url)
provide exactly the same curve over a set of discrete points and in some cases it may not be viable to integrate the function used, and so it is worth mentioning that the use of quadrature methods can provide a solution that is very close to the integral value as Table 3.1 shows. Numerical methods of quadrature are completely independent of the underlying function at hand and so may be preferable to evaluate when only limited knowledge about this function is available. In the case of Romberg integration there is the flexibility to choose how many steps of the algorithm are computationally economical in order to achieve a result of desired standard.

Although the information between each measured profile point in a real data set will never be known, the pattern that these points provide should be exploited to the full. The ‘real’ surface, from which the points were measured, will almost certainly not

<table>
<thead>
<tr>
<th>Method</th>
<th>Ra Result</th>
<th>Error Bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trapezoidal Rule</td>
<td>0.63623382412721</td>
<td>0.00302665254281</td>
</tr>
<tr>
<td>Simpson’s 1/3 Rule</td>
<td>0.63638420976812</td>
<td>n/a</td>
</tr>
<tr>
<td>Romberg ($T_n^0$)</td>
<td>0.63639118838757</td>
<td>0.15634703972455e-03</td>
</tr>
<tr>
<td>Romberg ($T_n^1$)</td>
<td>0.63638461231479</td>
<td>0.18612796557303e-05</td>
</tr>
<tr>
<td>Romberg ($T_n^2$)</td>
<td>0.63638423055495</td>
<td>0.17004174871449e-05</td>
</tr>
<tr>
<td>Romberg ($T_n^5$)</td>
<td>0.63638418279210</td>
<td>0.12312833404073e-10</td>
</tr>
<tr>
<td>Integral of $s(x)$</td>
<td>0.63657954228892</td>
<td>n/a</td>
</tr>
<tr>
<td>Old Method ($\frac{1}{N} \sum</td>
<td>z_i</td>
<td>)$</td>
</tr>
<tr>
<td>'True' Ra Value</td>
<td>0.63661977236758</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 3.1: Values computed for Ra by various quadrature methods and other sources
have been as smooth as what the fit suggests using natural cubic splines. However, it
does illustrate the most natural line through all of the given profile points. Therefore,
it presents a good reference in order to develop an algorithm for determining these
parameters that has universal interpretation with sound mathematical background.
4.1 Surface Profile Interpolation

The type of function demonstrated to fit to a series of measured profile points \((x_i, z_i)\) has been shown to obey certain criteria in order to faithfully represent the characteristics of a surface texture profile. This function, a RBF representation of the natural cubic spline (3.34), neither introduces nor subtracts characteristics implied by the measured points. This is an important aspect of the interpolant as the evaluation of surface texture parameters on the must quantify aspects of the profile, not the approximation or interpolation scheme imposed upon it. We have sought a reliable representation of the measured profile with which to work with.

Speculating what the ‘real’ surface may look like or attempting to reproduce it would be tantamount to speculation, see Figure 4.1. There is little to be gained in attempting this venture and given the available measured data this desire should be suppressed. For all interests and purposes the ‘real’ surface can be thought of as a mythical entity. We should extract the most information that we can from the measured coordinate values and the interpolating function described help us toward this goal by providing a robust and continuous data fit.
Additionally, this function, when computed, produces a stable and reliable output meaning small changes in the input profile data will only lead to small perturbations in the output function due to the minimum variance constraints imposed upon it. Since the co-ordinate measurements are usually extremely accurate, an ill-conditioned interpolation scheme could easily introduce numerical error larger than the uncertainty in the measurements. However, RBFs can become ill-conditioned for large data sets which is the case for a full measured surface profile. Therefore a series of refinements to the interpolation routine have been developed.
In order to illustrate each refinement we shall use a section extracted from a measured surface roughness profile, shown in Figure 4.2. Although this is a very small piece of what would be a very large set of coordinate values the following steps are applied to the entire profile length.

4.1.1 Mean line crossing points

As highlighted in the previous chapter the inclusion of the points where it is implied that the surface profile intersects with the mean line is extremely important in the safe calculation of surface texture parameters. Therefore, the first step of the algorithm is to calculate all mean line crossing points and add them to the coordinate values of the profile. These crossing points can be thought of as all the points along the $x$-axis where the $z$ ordinate value sits on the mean line ($z = 0$).

Figure 4.3 shows the profile section with the mean line crossing points highlighted. These mean line intersection points become the boundaries for the profile elements in the sampling length. The first and the final crossing point calculated should also form
Figure 4.3: Calculated mean line crossing points with profile element divisions shown.

the start and end points of the current profile length, effectively cropping the profile length to only include 'closed' profile elements where two crossing points have been found in opposing directions through the mean line. The data discarded by bringing this into effect, which is usually minimal, usually causes confusion in the subsequent process evaluating surface texture parameters [31].

4.1.2 Piecewise approach to data fitting

Now we have isolated the end points of each profile element in our sampling length we can use our RBF interpolant over a much smaller data set. We are now effectively interpolating the entire profile in pieces rather than one large calculation, which can
cause the matrix in equation (3.39) to be quite large. This piecewise approach removes the stress of having to perform such a large numerical calculation and such a technique is not unusual [2]. Using the crossing points as the boundary of each profile element as start and end points for the RBF interpolant each element can be fitted independently of the next, as can been seen in Figure 4.4.

Using this method the profile length becomes a series of profile elements each interpolated separately, see Figure 4.8. In this plot no discrimination levels have been applied. However, as the profile elements are independent this makes it a lot easier
It is important to note that a simple linear interpolation routine is used to calculate the set of mean line crossing points. This ensures continuity between profile elements when they are interpolated individually. Using a more exotic approach such as using the last point of the previous profile element and the first point of the next profile element could result in a profile where the elements overlap, shown in Figure 4.5, or discontinuous in the $x$-axis, shown in Figure 4.6. Neither of these two cases are acceptable and using a point on the mean line that is common to neighbouring profile elements eliminates these phenomena.

After the interpolation routine has been applied to each profile element it has been observed that even the constrained oscillation of a NCS interpolant may introduce further mean line crossing points, such as in the case illustrated in Figure 4.7. Any such instances of this should be virtually ignored and the range of data interpolated still recognised as only one profile element. This is because we would be changing
Figure 4.6: Example of a discontinuous profile caused by using points from the neighbouring profile element leaving a portion of the $x$-axis empty. The resulting profile can be seen more clearly inset.

the data that we are trying to represent and would therefore affect some parameter values, most notably that of the mean profile element widths $RSm$.

Translation of $x$ values

Figure 4.4 also shows that for each profile element in the profile length its respective $x$-axis values have been translated to the range from $-1$ to $+1$. This is to aid in the numerical stability of the interpolant calculation. Equation (3.40) shows that we are using the cubed distances between each $x$ value in our calculation. The distances between each $x$ ordinate value are usually very small due to the high precision of modern day measurement instruments [29] and the raising them to the power of three can make these values very small and can expose ill-conditioning problems when solving equation (3.38). It should be noted that the original $x$-axis values are preserved and the translated values are used purely in the computation of the interpolating function.
4.2 Abcissae spacing of profile points

It is not unknown that the spacing between the measured x-axis points are not consistent. This non-uniformity in the spacing is mostly caused by the design of stylus measurement instruments whereby the pivot arm moves vertically (z direction) as it traverses the surface, see Figure 4.9. This arcial movement can, in theory, be resolved mathematically by simple trigonometry. However, in practice it is not always possible to know the values involved to a sufficient accuracy and so this movement must be calibrated out of the system using known artefacts [37].

It has been found in an international comparison of measurements, EUROMET 600 [25], that the lack of uniform spacing can cause problems with the standard Gaussian
Figure 4.8: Measured profile (top) goes through a number of stages in order to be modelled as a series of profile elements each fitted with a NCS interpolant individually (bottom).

Filtering a profile that has non-uniform spacing in the \( x \)-axis can provide a dramatic difference in the wavelengths suppressed and therefore a difference in the roughness profiles produced from this process, see Figure 4.10.

### 4.2.1 Gaussian filter

The Gaussian filter documented in ISO 11562 [13] is used to separate the roughness and waviness components of a measured surface profile given a cut-off wavelength. The standard defines a Gaussian weighting function, given by
Figure 4.9: Arcial movement of the stylus on a surface profile measurement instrument.

\[ s(x) = \frac{1}{\alpha \lambda_c} \exp \left( -\pi \left( \frac{x}{\alpha \lambda_c} \right)^2 \right). \]  \hspace{1cm} (4.1)

Where \( x \) is the distance from the centre of the filter, \( \lambda_c \) the cut-off wavelength of the filter, and \( \alpha \) a constant chosen to give the filter a certain transmission characteristic.

The filter characteristic is determined by means of the Fourier transform from the weighting function, corresponding to the following equation

\[ S(\lambda) = \exp \left( -\pi \left( \frac{\alpha \lambda_c}{\lambda} \right)^2 \right), \]  \hspace{1cm} (4.2)

and its amplitude defines the amplitude spectrum for the filter. The constant \( \alpha \) is chosen so that this response function takes the value \( \frac{1}{2} \) when \( \lambda = \lambda_c \). Expressed mathematically this is
Figure 4.10: A non-uniformly spaced sinusoidal profile($\lambda = 0.4$) after filtering($\lambda_c = 0.1$).

\[ \frac{1}{2} = \exp\left(-\pi \alpha^2\right), \quad (4.3) \]

where $\alpha$ resolves to

\[ \alpha = \sqrt{\frac{\ln 2}{\pi}}. \quad (4.4) \]

4.2.2 Analysis of filtering non-uniformly spaced profiles

In an attempt to quantify the differences between filtering profiles with uniform and non-uniform spacing in the $x$-axis values a test routine was devised. This assessment
involved the filtering of many profiles of varying wavelength (\(\lambda\)) with a constant cut-off wavelength (\(\lambda_c\)). By plotting the calculated amplitude of the filtered profile against the wavelength of the input profile we can display the performance of the filter at that wavelength.

We defined a set of wavelengths, \(\lambda_i\) where \(i = 10^{-2}...10^0\), and the cut-off frequency to be used, \(\lambda_c\), was fixed at \(10^{-1}\). For each wavelength, \(\lambda_i\), the following process was carried out.

- Two sinusoidal profiles of unit amplitude with wavelength \(\lambda_i\). One profile is created with equidistant \(x\)-axis points and another with non-uniformly spaced \(x\) points. The non-uniformity in the point spacing was created by the addition of normally distributed noise to each point, using \(\sigma = \frac{x_s}{10}\) where \(x_s\) is distance between each \(x\)-axis point in a uniformly spaced profile.

- An additional input profile is created by taking the non-uniformly spaced profile and applying the piecewise data fitting regime using a RBF interpolant that have been previously described. Now the profile at hand is represented as a series of continuous functions we can resample at equidistant intervals along the \(x\)-axis.

- Apply the Gaussian filter to each of the three profiles to obtain the corresponding waviness components.

- The amplitudes of each of the waviness components are then estimated. The value for each, \(\gamma_i\), is calculated using the equation

\[
\gamma_i = || a ||_2, \tag{4.5}
\]

where the vector \(a\) is obtained by solving for
Figure 4.11: Transmission characteristics of the Gaussian filter using, from left, uniformly spaced profiles, non-uniformly spaced profiles and non-uniformly spaced profiles resampled at uniformly spaced intervals using an RBF natural cubic spline (NCS).

\[ w_i = B a. \]  

(4.6)

\( w_i \) is the waviness profile from filtering the profile with wavelength \( \lambda_i \) and \( B \) is defined as

\[ B = \left( \sin \left( 2\pi \frac{x}{\lambda_i} \right) \cos \left( 2\pi \frac{x}{\lambda_i} \right) \right). \]  

(4.7)
• The computed amplitudes are compared with the amplitude derived from the predicted transmission characteristic, which is calculated using the Fourier transform of the Gaussian weight function given in equation (4.2).

Figure 4.11 shows the computed transmission characteristics, the plot on the left using profiles with uniformly spaced points whereas the central plot uses profiles with non-uniformly spaced points. The plot on the right was the non-uniform spaced profiles resampled using our method of data fitting. In the central plot of Figure 4.11 it can be seen from the transmission characteristics that the Gaussian filter is not suppressing the higher frequency elements of the profile effectively, illustrated by the higher error values in the left hand side of the plot.

Therefore, the roughness profile that would be extracted after such filtering has taken place will not possess the same characteristics as a profile of the same function with uniformly spaced points. The errors in this extracted profile will be passed on to any parameters calculated, giving inaccurate and unreliable results. This would explain as to why some parameter values given in the international comparison [25] were noticed as being erroneous.

By plotting the difference between the predicted and the computed transmission characteristics for each transmission curve, which is essentially the error of the computed transmission characteristic, the difference is clearly illustrated, see Figure (4.12). These error plots clearly highlight the effect of using non-uniformly spaced data points with the Gaussian profile filter, with the middle plot clearly standing out as the filter has not suppressed certain frequencies adequately. The difference between the error plots using uniformly spaced profiles and profiles resampled using the piecewise RBF interpolant are negligible. This would indicate that resampling in such a way with
non-uniformly spaced data before filtration it is possible to neutralise the apparent inadequacy that the Gaussian filter has with such profiles.

The transmission characteristic for uniformly spaced points, which is acting as a ‘reference’ case for this test, will not be equal to the predicted characteristics due to the discretisation of the underlying continuous sinusoidal function. An effect similar to that of an aliasing effect, depicted in Figure 4.13.
The institution that noticed the effect of the Gaussian filter on non-uniform spaced points, the National Physical Laboratory (NPL), have stated that the problem was rectified by employing a simple linear interpolation routine [30] and resampling at equally spaced points. This case was added to the test routine for the Gaussian filter to see how this would compare against applying our more complex approach of piecewise RBF interpolants. This comparison of the error in the transmission characteristics computed for resampling via linear interpolation can be seen in Figure 4.14. It can be seen that the range in the $y$-axis of these plots is considerably smaller than the plots in Figure 4.12, meaning the error in transmission using a linear interpolation routine is substantially reduced rather than just filtering the non-uniformly spaced
Figure 4.14: Error between the predicted and computed transmission characteristics using linear and piecewise RBF interpolation to resample at equally spaced points. However, it is more obvious to see that the linear interpolation routine is not as effective as that of using the piecewise RBF approach to resample at uniform spacing. Therefore, it can be deduced that by going down the avenue of using a linear interpolation routine to resample surface profile coordinates will not fully counteract the inadequacy in the Gaussian filter and should only be used with this caveat in mind.
4.3 Summary

The full process of taking a discretely sampled measured profile and converting it into an arguably more useful series of robust interpolating functions has been outlined here. The definite integral can now be calculated exactly over the range of each profile element as it is represented as a series of continuous functions. This methodology has been adopted into the University of Huddersfield and National Physical Laboratory SOFTGAUGES project [12] for use in the national software reference library for surface texture parameters. Unequal spacing in profile points can be overcome safely by using the interpolation routine and thereby avoid the deficiency of the standard Gaussian filter with such spacing. We can now review the parameters and see what this process means to each set from the standard.
5.1 Overview

In this brief chapter we state the main surface parameters of ISO 4287:1997 [15] again but this time we directly relate them with the method of data fitting that has been presented in the previous chapters. A brief comparison of parameter values is included using a test profile shown in Figure 5.1. This is a profile containing 21 equally spaced points sampled from the sine function between 0 and $10\pi$. The number of points used have been deliberately chosen so that no point coincides with the maximum or minimum values (1 and $-1$ respectively) of the sine function in order to illustrate the reconstructive properties of the data fitting algorithm.

5.2 Representation of the surface profile

The measured surface profile can be represented in some way other than merely a set of $z$ ordinate values. The new method of data fitting for surface profiles describes how the profile can be interpolated by a RBF representation of the natural cubic spline in a piecewise approach. Instead of a vector of profile ordinate values, $z$, we can model
Figure 5.1: 21 point test profile plotted against its piecewise natural cubic spline interpolant and the underlying sine function from which the points were sampled.

A profile $p$ as the set of interpolated profile elements in the profile length, where

$$p = [s(E_1), \ldots, s(E_m)]$$  \hspace{1cm} (5.1)

and each element in $p$ can be referred to as

$$p_i = s(E_i) \quad i = 1, \ldots, m.$$  \hspace{1cm} (5.2)

Here $E$ is the set of $x$-axis values for each profile element detected in the profile and $s(x)$ is stated back in equation (3.34). There are $m$ profile elements in a profile length corresponding to the $m + 1$ implied mean line crossing points, which we designate as $\chi$. Each element in $E$ also contains the consecutive crossing points that define the start and end points on the $x$-axis of this profile element, so it can stated that
\[ E_i = [\chi_i, (\chi_i \leq x \leq \chi_{i+1}), \chi_{i+1}] \quad i = 1, \ldots, m. \]  

(5.3)

The surface texture parameters can now be expressed with respect to the modelled surface profile, \( p \).

### 5.2.1 Refinement of peak to valley parameters

Only \( R_p \) and \( R_v \) need to be stated here as the other parameters, \( R_z \), \( R_c \) and \( R_t \) are just a summation of these two parameters evaluated over different lengths (sampling length, profile element width and evaluation length respectively). In essence \( R_p \) and \( R_v \) are the same, which is the greatest distance perpendicular from the mean line to the profile outline, the only difference being that \( R_p \) is concerned with data above the mean line and \( R_v \) below it.

The maximum and minimum values of the interpolating function can be calculated analytically by evaluating the first derivative of equation (3.34). This can be written as

\[
s'(x) = \sum_{i=1}^{n} 3\lambda_i |x - x_i|^2 + \lambda_{n+2}. \tag{5.4}
\]

The maximum profile peak height and minimum valley depths occur when

\[
s'(x) = 0. \tag{5.5}
\]

In practice this value is notoriously difficult to compute, especially with many local minima and maxima as a surface profile will have. The best option would be to resample the interpolating function with a much denser point spacing and take the maximum or minimum value from this.
Table 5.1: Comparison of results for peak to valley parameters using the test profiles in Figure 5.1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>'True' value</th>
<th>Discrete Method</th>
<th>Refined Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_p$</td>
<td>1.00000000</td>
<td>0.9510565</td>
<td>0.9954397</td>
</tr>
<tr>
<td>$R_v$</td>
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<td>0.9954397</td>
</tr>
<tr>
<td>$R_z$</td>
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<td>$R_c$</td>
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</tr>
<tr>
<td>$R_t$</td>
<td>2.00000000</td>
<td>1.9021130</td>
<td>1.9908793</td>
</tr>
</tbody>
</table>

5.2.2 Refinement of average of ordinate parameters

In the case of the $R_a$ parameter this can now be written as

$$R_a = \frac{1}{l} \sum_{i=1}^{m} \left( \int_{\chi_i}^{\chi_{i+1}} |p_i| \, dx \right), \quad (5.6)$$

where the limits of the definite integral stated as $\chi_i$ to $\chi_{i+1}$ are the implied crossing points for the profile element $p_i$. As we can now evaluate this definite integral exactly over the span of each profile element. The generic form for the $R_a$ and $R_q$ parameters can be written as

$$R_{a(k=1)}, R_{q(k=2)} = \left( \frac{1}{L} \sum_{i=1}^{m} \left( \int_{\chi_i}^{\chi_{i+1}} |p_i|^k \, dx \right) \right), \quad (5.7)$$

and the remaining $R_{sk}$ and $R_{ku}$ parameters have the form

$$R_{sk(k=3)}, R_{ku(k=4)} = \frac{1}{R_q^k} \left( \frac{1}{L} \sum_{i=1}^{m} \left( \int_{\chi_i}^{\chi_{i+1}} |p_i|^k \, dx \right) \right). \quad (5.8)$$

5.2.3 Refinement of mean width of the profile elements $R_{Sm}$

If we say that $\chi$ is the set of profile elements crossing points after the desired discrimination levels have been applied then
<table>
<thead>
<tr>
<th>Parameter</th>
<th>'True' value</th>
<th>Discrete Method</th>
<th>Refined Method</th>
</tr>
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<tr>
<td>$Rku$</td>
<td>0.4089404</td>
<td>0.3845912</td>
<td>0.4143784</td>
</tr>
</tbody>
</table>

Table 5.2: Comparison of results for average of ordinate parameters using the test profiles Figure 5.1.

\[ RS_m = \frac{|x_{m+1} - x_1|}{m}. \]  (5.9)

As each profile element is already defined individually then this makes it considerably easier to merge in existing methods for the stable evaluation of this parameter such as [61]. No comparison of results have been included for this parameter as both test profiles would use a linear interpolation method in order to compute the widths of profile elements and therefore the result would be the same.

5.3 **Summary**

The parameters have been stated in a new way that removes the ambiguity that was present beforehand. The new format is based upon representing the profile as a set of natural cubic spline interpolants and no longer a series of discrete data points.
6.1 Measurement Uncertainty

All measurements are flawed. Measurement units and instruments have all been made by man and are therefore inherently imperfect. When a quantity is measured by separate instruments the values obtained will, in general, be different. In order to make a statement concerning the measurement of the quantity of interest it is usual to provide an estimate of the quantity and an associated uncertainty. Without an evaluation of the quantities that make up this combined uncertainty it is almost impossible to compare values from different sources.

The area of surface texture measurement is no exception. Unless a statement of uncertainty is given with a calculated surface texture parameter it is difficult to assess whether the difference in the results obtained from two interpretations of the same parameter is critical to understanding the surface being measured. The problem of uncertainty analysis is complex and existing approaches to solving this problem are not always appropriate or straightforward to apply.

Every measured point that makes up a profile is assigned the same standard uncertainty and so we assume that if a continuous function were to interpolate, such
Figure 6.1: Plot illustrating the concept of the uncertainty coverage intervals.

as that presented previously, then the profile could be visualised with this interval along its range. Figure 6.1 demonstrates this point as the blue plot shows the given measured profile and the red plots show the 95% confidence boundary of the given associated standard uncertainty value. Inset in the same figure is a close up showing the uncertainty interval of the measured points and how the red plots have been constructed. An insight into the area of measurement uncertainty will be given here. Ultimately such methodologies will need to be coupled with reliable and stable software algorithms that this document concerns in order to provide a complete scope of the quantities involved when quoted the value of a surface texture parameter.
6.1.1 The Guide to the Expression of Uncertainty in Measurement

The authoritative document published by the International Standardisation Organisation that addresses the fundamental principles of the problem of uncertainty evaluation is the Guide to the Expression of Uncertainty in Measurement [19], known as the 'Guide'. This document commands the use of a model for the measurement, a concept illustrated in Figure 6.2. This figure shows a model that has $n$ sets of input quantities $X$ and $Z$, that are the profile co-ordinate values estimated by $x$ and $z$ with associated standard uncertainty $u(z)$. There is a single output quantity $Y$, estimated by the measurement result $y$ with associated standard uncertainty $u(y)$. This approach is used by the Guide to the Expression of Uncertainty in Measurement [19]. This is a rule or procedure that enables us to calculate from a set of input quantities the value of the output quantity, or measurand, that is of interest. In the case of surface roughness parameters the model could be the formula that defines the parameter in terms of the profile ordinate values. Each of the ordinate values that make up a roughness profile will only be estimates, as they are individual measurements. The evaluation of uncertainty is concerned with quantifying the inexactness of the measurand given the model and information about the inexactness of the input quantities. Knowledge about an input quantity is conveyed mathematically by use of a probability density function (PDF). If a PDF can be derived for an output quantity then it can be used
Figure 6.3: Two commonly encountered probability density functions in metrology, on the left the uniform distribution and on the right the normal or Gaussian distribution to produce certain pieces of information such as a mean and standard deviation for that measurand. Two most commonly encountered PDFs in metrology are depicted in Figure 6.3, these being the uniform and normal, or Gaussian, distributions.

A general approach advocated in the GUM is the 'law of propagation of uncertainty' and the use of the central limit theorem. The central limit theorem is invoked to assign a normal distribution

$$N(y, u^2(y)),$$  \hspace{1cm} (6.1)

to the PDF of the measurand, $Y$, with the mean value $y$ (the standard uncertainty value for the measurand) which is obtained by evaluating the model with the values of the input quantities ($z_i$ for surface profiles). A variance, $u^2(y)$, for this distribution is obtained by the law of propagation of uncertainty applied to linearisation of the model in the process of summing in quadrature the variances if the input quantities where these variances are weighted according to the model sensitivities,

$$u^2(y) = \sum_{i=1}^{N} u_i^2 = \sum_{i=1}^{N} (c_i u(z_i))^2.$$  \hspace{1cm} (6.2)

This approach only uses a limited amount of information. It does not use the PDFs of the input quantities only their mean values and the standard deviations relating
to these PDFs. This methodology is not sufficient to apply to the complex nature of surface texture measurement. The problem lies in the process of having to linearise the model and assign a normal distribution to the measurand value as this involves delivering an approximate solution where the degree of approximation is outside the user’s control.

6.1.2 Monte-Carlo Simulation

More general approaches are gaining recognition that do not possess the limitations of the GUM approach. Monte-Carlo simulation [8] (MCS) is an alternative method to propagate measurement uncertainty through the calculation of surface texture parameters. MCS is a computationally intensive iterative approach where each iteration samples randomly from the PDFs of the input quantities and evaluates the model with these random samples. The results of performing many trials are used to build distributional information about the value of the measurand and hence approximate the required PDF.

Figure 6.4 illustrates the distribution obtained from 100,000 trials of MCS (histogram plot) compared with the distribution given by the values from the methodology of the GUM (dashed plot) for the calculation of the parameter $Ra$. Both methodologies used the same evaluation method for $Ra$ and the same measurement uncertainty for the profile points, which were assigned normal (Gaussian) PDFs. It is interesting to see that the GUM technique gives a larger standard deviation for the distribution of the measurand than the MCS, which shows it to be smaller from repeated trials. This counter-intuitive situation, where the uncertainty of the result is smaller than the uncertainty of the input quantities combined, can occur in averaging parameters such as $Ra$ especially when the value for the parameter over an evaluation length is taken as an average of the values calculated from each sampling length. This phenomenon can be observed in the PDFs on the left-hand side in Figure 6.5 where bottom row
contains PDFs produced from averages of the five sampling lengths in the top rows, and it can be seen that these PDFs show a higher standard deviation similar to that given by the GUM methodology in Figure 6.4.

In both cases in Figure 6.5 concerning $Ra$ the probability density function (PDF) of the result using profile fitting has more overlap with the reference result than the results obtained from evaluating the raw profile data. The $Rv$ parameter is the absolute minimum value of the profile and for evaluation by GUM methods it requires certain
approximation methods to be used, and assigns the output PDF to be Gaussian (the MCS results clearly show a skewed PDF). The plots for the PDFs of the reference profile and the NCS fitted profile overlay one another in the figure for the $R_v$ results using the GUM methodology (bottom right of the figure).

### 6.2 Summary

This chapter has outlined the most common methods for calculating the uncertainty in measurement. Due to timescale limitations in this project we have not been able
to present a satisfactory method to couple with the computation of surface texture parameters and so this part of the document serves as an introduction into this field. However, it has been indicated that an empirical methodology (such as Monte-Carlo simulation) may work better with surface parameter algorithms than that of an analytical approach (such as the GUM) due to the latter not being inherently compatible with the complex nature of surface profile data.

The examples of uncertainty analysis provided here have utilised basic uncertainty evaluation methodologies and these techniques do not account for correlation effects inevitably caused by the standard Gaussian filter [13] or uncertainty in the traverse direction (x-axis). This in particular will certainly influence the $RSm$ and hybrid parameters. Some work has already been attempted in this area [28], there is a definite need to establish a more extensive and rigorous uncertainty analysis that accounts for both measurement and algorithmic uncertainty contributions. Unfortunately, as previously mentioned, this kind of analysis could not be displayed here but it is essential to underline the complicated, intricate and needed world of measurement uncertainty. It is hoped from this that the user can gain an appreciation of the task involved in order to fulfil the aim of presenting the result of a parameter with a complete statement of uncertainty.
'You’re gonna need a bigger boat.'

Chief Brody, *Jaws*

Research strives to improve things. We always want to have better things, better tools and better options available. In other words we will always want ‘a bigger boat’.

### 7.1 Aims Achieved

Relating back to the objectives outlined at the beginning of this document we can identify that the following aims have been achieved in the duration of this study:

- The standard definitions for surface texture profile parameters have been presented and annotated. The main flaws associated with definitions were highlighted in order to show areas where they can be improved. It was exposed that the main deficiency is caused by using a definite integral in the definition of a function for discrete data.

- A novel application of data fitting for surface texture profiles using a natural cubic spline (NCS) interpolating function has been presented. This function was found to
fulfil all the criteria that was marked out as being required for any function used to fit to the set of measured profile points. Additionally it was shown that the definite integral can be calculated exactly and therefore disposing of the need for any kind of quadrature algorithm. This new method represents the profile as a continuous series of NCS interpolating functions that respect the implied profile of the discrete points by neither introducing nor removing characteristics of the profile. It has introduced a considerable advantage over just using a set of discrete co-ordinate values as we can extract more information from this new representation of the profile, such as the mean line crossing points and profile element boundary points, which are inherently absent in co-ordinate data.

- The full process of taking a discretely sampled measured profile and converting it into an arguably more useful series of robust interpolating functions was presented. The research from this study has been incorporated into the University of Huddersfield and National Physical Laboratory Softgauges project [12], which developed Type F2 software measurement standards for surface texture parameters. This is part of the national software reference library.

Outside of the original scope of objectives it has been demonstrated that the standard Gaussian filter is deficient when dealing with non-uniform point spacing. The new method showed that this deficiency can be overcome by resampling from its continuous representation at equally spaced intervals, and is superior to just using simple linear interpolation to accomplish the same goal.

The parameters have been stated in a new way that removes the ambiguity that was present before. This new format is based upon representing the profile using the new method and longer a series of discrete data points. Whilst using mathematical representations for surface roughness is not new [41] this method is novel in the field
of surface texture parameters as well as the use of reference software. When compared to other Type F2 software measurement standards developed by other national institutions [35], although the results were in general agreement, the parameter software utilising the research contained in these pages was noticeable by its superior performance. This comparison study showed that this software delivered seven to ten accurate significant digits in the results, even higher than the precision of measuring data.

*Softgauge* measurement standards are used by software developers as part of instrument manufacture to test metrology software by helping them locate software bugs and check the correctness of their algorithms. Software measurement standards are also used by users, such as those in the manufacturing industry, of the software to give them confidence in the correctness of the algorithms and software in their metrology instruments. It is critical that these *softgauges* are correct and robust and for the national measurement institution to incorporate the research here into their development mean that is a massive aim achieved.

It is also quite possible to define a new generation of standards for surface texture parameters using the data fitting method we have proposed. In this case the parameters would be based upon a continuous profile and not a co-ordinate based one as published in ISO 4287, this alone would remove a lot of the ambiguity in definition.

### 7.2 Possibilities for the future

#### 7.2.1 Investigation into the propagation of uncertainty

Although the methods to quantify measurement uncertainty were not explored in great detail and the aim of providing a complete result to the calculation of a surface texture parameter was not met it has shown there is a significant case to explore
this area. One idea was born during this project: the application of Bayes’ theorem to uncertainty evaluation [44], [36] for surface texture parameters. This idea is not widely known to metrologists and is virtually non-existent in the field of surface texture parameters. Bayesian inference may provide a rigorous means of using all known prior information in calculating a measurand. It would allow the current state of knowledge about the measurand to be refined in the light of new information acquired through the measurement process. The nature of some of the standard surface texture parameters is inherently incompatible with the methodology stated in the aforementioned ’Guide’ [19], especially those such as $R_p$ which is discontinuous, and $R_v$, which is non-linear. The Guide approach applies the Law of Propagation of Uncertainty (LPU) and requires the following conditions to hold:

- the non-linearity of $f$ must be insignificant.

- the Central Limit Theorem (CLT) must apply and the output quantity be characterised by a Gaussian or t-distribution.

It has been shown that the second point cannot always be assumed [34]; however, this is largely a result of the first point not holding. When LPU is used in violation of the above conditions (one is usually unaware of this), the results produced can only be regarded as approximate, with an unquantified degree of approximation. Further, the Guide is often applied by disregarding mutual dependencies in the input quantities. Here, however, the measured values constituting a profile have associated correlation due to the filtration process [13] and non-linearity as a result of the inherent nature of contact stylus measurement [37]. Additional information is needed to quantify these attributes.

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

A method using a Bayesian approach will also allow certain prior rules to be observed.

Figure 7.1: Part of the PDF indicates that this $Ra$ value could be negative.
that could be overlooked using an analytical approach. In the case of an ultra flat surface, the magnitude of a parameter value could be overshadowed by that of the associated uncertainty. Figure 7.1 shows such a case where the probability density function (PDF) of the calculated \( Ra \) value crosses over the zero threshold. Therefore, when determining a coverage interval for a parameter, it could lead to the belief that the parameter has a finite probability of being negative or taking some other infeasible value. A Bayesian method would not allow this as part of the prior knowledge would simply state that this value cannot be negative.

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

### 7.2.2 Areal surface texture parameters

The next generation of ultra-precision surfaces will not only be incredibly smooth [38], [62] but also have the specification of surface format levels approaching atomic magnitude. Such surfaces will relate to a wide range of devices and components and the desire in surface metrology is changing profile to areal characterisation, see Figure 7.2.

The use of areal measurement attempts to characterise the fundamental and func-
Figure 7.2: Example of areal surface measurement. This provides us with a lot more information than profile measurement does but is young in comparison.

Ftional topographical features of the surface and a lot of research has gone into developing parameters for areal surface texture [22] but they have still not reached the stage of being incorporated into ISO standards. It is not the purpose here to discuss the problems associated with defining parameters for areal texture but the use of a natural cubic spline interpolant presented in this study to determine profile parameters is based around radial basis functions and it is easily extensible to apply to these increasingly areal domain [46]. Therefore it is a possibility that the definition of areal parameters can be directly related to the definition of profile parameters with the work introduced in this document. With the focus turning more and more to areal surface measurement the need for an international standard to define parameters in this field is inevitable, and with ambiguous definitions being published in the past we would hope that this does not happen again.
7.3 Final Remark

It is hoped that the course of this study and its findings have provided the field of surface texture profile parameters with, metaphorically speaking, 'a bigger boat', and to move a step further down the evolutionary path for better software and a better approach in the calculation of these parameters.


Parameter Function Specifications

These specifications and definitions of the software developed during the course of this study are included here for completeness and to provide some scope as to the extent of the software library created.

A.1 RProfile

Inputs

- **x**: Vector of dimension n of the x-axis values
- **z**: Vector of dimension n of the profile (z-axis) values
- **Lc**: OPTIONAL. Numerical value of the wavelength of the profile filter Lambda c used to extract the roughness profile values. DEFAULT = 0.8

Outputs

- **r**: RProfile MatLab Object

Call

```matlab
r = RProfile(x,z,Lc)
r = RProfile(x,z)
```
A.2 Maximum profile peak height, $R_p$

**Inputs**

$r$ RProfile object

**Outputs**

$R_p$ Vector of values representing the maximum profile peak height for each sampling length of the evaluation length. The last value in the vector is the average of all the $R_p$ values from each sampling length.

**Call**

$R_p = \text{getRp}(r)$

A.3 Maximum profile valley depth, $R_v$

**Inputs**

$r$ RProfile object

**Outputs**

$R_v$ Vector of values representing the maximum profile valley depth for each sampling length of the evaluation length. The last value in the vector is the average of all the $R_v$ values from each sampling length.

**Call**

$R_v = \text{getRv}(r)$
A.4 Maximum height of profile, $R_z$

**Inputs**

$r$  
RProfile object

**Outputs**

$R_z$  
Vector of values representing the maximum height of profile for each sampling length of the evaluation length. The last value in the vector is the average of all the $R_z$ values from each sampling length.

**Call**

$R_z = \text{getRz}(r)$
A.5  **Mean height of profile elements, $R_c$**

**Inputs**

- $r$: RProfile object
- $\text{heigD}$: OPTIONAL. Height discrimination tolerance level expressed as a percentage of maximum height of profile parameter $R_z$. DEFAULT = 0.1 (10%)
- $\text{spacD}$: OPTIONAL. Spacing discrimination tolerance level expressed as a percentage of the sampling length. DEFAULT = 0.01 (1%)

**Outputs**

- $R_c$: Vector of values representing the mean value of profile element heights for each sampling length of the assessed profile. The last value in the vector is the average of all the $R_c$ values from each sampling length.

**Call**

- $R_c = \text{getRc}(r)$
- $R_c = \text{getRc}(r, \text{heigD})$
- $R_c = \text{getRc}(r, \text{heigD}, \text{spacD})$

A.6  **Total height of profile, $R_t$**

**Inputs**

- $r$: RProfile object

**Outputs**

- $R_t$: Value representing the total height of profile for the evaluation length.

**Call**

- $R_t = \text{getRt}(r)$
A.7  Arithmetical mean deviation of the assessed profile, $Ra$

**INPUTS**

$r$  
RProfile object

**OUTPUTS**

$Ra$  
Vector of values representing the arithmetical mean deviation for each sampling length of the assessed roughness profile. The last value in the vector is the average of all the $Ra$ values from each sampling length.

**CALL**

$Ra = \text{getRa}(r)$

A.8  Root mean square deviation from the assessed profile, $Rq$

**INPUTS**

$r$  
RProfile object

**OUTPUTS**

$Rq$  
Vector of values representing the root mean square deviation for each sampling length of the assessed profile. The last value in the vector is the average of all the $Rq$ values from each sampling length.

**CALL**

$Rq = \text{getRq}(r)$
A.9  **Skewness of the assessed profile, Rsk**

**Inputs**

- \( r \)  
  RProfile object

**Outputs**

- \( Rsk \)  
  Vector of values representing the skewness for each sampling length of the assessed profile. The last value in the vector is the average of all the Rsk values from each sampling length.

**Call**

\[
Rsk = \text{getRsk}(r)
\]

A.10  **Kurtosis of the assessed profile, Rku**

**Inputs**

- \( r \)  
  RProfile object

**Outputs**

- \( Rku \)  
  Vector of values representing the kurtosis for each sampling length of the assessed profile. The last value in the vector is the average of all the Rku values from each sampling length.

**Call**

\[
Rku = \text{getRku}(r)
\]
A.11 Mean width of the profile elements, $R_{Sm}$

**Inputs**

- $r$: RProfile object
- $heigD$: OPTIONAL. Height discrimination tolerance level expressed as a percentage of maximum height of profile parameter Rz. DEFAULT = 0.1 (10%)
- $spacD$: OPTIONAL. Spacing discrimination tolerance level expressed as a percentage of the sampling length. DEFAULT = 0.01 (1%)

**Outputs**

- $R_{Sm}$: Vector of values representing the mean width of the profile elements for each sampling length of the assessed profile. The last value in the vector is the average of all the $R_{Sm}$ values from each sampling length.

**Call**

- $R_{Sm} = \text{getRSm}(r)$
- $R_{Sm} = \text{getRSm}(r,heigD)$
- $R_{Sm} = \text{getRSm}(r,heigD,spacD)$
A.12 *Root mean square slope of the assessed profile, $R\Delta q$*

**Inputs**

- $r$  
  RProfile object

**Outputs**

- $Rdq$  
  Vector of values representing the root mean square of each sampling length of the assessed profile. The last value in the vector is the average of all the $Rdq$ values from each sampling length.

**Call**

$$Rdq = \text{getRdq}(r)$$
**Inputs**

- **x**: Vector of dimension n of the x-axis values.
- **z**: Vector of dimension n of the profile (z-axis) values.
- **Lc**: OPTIONAL. Numerical value of the wavelength of the profile filter Lambda c used to extract the roughness profile values. DEFAULT = 0.8

**Outputs**

- **lx**: Matrix of l x m, where l is the number of sampling lengths and m is the number of x values in each sampling length.
- **lz**: Matrix of l x m, where l is the number of sampling lengths and m is the number of z values in each sampling length.
- **ex**: x-axis values for the entire evaluation length. This will differ from the input argument x only when values from x are unused, ex being x with these unused values removed.
- **ez**: Profile (z-axis) values for the entire evaluation length. This will differ from the input argument z only when values from z are unused, ez being z with these unused values removed.
- **sLengths**: Number of sampling lengths extracted from the profile. This is equal to n when [m,n] = size(r.lz).

**Call**

```
[lx,lz,ex,ez,sLengths] = samplingLengths(x,z,Lc)
[lx,lz,ex,ez,sLengths] = samplingLengths(x,z)
```
Inputs

lx Vector of dimension n of the x-axis values
lz Vector of dimension n of the profile (z-axis) values
heigd OPTIONAL. Height discrimination tolerance level expressed as a percentage of maximum height of profile parameter Rz. DEFAULT = 0.1 (10%)
spacD OPTIONAL. Spacing discrimination tolerance level expressed as a percentage of the sampling length. DEFAULT = 0.01 (1%)

Outputs

pElements 2 x m matrix where the given sampling length contains m profile elements passing the discrimination level.

Call

pElements = profileElements(lx, lz, heigD, spacD)
pElements = profileElements(lx, lz, heigD)
pElements = profileElements(lx, lz)

Inputs

lxP Vector of dimension n of the x-axis values
lzP Vector of dimension n of the profile (z-axis) values
elementsSF 1 x 2 vector containing the start and finish x values of this profile element

Outputs

pElement m x 2 matrix where the profile element is found to contain m x,z co-ordinate values.

Call

pElement = getElements(lx, lz, eSF)
The international standard in the title of document refers to ISO 4287:1997 Geometrical Product Specifications (GPS) - Surface Texture: Profile method - Terms, definitions and surface texture parameters. This means that this is the standard that specifies the terms, definitions and parameters to be used in the determination of surface texture by stylus measurement instruments. These terms are stated here for the readers convenience of quick reference.

B.1 General Terms

Most of these definitions are taken from ISO 4287:1997. Surface texture can be considered to be what remains after the application of a filter to a measured profile to remove the form of the surface. This can be thought of as the overall shape or angle of the surface being measured, for example when measuring a spherical object it is favourable ignore the curvature and only examine the surface as though it were flat. Once this has been removed the surface texture is made up of three components that are known as form, waviness and roughness. This document mainly concerns the roughness component. However all is described here.
B.1.1 Real Surface

This is the surface limiting the body and separating it from the surrounding medium.

B.1.2 Surface Profile

This is the profile that results from the intersection of the real surface by a specified plane. See figure B.1.

B.1.3 Traced Profile

This is the trace of the locus of the centre of a stylus tip that has an ideal geometrical form (conical with spherical tip) and nominal dimensions with nominal tracing force as it traverses the surface within the intersection plane.

Figure B.1: Surface profile and co-ordinate system convention, from ISO 4287:1997
B.1.4 Reference Profile

This is the trace reported by the probe as it moved with the intersection plane along a perfectly smooth and flat workpiece. The shape of the reference profile is a realisation of a theoretical exact profile. Its nominal deviations depend on the deviations of the guide as well as on external and internal disturbances. This profile arises from the movement caused by an imperfect datum guideway and therefore if the datum were perfectly flat and straight, the reference profile would not affect the total profile.

B.1.5 Total Profile

The is the digital form of the traced profile relative to the reference profile, with the vertical and horizontal coordinates assigned to each other. Most surface texture measurement instrument do not take account of the error introduced by datum imperfections, as this is not practical, and the total profile is the only available information concerning the traced profile.

B.1.6 Profile Filter

Filters play a fundamental role in the analysis of surface texture measurement. It is the process of extracting, or suppressing, certain wavelengths or spatial frequencies in the total profile, for example the attempts to reduce the effects of instrument noise and imperfections.

The Profile filter is the filter that separates profiles into longwave and shortwave components. There are three filters used in instruments for measuring surface roughness, waviness and primary profiles (see ISO 11562 for more details). For completeness all are defined here, however this document only concerns the \( \lambda_c \) filter. They all possess the same transmission characteristics, but have differing cut-off wavelengths.
Figure B.2: Transmission characteristic of roughness and waviness profiles, from ISO 4287:1997

B.1.7 $\lambda_s$ Profile Filter

This is the filter that defines the intersection between the roughness and shorter wave components, such as instrument noise, present in a surface. See figure B.2.

B.1.8 $\lambda_c$ Profile Filter

This is the filter that defines the intersection between the roughness and waviness components. See figure B.2.

B.1.9 $\lambda_f$ Profile Filter

This is the filter that defines the intersection between the waviness and longer wave components, such as form, present in a surface. See figure B.2.

B.1.10 Primary Profile

The primary profile is the basis for the evaluation of the primary profile parameters from ISO 4287. It is defined to be the total profile after the application of the short
wavelength filter with cut-off $\lambda_s$.

**B.1.11 Roughness Profile**

This is defined to be the profile derived from the primary profile by suppressing the long wave components using a long wavelength filter with cut-off $\lambda_c$. The roughness profile is the basis for evaluation of the roughness profile parameters that have been implemented in this text. Such evaluation automatically includes the use of the $\lambda_s$ filter since it is derived from the primary profile.

**B.1.12 Waviness Profile**

This is the profile derived by the application of the $\lambda_c$ and $\lambda_f$ profile filters and is the basis for the evaluation of the waviness parameters. This text is not concerned with the waviness profile and this definition is included for completeness.

**B.1.13 Coordinate System**

For two-dimensional surface texture measurement it is usual to use a rectangular coordinate system in which the axes form a right-handed Cartesian set, the $x$-axis being the direction of tracing co-linear with the mean line, the $y$-axis also nominally lying on the real surface and the $z$-axis being in an outward direction from the material to the surrounding medium. This convention, illustrated in figure B.1, is used throughout this text and the International Standard ISO 4287.

**B.1.14 Mean Line for the Roughness Profile**

The mean line used for the roughness profile, where $z = 0$, is a reference line for parameter calculation. It is the mean line corresponding to the long wave profile component suppressed by the profile filter $\lambda_c$. 
B.1.15  Sampling Length \( lr \)

This is length in the \( x \)-axis used for identifying the irregularities that characterise the profile under evaluation. The sampling length for \( lr \), roughness (\( lw \) for waviness and \( lp \) for the primary profile) is numerically equal to the wavelength of the profile filter \( \lambda_c \). Almost all parameters should be evaluated over the sampling length, however reliability is improved if an average is taken from several sampling lengths.

B.1.16  Evaluation Length \( ln \)

This is length in the direction of the \( x \)-axis used for assessing the profile under evaluation. It is normal practice to evaluate roughness (and waviness) profiles over several successive sampling lengths the sum of which gives the evaluation length. The standard advocates the use of five sampling lengths as the default for roughness evaluation, if another is used then the assessment parameter will have that number included in its symbol, for example \( Ra6 \) or \( Rt2 \). The parameters should be evaluated in each successive sampling length and then an average taken of sampling lengths in the evaluation length. A few exceptions exist and some parameters are assessed over the entire evaluation length. To allow for acceleration at the start of a measurement and deceleration at the end, the instrument traverse length is normally longer than the evaluation length.

B.1.17  Total Traverse Length

This is the total length of surface traversed in making a measurement. It is usually greater than the evaluation length due to the need to allow a short period at both end of the measured profile to allow mechanical and electrical transients to be excluded from the measurement and to allow for edge effects of filters.
B.2 Geometrical Parameter Terms

This document mainly concerns what is defined by ISO 4287:1997 to be $R$-parameters, those that are calculated from the roughness profile. For these $R$-parameters that have been implemented there are equivalent $W$ and $P$-parameters that are calculated from the waviness and primary profiles respectively. These parameters can be distinguished from one another by their prefixes of $R$, $W$ and $P$. For example $Ra$, $Wp$ and $Pt$ are calculated from their respective profile.

All the parameters described below are calculated once the form has been removed from the measurement (wavelengths greater than $\lambda f$). It is important to understand the concept that a profile consists of alternating ‘peaks’ and ‘valleys’ in order to evaluate surfaces. Also the application of discrimination levels to these profile to remove insignificant profile events.

B.2.1 Profile Peak

This is a part of the assessed profile connecting two adjacent points of the intersection of the profile with the $x$-axis, firstly in the positive direction and secondly in the

Figure B.3: Profile element definitions, from ISO 4287:1997
negative direction. In this part of the profile all $Z(x)$ ordinate values are positive.

**B.2.2 Profile Valley**

This is a part of the assessed profile connecting two adjacent points of the intersection of the profile with the $x$-axis, firstly in the negative direction and secondly in the positive direction. In this part of the profile all $Z(x)$ ordinate values are negative.

**B.2.3 Profile Element**

This is profile peak and the adjacent profile valley. A section of the profile at which it crosses the mean line to point at which it next crosses the mean line in the same direction, for example from above to below the mean line. This is shown graphically in figure B.3.

**B.2.4 Height and/or Spacing discrimination**

In order to prevent software and other systems counting very slight fluctuations in a profile, where it crosses the mean line and almost immediately crosses it again, that may be considered insignificant and not really a true profile feature discrimination levels are applied. Theses discrimination levels allow only profile peaks, valleys or elements larger than a specified height and width to be counted. In the absence of other specifications the default levels are that a profile peak or valley must exceed 10% of the $Rz$ parameter value and that the width of the profile peak or valley must exceed 1% of the sampling length. Both criteria must be met simultaneously for the profile feature to be counted.

**B.2.5 Ordinate Value $Z(x)$**

This is the height of the assessed profile at any position $x$. The height is regarded as negative if the ordinate lies below the $x$-axis and positive otherwise.
B.2.6  **Local Slope** $dZ/dX$

This is the local slope of the assessed profile at position $x_i$. The numerical value of the local slope, and thus the parameter $R\Delta q$ depends critically on the ordinate spacing.

B.2.7  **Profile Peak Height** $Z_p$

This is the distance between the $x$-axis and the highest point of the profile peak, the greatest value of $Z(x)$ contained within the profile peak.

B.2.8  **Profile Valley Depth** $Z_v$

This is the distance between the $x$-axis and the lowest point of the profile valley, the absolute smallest value of $Z(x)$ contained within the profile valley.

B.2.9  **Profile Element Height** $Z_t$

This is the sum of the height of the peak and depth of the valley of a profile element, i.e. $Z_p$ and $Z_v$.

Figure B.4: Local slope definition, from ISO 4287:1997
B.2.10  Profile Element Width \(X_s\)

The is the length of the \(x\)-axis segment intersecting with the profile element.

B.2.11  Material Length of Profile at the Level \(c\), \(Ml(c)\)

This is the sum of section lengths obtained, intersecting with the profile element by a line parallel to the \(x\)-axis at a given level (in the range of \(Rl\) \(c\)), see figure B.5.

B.3  Text Equivalents

In order to facilitate alphanumeric notation by means of computer the text equivalents listed in figure B.1 have been implemented in all of the code as recommended by ISO 4287:1997.

\[Ml(c) = Ml_1 + Ml_2\]

Figure B.5: Material length definition, from ISO 4287:1997
Table B.1: Text equivalents recommended by ISO 4287:1997

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Text Equivalent</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R\Delta q$</td>
<td>Rdq</td>
</tr>
<tr>
<td>$R\delta c$</td>
<td>Rdc</td>
</tr>
<tr>
<td>$\lambda s$</td>
<td>Ls</td>
</tr>
<tr>
<td>$\lambda c$</td>
<td>Lc</td>
</tr>
<tr>
<td>$\lambda f$</td>
<td>Lf</td>
</tr>
</tbody>
</table>
The following publications have been produced as a result of the research contained in this thesis:


Approximation of Surface Texture Profiles and Parameters

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Abstract

This paper provides an overview for a project in progress, at the University of Huddersfield in collaboration with the National Physical Laboratory, concerning the development of algorithms and software to compute standard surface texture parameters accurately with elements of numerical safety. The paper describes the problems associated with ambiguously defined ISO parameters and the resulting complications for their implementation. Also illustrated in the paper is the issue of propagating the uncertainty of measurement through the software processes applied to the measured profile, in order to assign a parameter value. Results obtained from the research to date will also be presented.

Introduction

Every surface has some form of texture structure that takes the form of a series of peaks and valleys. This texture has properties that are a result of the way the surface was produced as well as other factors (e.g. crystal structure, paint on the surface). These factors combine to make up the characteristics of a surface’s profile and often affect the performance, quality and service life of the product. If we could control surface texture then we could control these aspects of a product, in order to do this we must measure it. Measuring surface texture during the production cycle allows the product to be improved by controlling and optimising the manufacturing processes, and measuring at the end of the cycle provides a guide to the performance capability of the product.

Today a range of instruments are available for surface texture measurement. The instruments record the coordinates of data points that represent a surface profile, apply software to filter the data (e.g. to separate the measured primary profile into waviness and roughness profiles) and compute various surface texture parameters that aim to describe properties of the surface. The most common surface texture parameters in use today have been published as an ISO specification standard for two-dimensional profiles\(^1\). This standard, ISO 4287: 1997\(^2\) provides eleven different parameters for the quantification of different surface profile characteristics, of which nine are calculated from profile height measurements (z data), one from profile spacing measurements (x data) and one is a hybrid combination of both. The work described in this report is timely because a number or recent comparisons of surface texture measurements have shown some alarming spreads in the results\(^3\). It is difficult to say whether such variations are due to the instrument performance, the variation over the surface or the software employed to calculate the parameters. The consolidation and development of algorithms and software to compute surface texture parameters accurately with elements of numerical safety is the immediate focus of this study and will help to ensure that the uncertainty contribution caused by the software is minimised and well quantified.

Ambiguity of Definition

The information conveyed by surface texture parameters is legitimate only if those parameters are based upon mathematically unambiguous definitions. In the absence of such a requirement it may be possible that these definitions could be understood in different ways. This will lead to different interpretations in the way the parameters should be calculated, and as a consequence, different software developers will implement mathematically different algorithms to compute the same surface parameter. Leach and Harris\(^3\) have discussed one particular surface texture parameter, the two-dimensional spacing parameter, \(R_{Sm}\), in order to illustrate the difficulties of interpreting such parameters unambiguously. It is shown that the ISO definition of the parameter is ambiguous and its evaluation open to interpretation. Such ambiguities in the definitions of surface texture parameters can lead to serious problems in ensuring traceability of surface texture measurement to national and international standards as well as in interpreting the functionality of a surface. Results from this study\(^3\) show that the \(R_{Sm}\) parameter value can vary by nearly 10% simply by reversing the order of the data under examination.

In Section 4.2 of ISO 4287: 1997 four amplitude parameters are defined and all require the evaluation of a definite integral over the sampling length (a length of the measured surface profile). Surface profiles are measured discretely and, therefore, these parameters can only be evaluated approximately. These parameter definitions imply, although not explicitly stated, that a quadrature method needs to be implemented in order to compute approximations for these parameters. This process of quadrature introduces a certain amount of discretisation error and the option to implement one of many different methods of quadrature lies at the discretion of the software developer in question. In order to evaluate the integral and discretisation error a suitable underlying function needs to be applied to the discrete measured profile points. The use of a natural cubic spline interpolant, Fig 1, for this purpose has been explored in the course of this study using reliable numerical methods\(^4, 5\) in the
computation of such functions to ensure a smooth approximation to the underlying function, without undue oscillation, in contrast to polynomial interpolation at all data points. This enables the quantification of an upper bound for the discretisation error associated with the chosen method of quadrature. Table 1 shows some results obtained by taking advantage of this technique, in comparison with the alternative of implementing a discrete sum to estimate a definite integral. The profile used for this test was a sinusoidal profile sampled at fifty points over five complete wavelengths. The ‘true’ $Ra$ value stated in the table is calculated from a continuous sinusoidal plot and included for comparison.

<table>
<thead>
<tr>
<th>Method</th>
<th>$Ra$ result</th>
<th>Error bound</th>
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<tr>
<td>Trapezoidal Rule ($T_n$)</td>
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<td>-</td>
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</tbody>
</table>

Propagation of Uncertainty

Unless a statement of uncertainty is given with a calculated surface texture parameter it is difficult to assess whether the difference in the results obtained from two interpretations of the same parameter is critical to understanding the surface being measured.

Fig 2. Comparison of distributions obtained by using Monte-Carlo simulation and GUM
dashed) for the calculation of the parameter $Ra$. Both methodologies used the same evaluation method for $Ra$ and the same measurement uncertainty for the profile points, which was assigned to be Gaussian. It is interesting to see that the GUM technique gives a larger standard deviation for the distribution of the measurand than the MCS, which shows it to be smaller from repeated trials. Further comparison and examination of both methodologies is under development in order to provide robust functionality for the evaluation of measurement uncertainties in surface texture parameter and filtration operations.

Conclusions

The definitions of measurement parameters, and subsequently the implementation of software for their evaluation, will benefit greatly from a mathematical treatment founded on sound approximation theory and numerical analysis. Subsequently it will be necessary for the development of a deeper understanding of uncertainty evaluation in the processes applied to measured surface profiles, to extract and quantify desired characteristics, in order to provide traceable and reliable measurement results in the calculation of surface parameters.

Acknowledgements

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References

Reconstruction of continuous surface profiles from discretely sampled data

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Abstract
The need to produce a continuous representation of a curve (or part of a curve) from a set of discretely defined data arises in many metrological applications. In this paper we are interested in the reconstruction of continuous surface texture profiles defined only at discretely obtained points. By reconstructing surface profiles accurately, with elements of numerical safety being taken into account, we can provide a mathematically sound basis on which to compute surface texture profile parameters [1], especially those that do not allow exact evaluation with discrete data points. Examples are given to illustrate the advantages of using this reconstruction method.

Introduction
Measuring a surface with a contact stylus instrument reveals the surface’s complex structure of peaks and valleys. This structure is represented by a series of discrete measured co-ordinate values returned from the instrument. It is important to note that these points are not uniformly spaced along the x-axis because during the measurement process the stylus moves in an arc as it traverses the surface [2], and this is influenced by subsequent electronic processing within the instrument. The inconsistency in the spacing of points causes noticeable errors in the calculation of surface texture parameters due to the apparent incompatibility with standard filtering software [3]. This process of filtration is an important element of surface profile analysis, its purpose is to separate the measured primary profile into waviness and roughness profiles. These profiles form the basis upon which the various surface texture parameters are calculated. Any errors in the extraction of these waviness and roughness profiles from the measured profile greatly influence the value of the calculated parameters. Combined with the fact that research has shown that some ISO surface parameters possess ambiguous definitions [4], this highlights the need to apply a robust mathematical method to eliminate the effects of non-uniform spacing in the filtration process. Implementation of such a method can also provide scope for the development of parameter algorithms that can achieve more accurate results when coupled with such a methodology. This paper presents an approach for profile data fitting in response to this need.

Profile Data Fitting
Research has already shown that using a sensible form of data fitting to roughness profile data before calculating certain parameters provides a more reliable result than just using the discrete points as input to the parameter functions [5]. This paper applies this method of data fitting at the stage where the measurement co-ordinates are first attained, not only before the process of applying parameter functions but also before profile filtration. In many cases,
simple polynomial approximation schemes are adequate for this task providing the order of the polynomial is sufficiently small to allow safe numerical computation of the solution parameters. However, polynomials can often fail to encompass all the desired properties in the approximant. The use of a natural cubic spline interpolant for the purpose of profile data fitting has been explored in the course of this study using reliable numerical methods [6] in their computation to ensure a smooth approximation to the underlying function, without undue oscillation, in contrast to polynomial interpolation at all data points.

![Non-uniform spaced profile fitted with a natural cubic spline interpolant](image)

**Fig. 1** Sinusoidal profile sampled at non-uniform spaced points and interpolated by a natural cubic spline in a piecewise way. The interval end points are determined by crossing points of the x-axis.

To avoid computation with large matrices that would occur if the whole profile were to be interpolated at once this research has taken a piecewise approach to data fitting. Taking each profile peak and valley as individual segments, together with the x-axis values that determine their respective start and end points, each element is fitted separately, see Figure 1. This allows for a more stable data fit as considerably fewer points are used than if the whole profile were interpolated. The calculation of most surface texture parameters will benefit from such an approach as their definitions are basically functions of separate profile elements. The result of the parameter being either the maximum, minimum or sum of the function applied to each element.

The transmission characteristic shown in Figure 2 clearly highlights the problem of using non-uniform spaced data points. Figure 2 was computed using sinusoidal profiles of varying wavelength ($\lambda$), the figure on the left used profiles with uniform spaced points whereas the central figure used profiles with non-uniform spaced points. The figure on the right was generated using sinusoidal profiles with non-uniform spaced points that were fitted using a natural cubic spline interpolant and then re-sampled at uniform spaced points using the spline coefficients. The Gaussian filter with a fixed cut-off frequency ($\lambda_c$) was then applied to each profile and the amplitude of the filtered profile calculated.
In the central plot of Figure 2 it can be seen from the transmission characteristics that the Gaussian filter is not suppressing the higher frequency elements of the profile effectively, illustrated by the higher error values in the left hand side of the plot. Therefore, the roughness profile that would be extracted after such filtering has taken place will not possess the same characteristics as a profile of the same function with uniform spaced points. The errors in this extracted profile will be passed on to any parameters calculated, giving inaccurate and unreliable results.

Using the method of piecewise natural cubic spline interpolation on profiles that do not possess equidistant spacing before filtration eliminates any problems that the Gaussian filter has with these profiles. The comparison of error plots shown on the left and right hand-sides of Figure 2 illustrate this. The comparison of the roughness profiles extracted from the different profiles can be seen in Figure 3. The roughness profiles with uniform spaced data and that fitted with the natural
cubic spline are virtually identical, however, the non-uniform spaced roughness profile is noticeably different. The amplitude of this profile is greater than it should be because the filter has not suppressed certain frequencies adequately.

**Results**
A variety of surface texture parameters were calculated using the three types of profiles used throughout the course of study. Table 1 shows the results for some of these parameters. The parameters that require the evaluation of a definite integral, the Amplitude Parameters (Average of Ordinates) from ISO: 4287 ($R_a$, $R_q$ etc.), have the advantage of being able to be calculated exactly when a continuous function (i.e. natural cubic spline interpolant) is fitted to the data, this makes the need for a quadrature rule obsolete.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Uniform Spacing</th>
<th>Non-uniform spacing (A)</th>
<th>NCS fitted profile (B)</th>
<th>Error between A &amp; B (%)</th>
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</thead>
<tbody>
<tr>
<td>$R_p$</td>
<td>0.5922719</td>
<td>0.6692481</td>
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<tr>
<td>$R_a$</td>
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<td>0.3273360</td>
<td>0.3199791</td>
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<tr>
<td>$R_q$</td>
<td>0.3556151</td>
<td>0.3661291</td>
<td>0.3556124</td>
<td>2.96</td>
</tr>
</tbody>
</table>

Table.1 Results of various surface texture parameters applied to each profile type

**Conclusion**
A novel approach to surface profile data fitting has been presented that overcomes the ineffectiveness of the Gaussian profile filter with non-uniform spaced profile points. This process allows more efficient and reliable computation of the surface profile parameters because it represents the discrete profile as a series of continuous functions. This feature permits definite integrals and other phenomena in the definition of surface profile parameter definitions to be calculated exactly.

**Acknowledgements**
This research was carried out under a CASE Studentship Project funded in full by EPSRC and the National Physical Laboratory.

**References**
The need to evaluate the value for the combined standard uncertainty of an output quantity that itself is a function of many input quantities each with their own associated standard uncertainties is a problem of surface profile metrology. This paper presents research in progress that attempts to combat complications when trying to compute a robust value for this combined standard uncertainty.

1. Introduction

Measuring a surface with a contact stylus instrument and then evaluating surface texture profile parameters, such as those defined in ISO: 42871, quantifies certain aspects of the surface. It is important to note that these surface profile points are not uniformly spaced along the \( x \)-axis because of many influences during the measurement process2. This inconsistency in the spacing of points causes noticeable errors in the calculation of surface texture parameters due to the apparent incompatibility with standard filtering software3. The magnitude of the co-ordinate values that make up a surface profile are very small and susceptible to error in numerical computation and the standard uncertainty associated with these values is equally small. Compound this with the facts that the ISO parameters are defined in terms of a continuous function and have ambiguities in some definitions, there is a need to develop robust software for the safe calculation of these parameters and their subsequent standard uncertainty values.
Figure 1. Input-output model illustrating the propagation of uncertainty. The model has \( n \) sets of input quantities \( X \) and \( Z \), that are the profile co-ordinate values estimated by \( x \) and \( z \) with associated standard uncertainty \( u(z) \). There is a single output quantity \( Y \), estimated by the measurement result \( y \) with associated standard uncertainty \( u(y) \). This concept can be extended to incorporate the standard uncertainty associated with the traverse axis \( x, u(x) \).

2. Profile Fitting

A novel method of data fitting has already been presented\(^4\). The advantages of using this method are that, firstly, it fits a series of continuous functions to the profile and thereby represents the profile in the same format that the ISO standard parameters are defined for. Secondly, because the profile is now a series of continuous functions it can be re-sampled at equidistant points so it is compatible with standard filtering procedures. This method for data fitting has been extended to incorporate the propagation of uncertainty for surface texture parameters, utilising both the methodology from the Guide to the Uncertainty of Measurement (GUM)\(^5\) and Monte-Carlo simulation (MCS) approach\(^6\).

3. Propagation of Uncertainty

The software has been developed to replicate the concept shown in Figure 1, and output a parameter value together with its associated standard uncertainty. The model aims to quantify the extent of the inexactness of the parameter value with respect to the inexactness of the input quantities. Every measured point that makes up a profile is assigned the same standard uncertainty and so we assume that if a continuous function were to interpolate this profile then this would inherit the same value along its range, see Figure 2. As a result of this, the advantages of the profile fitting method hold when propagating uncertainties for parameter values. From the results gathered so far it can be seen that using this method, with both GUM and MCS procedures, it seems to provide a more accurate result for the parameter value and the uncertainty coverage interval. This is compared to results that were generated from an equally spaced reference.
Figure 2. Plot illustrating the concept of the uncertainty coverage intervals. The blue plot shows the given measured profile. The red plots show the 95% confidence boundary of the given associated standard uncertainty value. Inset, a close up showing the uncertainty interval of the measured points and how the red plots have been constructed.

profile and using the same software, see Figure 3.

4. Conclusions

A robust method of propagating uncertainty through surface texture profile parameters has been presented. The method of data fitting has already shown to overcome the ineffectiveness of the Gaussian profile filter with non-uniform spaced profile points and using this method in conjunction with existing methods for the evaluation of uncertainty show a more accurate approximation to both the measurand (parameter value) and its associated uncertainty value. This process of data fitting represents the discrete profile as a series of continuous functions permitting the exact calculation of definite integrals and other phenomena such as maximum peak height, and therefore provides a stable basis for both mainstream GUM and Monte-Carlo methods to compute sensitive uncertainty estimates.

Acknowledgements

This research was carried out under a CASE Studentship Project funded in full by EPSRC and the National Physical Laboratory.
Figure 3. These plots show results for the uncertainty evaluation of two surface profile parameters, $Ra$ (top) and $Rv$ (bottom), for both MCS (left) and GUM (right) methodologies. In both cases concerning $Ra$ the probability density function (pdf) of the result using profile fitting has more overlap with the reference result than the results obtained from evaluating the raw profile data. The $Rv$ parameter is the absolute minimum value of the profile and for evaluation by GUM methods it requires certain approximation methods to be used, and assigns the output pdf to be Gaussian (the MCS results clearly show a skewed pdf). The plots for the pdfs of the reference profile and the NCS (Natural Cubic Spline) fitted profile overlay one another in the figure for the $Rv$ results using the GUM methodology (bottom, right).

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6. Cox M and Harris P 2001 Measurement uncertainty and the propagation of distributions 10th Int. Metrology Congress, Saint Louis, France
Approximation of Surface Texture Profiles

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Abstract. In this paper we are interested in the approximation of continuous surface texture profiles defined only at discretely obtained points. A continuous representation is required in order to be able to apply filtration methods that assume uniform data spacing to practical data that in general is not uniformly spaced. By reconstructing surface profiles as natural cubic spline interpolants accurately using numerically stable fitting algorithms, we can provide a mathematically sound basis on which to compute surface texture profile parameters. As an important direct benefit, parameters involving the integrals of surface profiles can be calculated directly from the spline interpolant. Examples are given to illustrate the advantages of using this reconstruction method.

1. Introduction
Measuring a surface with a contact stylus instrument reveals the surface's structure of peaks and valleys. This structure is represented by a series of discrete measured co-ordinate values returned from the instrument. It is important to note that these points are not uniformly spaced along the measuring line because of a number of factors relating to the mechanical movement of the instrument during the measurement process [1] and the subsequent electronic processing within the instrument. The inconsistency in the spacing of points can cause noticeable errors in the calculation of surface texture parameters [2] due to the incompatibility with standard filtering software [3]. The filtration process separates the measured primary profile into waviness and roughness profiles, which form the basis upon which the various surface texture parameters are calculated. Any errors in the extraction of the waviness and roughness profiles from the measured profile will influence the value of the calculated parameters. Combined with the fact that research has shown that some ISO surface parameters possess ambiguous definitions [4], this highlights the need to apply a robust mathematical method to eliminate the effects of non-uniform spacing in the filtration process. Implementation of such a method can also provide scope for the development of parameter algorithms that can achieve more accurate results when coupled with such a methodology. Research has already shown that using a sensible form of data fitting to roughness profile data before calculating certain parameters provides a more reliable result than simply using the discrete points as input to the parameter functions [5]. This paper applies this method of data fitting at the stage where the measurement co-ordinates are first obtained, not only before the process of applying parameter functions but also before the profile is filtered.
2. Representation of profile data
The type of function needed to fit to a series of measured profile points \((x_i, z_i)\) must obey certain criteria in order to represent faithfully the characteristics of a surface texture profile. The fitted function must be an interpolant passing through all the measured points. Failing to meet this requirement will result in some peaks, valleys or points where the profile intersects with the mean-line \((z = 0)\) being lost (leading to a change in some of the evaluated parameters). The function must be continuous throughout the range and have no large oscillations between interpolated points. Additionally, when the function is computed, it must produce a stable and reliable output. Small changes in the input profile data must only lead to small perturbations in the output function. Since the \(z\) measurements are extremely accurate, an ill-conditioned interpolation scheme could easily introduce numerical error larger than the uncertainty in the measurements.

Candidate interpolant functions include polynomials, radial basis functions and splines. In many applications, simple polynomial interpolants can be effective. Using orthogonal polynomials such approaches can be implemented in a numerically stable way. However, polynomial interpolants are prone to large oscillations between interpolated points and are therefore unsuitable for this application. Radial basis functions can also be used for interpolation but can become ill-conditioned for large data sets and are also prone to unwanted oscillatory behaviour. As an alternative, the use of a natural cubic spline interpolant for the purpose of profile data fitting has been explored in the course of this study [6].

![Figure 1. (1a, left) Sinusoidal profile sampled at non-uniform spaced points and interpolated by a natural cubic spline in a piecewise way. (1b, right) Measured data set with the same data fitting method applied.](image)

Natural cubic spline interpolants to functions of one variable are solutions of a variational calculation [7] designed to ensure a smooth approximation to the underlying function free from undue oscillation. The general form of these interpolants is as follows

\[
s(x) = \sum_{i=1}^{n} \lambda_i \left| x - x_i \right|^3 + \lambda_{n+1} + \lambda_{n+2} x \text{ for } x \in \mathbb{R},
\]

the parameters \(\{\lambda_i : i = 1, 2, 3, \ldots, n\}\) being restricted not only by the interpolation requirements but also by other related constraints [8]. The resulting spline has minimal average curvature amongst all interpolating splines and as such can be regarded as the smoothest interpolating spline. This research has taken a piecewise approach to data fitting by taking each profile peak and valley as individual segments, together with the \(x\)-axis values that determine their respective start and end points, each element is fitted separately, see figure 1. This allows for a more stable data fit as considerably fewer points are used than if the whole profile were interpolated. The calculation of most surface texture parameters will benefit from such an approach as their definitions are basically
functions of separate profile elements. The result is that the parameter is either the maximum, minimum or sum of the function applied to each element.

2.1. Calculated transmission characteristics for Gaussian filters on non-uniform data

The transmission characteristic shown in figure 2 clearly highlights the effect of non-uniform spaced data points on Gaussian profile filter transmission characteristics. Figure 2 was computed using sinusoidal profiles of varying wavelength ($\lambda$), the plot on the left uses profiles with uniform spaced points whereas the central plot uses profiles with non-uniform spaced points. The plot on the right was generated using sinusoidal profiles with non-uniform spaced points that were fitted using a natural cubic spline interpolant and then re-sampled at uniform spaced points using the spline coefficients. The Gaussian filter with a fixed cut-off frequency ($\lambda_c$) was then applied to each profile and the amplitude of the filtered profile calculated.

In the central plot of figure 2 it can be seen from the transmission characteristics that the Gaussian filter is not suppressing the higher frequency elements of the profile effectively, illustrated by the higher error values in the left hand side of the plot. Therefore, the roughness profile that would be extracted after such filtering has taken place will not possess the same characteristics as a profile of the same function with uniform spaced points. The errors in this extracted profile will be passed on to any parameters calculated, giving inaccurate and unreliable results.

Using the method of piecewise natural cubic spline interpolation on profiles that do not possess equidistant spacing before filtration eliminates any problems that the Gaussian filter has with these profiles. The comparison of error plots shown on the left and right hand sides of figure 2 illustrates this. The roughness profiles with uniform spaced data and that fitted with the natural cubic spline are virtually identical. However, the non-uniform spaced roughness profile is noticeably different. The amplitude of this profile is greater than it should be because the filter has not suppressed certain frequencies adequately.

3. Effect of interpolation scheme on calculated surface parameters

Although the information between each measured profile point in a real data set will never be known, the pattern that these points provide should be exploited to the full. The 'real' surface, from which the points were measured, will almost certainly not have been as smooth as the fitted natural cubic spline.
However, the fitted spline does represent faithfully the surface profile on the basis of the information provided in terms of the given profile points. Therefore, it presents a good reference in order to develop an algorithm for determining these parameters that has universal interpretation with sound mathematical background.

A variety of surface texture parameters were calculated using the three types of profiles used throughout the course of study. Table 1 shows the results for some of these parameters. For parameters that require the evaluation of a definite integral such as the amplitude parameters (average of ordinates) from ISO: 4287 [1] (Ra, Rq, etc.), a spline interpolant offers a significant advantage in that the required integrals can be determined directly from the fitted spline parameters, obviating the need to apply quadrature algorithms.

<table>
<thead>
<tr>
<th>Parameter</th>
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4. Conclusion

A novel approach to surface profile data fitting has been presented that overcomes the ineffectiveness of the Gaussian profile filter with non-uniform spaced points. This process allows more efficient and reliable computation of the surface profile parameters because it represents the discrete profile as a series of continuous functions. The use of spline interpolants means that surface texture parameters defined in terms of integrals of the (real) surface profile can be calculated directly from the spline interpolant.

Acknowledgements

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