Uncertainty calculation of roundness by automatic differentiation

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Abstract

According to the Guide to the Expression of Uncertainty in Measurement (GUM), all measurement results must have a stated uncertainty associated to them. But in most cases of roundness measurement either no uncertainty value is given, or the calculation is not based on the model of the respective association criterion for the geometrical feature, because no suitable measurement uncertainty calculation procedure does exist. For the case of roundness measurement in coordinate metrology, this paper will suggest algorithms for the calculation of the measurement uncertainty of the roundness deviation based on the two mainly used association criteria LSC and MZC. The calculation of the sensitivity coefficients for the uncertainty calculation can be done by automatic differentiation, in order to avoid to introduce additional errors by the traditional difference quotient approximations. The proposed methods are exact and need as input data only the measured co-ordinates of the data points and their associated uncertainties.

Keywords: Measurement uncertainty, roundness, automatic differentiation.

1. Introduction

All international, as well as national standards existing today leave it open to the designer, which method for the assessment of roundness he would like to indicate on the technical drawing. The four possibilities given by ISO 1101:2004 [1] or the US standard ANSI B89.3.1-1972 (reaffirmed 1997) [2] are the least squares circle (LSC), the minimum circumscribed circle (MCC), the maximum inscribed circle (MIC), and the minimum zone circle (MZC).

Although it is guaranteed by a theorem of Chebyshev, that the MZC always yields the smallest value for the roundness deviation, all other methods are still in use. This is either due to the fact, that the calculation of the roundness deviation is not strictly based on the MZC by a rule or standard (although strongly recommended by ISO and ANSI), or that no suitable algorithms for the calculation of the MZC are available for the user. Sometimes also functional needs, like mating of parts, might force designers to use one of the other methods.

According to the Guide to the Expression of Uncertainty in Measurement (GUM) [3], all measurement results must have a stated uncertainty associated to them. But in most cases of roundness measurement either no uncertainty value is given, or the calculation is not based on the model of the respective association criterion for the geometrical feature, because no suitable measurement uncertainty calculation procedure does exist. This is especially true for the case of the MZC.
For the case of roundness measurement in coordinate metrology, this paper will suggest algorithms for the calculation of the measurement uncertainty of the roundness deviation based on the two mainly used association criteria LSC and MZC. In this connection, the calculation of the sensitivity coefficients for the uncertainty calculation shall be done by automatic differentiation, in order to avoid to introduce additional errors by the traditional difference quotient approximations. The proposed methods are exact and need as input data only the measured co-ordinates of the data points and their associated uncertainties.

2. Definition and calculation of roundness

The following definition of roundness is given in the normative Annex B of the international standard ISO 1101:2004 [1]:

The roundness of a single tolerated feature is deemed to be correct when the feature is confined between two concentric circles such that the difference in radii is equal to or less than the value of the specified tolerance. The location of the centres of these circles and the value of their radii shall be chosen so that the difference in radii between the two concentric circles is the least possible value.

Figure 1 demonstrates, what the ISO standard requires. The annulus $A_2$ on the right side with the width $\Delta r_2$ and the centre $C_2$ is the smallest one including all measured points. Thus its width is identical to the roundness, which is denoted in the main body of the standard by $RON_i$.

The ISO definition clearly favours the minimum zone circle (MZC) association criterion. However, in practise the least squares circle (LSC) association criterion is also used quite often today and thus can not be ignored completely.

For the LSC criterion the roundness is defined as the difference of the maximum and the minimum distance of the measured points from the centre of the LSC with the co-ordinates $(x_0, y_0)$ (if it

$$RON_i = \sqrt{(x_1 - x_0)^2 + (y_1 - y_0)^2} - \sqrt{(x_2 - x_0)^2 + (y_2 - y_0)^2},$$

where $(x_1, y_1)$ and $(x_2, y_2)$, respectively, are the co-ordinates of two measured points having the largest and the smallest distance from the centre of the LSC with the co-ordinates $(x_0, y_0)$ (if it
should happen, that we have more than one point of the one or the other kind, we may select just one of them arbitrarily). However, the centre co-ordinates \((x_0, y_0)\) are dependend of the co-ordinates of all measured points.

On the first sight this looks not very promising for the uncertainty calculation of the roundness for the LSC criterion, but applying the method proposed in [4], we can easily obtain the uncertainty matrix of the centre co-ordinates, which subsequently can be used to propagate the uncertainties and covariances of these two parameters to the uncertainty of the roundness itself, as described in detail in the GUM [3].

In order to determine the necessary sensitivity coefficients, the calculation of the partial derivatives of equation (1) with respect to the parameters \((x_0, y_0)\), as well as with respect to the co-ordinates \((x_1, y_1)\) and \((x_2, y_2)\), respectively, is required. This task can most suitable be performed by a computer program using automatic differentiation not only for the LSC association [4], but also for the uncertainty calculation of the roundness. Thus the uncertainty calculation for the roundness in case of the LSC association criterion can be considered as to be solved.

Let us now turn to the MZC association criterion. For lack of space we can not go into detail here, how the centre and the two radii for the MZC can be obtained, because the problem is much more complex than solving the LSC case. However, optimisation theory allows us to derive conditions, which must be obeyed by any valid solution.

The MZC association belongs to a group of optimisation problems, which are summarised under the term Chebyshev approximation. This optimisation problems are non-linear and as such do not guarantee to provide a unique solution, and even if they do, this solution is not necessarily a global optimum, but can be as well a local one. However, if the deviation of the measured points is not too big, i.e. in our case if the roundness is small, as it is usually the case in practise, we can be more optimistic and may expect to obtain a unique solution, which does not deviate very much from the global optimum, if it deviates at all.

If degeneracy can be ignored, which under practical circumstances is mostly the case, the problem has a unique solution, which is controlled by four so called critical points. There are exactly two critical points on the outer circle and two critical points on the inner circle of the minimum zone annulus, and the cords connecting the projections of the respective points of

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Fig. 2. Typical solution of a MZC approximation.
each of the pairs onto the outer circle do intersect [5]. Figure 2 shows a typical solution of a MZC approximation.

As can be shown by the theory of computational geometry, the centre of the two concentric circles is inside of the convex hull of the measured data points at an intersection of a nearest Voronoi edge and a farthest Voronoi edge. This fact is convenient for the application of a fast and reliable exhaustive search algorithm, after the two Voronoi diagrams have been constructed. This does not only guarantee the termination of the algorithm, which otherwise is not always easy to prove, but allows also to check for the uniqueness of the solution.

A Voronoi edge is defined to be a line segment separating two adjacent regions of a Voronoi diagram. Each point on a Voronoi edge is equidistant from two sites associated to these regions. The nearest point Voronoi region associated with a certain point is the set of all points in the plane that are closer to that particular point than to any other point, while the farthest Voronoi region associated with a certain point is the set of points in the plane that are farther from that particular point than from any other point. For more details about Voronoi diagrams see any suitable text book on computational geometry, for example [6].

After the centre co-ordinates and the critical points have been obtained, we can again apply equation (1) to calculate the roundness, where \((x_0, y_0)\) now denotes the centre co-ordinates of the MZC and \((x_1, y_1)\) and \((x_2, y_2)\), respectively, the co-ordinates of one of the critical points on the inner and the outer circle at a time. In order to calculate the associated uncertainty, we need the uncertainty matrix of the centre co-ordinates, but there is no formula which can be used for this purpose, because the exhaustive search is not an algebraic algorithm. To overcome this problem, we recalculate the centre co-ordinates as the co-ordinates of the intersection point of the two perpendicular bisectors of the line segments, which connect the two points of each pair of the critical points on the inner and the outer circle of the minimum zone annulus, respectively. This yields a function depending on all four critical points and allows thus an uncertainty calculation for the centre co-ordinates by applying the usual rules as given in the GUM. The task to calculate the necessary partial derivatives should again most suitable be performed by a computer program using automatic differentiation.

3. Automatic differentiation

The preceding section has shown, that partial derivatives are essential for the calculation of the measurement uncertainty. Two methods are frequently used today to compute partial derivatives of given functions numerically, firstly to derive the necessary formulae analytically by hand or by using a suitable computer algebra system, and subsequently to code the expressions in a computer program, or secondly to apply a finite difference approximation. However, there is another technique available since long, namely automatic differentiation (sometimes also called algorithmic differentiation). Unfortunately this approach is not widely known within the engineering community, although it provides the possibility to compute partial derivatives of arbitrary order of functions efficiently and accurately. Thus this method is well suited to calculate the necessary partial derivatives.

The idea behind automatic differentiation is, that differentiation in principle, as is well known from calculus, is a rule based procedure, which thus can easily be programmed to be done by a computer. The computer program parses a given expression and uses term rewriting methods to apply successively the rules of differentiation to each subterm resulting from the parsing process. Details of the underlying ideas to construct suitable algorithms can, for example, be found in [7] or [8].

The code, representing the formula to be differentiated, is automatically generated from the input expression by a suitable parsing algorithm and usually stored in the computer memory as
an abstract syntax tree (AST). The derivative of the code is subsequently obtained by simply applying the rules given in table 1 step by step, using a suitable pattern matching algorithm, while traversing the AST depth first, left to right. The resulting code is generally much longer than the original code and contains superfluous expressions. Thus a subsequent code optimisation process is needed, in order to simplify the code. The optimisation algorithm uses the well known algebraic rules and is based on techniques, which have been developed for optimising compilers.

Table 1. Differentiation rules.

<table>
<thead>
<tr>
<th>rule</th>
<th>expression</th>
<th>derivative</th>
<th>comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$a = c$</td>
<td>$da = 0$</td>
<td>$c$ is a constant</td>
</tr>
<tr>
<td>2</td>
<td>$a = x$</td>
<td>$da = 1$</td>
<td>$x$ is the dependent variable</td>
</tr>
<tr>
<td>3</td>
<td>$a = u + v$</td>
<td>$da = du + dv$</td>
<td>$u$ and $v$ are expressions, depending on the variable $x$</td>
</tr>
<tr>
<td>4</td>
<td>$a = u - v$</td>
<td>$da = du - dv$</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>$a = u * v$</td>
<td>$da = u * dv + v * du$</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>$a = u / v$</td>
<td>$da = (du - a * dv) / v$</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>$a = f(u)$</td>
<td>$da = du * f'(u)$</td>
<td>$f$ is an arbitrary function, $f'$ is the derivative of $f$</td>
</tr>
</tbody>
</table>

By application of the outlined methods, a computer program can be written, which automatically calculates the sensitivity coefficients needed for the uncertainty calculations.

4. Conclusion

It has been shown, how automatic differentiation can be applied to the uncertainty calculation of the roundness for the two practically important cases of the least squares circle (LSC) and the minimum zone circle (MZC) association criterion. The proposed methods avoid additional errors, which otherwise are caused by the traditionally used difference quotient approximation, are exact and need as input data only the measured co-ordinates of the data points and their associated uncertainties.

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