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Data-Driven Framework for Machine Learning-Based Uncertainty Evaluation in Coordinate Measuring Machines

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Abstract
The increasing use of Coordinate Measuring Machine (CMM) systems for high-precision dimensional metrology in industrial environments demands not only accurate data but also reliable quantification of measurement uncertainty. Traditional methods, such as ISO 15530-3 and the Guide to the Expression of Uncertainty in Measurement (GUM), require extensive experimental effort and are often directly applicable only to prismatic geometries, limiting their use for novel geometries or conditions. Freeform geometries are increasingly applied in manufacturing for topological and functional optimization, yet conventional CMM uncertainty evaluation methods are tailored to primitive geometries, restricting their applicability.
This work proposes a novel data-driven framework that leverages machine learning (ML) prediction models trained on actual CMM measurement data and integrates an uncertainty analysis to provide predictions with metrological trustworthiness. The approach begins with collecting an extensive dataset, through a factorial design structured by design of experiment (DOE), from tactile CMM measurements on calibrated artefacts with prismatic and freeform geometries. Influential factors such as sampling density, measurement strategy, probe configuration, and alignment are considered as model inputs. A supervised ML algorithm is trained to predict measurement outcomes (e.g., geometric deviations, form errors) as a function of these parameters. Unlike classical statistical models, the ML model captures complex interactions among process parameters and machine behaviour.
Uncertainty is evaluated using a statistical resampling approach based on bootstrap methodology. Multiple bootstrapped samples are generated, and the ML model is retrained for each, producing an ensemble of prediction models. The variability in coefficients and outputs provides estimates of standard and expanded uncertainty in accordance with GUM principles.
The framework bridges conventional DOE-based metrological modelling and modern data-driven methods. It enables quantification of ML prediction uncertainty for CMM processes, supporting virtual validation, metrological digital twins, and bridging towards complex measurement tasks' error compensation strategies.

Keywords: Accuracy, Coordinate measuring machine (CMM), Metrology, Uncertainty

1. Introduction

Coordinate Measuring Machines (CMMs) remain a cornerstone of high-precision dimensional metrology for industrial qualification and conformity decisions, where the credibility of inspection results depends on traceable uncertainty statements rather than nominal deviations alone. In recent work, uncertainty evaluation and optimization for CMM measurement planning have been revisited with stronger emphasis on industrial feasibility and economic impact, highlighting that measurement strategy choices can materially affect both uncertainty and inspection cost. [1]
The challenge becomes more pronounced as inspection tasks shift from mostly prismatic features toward freeform and geometrically complex surfaces, driven by functional design and optimization in modern manufacturing. For such surfaces, the layout of measurement points and sampling strategies can strongly influence achievable accuracy and robustness, motivating dedicated research on measurement point distribution and strategy selection for freeform CMM inspection. [2] In parallel, recent studies on strategy-driven evaluation (e.g., form and orientation assessments) further reinforce that uncertainty is not a fixed "machine constant," but depends on how the measurement is executed (alignment, point selection, probing configuration, and data processing). [3]
Alongside these metrology-specific developments, the broader field is increasingly adopting virtual experiments and digital-twin concepts to support trustworthy prediction and decision-making. Recent frameworks explicitly argue that virtual/DT-based measurement systems must include uncertainty propagation and traceability principles if they are to be used for metrological purposes. [4] Complementary contributions expand on how uncertainty evaluation methods differ when implemented within virtual measurement pipelines and how they should be interpreted for complex measurement tasks. [5]
At the same time, machine learning (ML) has gained traction as a practical way to model highly nonlinear interactions among measurement strategy parameters, probe configuration, alignment choices, and machine behaviour relationships that are difficult to capture with classical linear/statistical models. However, ML predictions are insufficient for metrology unless paired with uncertainty evaluation to communicate the trustworthiness of

predictions. Recent reviews in ML uncertainty quantification provide structured overviews of uncertainty evaluation families and their suitability for safety- and decision-critical deployments. [6]
For data-driven regression models, ensemble and resampling-based approaches remain attractive due to their conceptual simplicity and compatibility with existing pipelines. Also, recent work has shown that bootstrap ensemble spread can be employed to improve uncertainty evaluation accuracy, an insight directly relevant when using bootstrap-based ML ensembles for uncertainty-aware CMM predictions. [7]
Motivated by these needs, the present work proposes a data-driven framework that couples DOE-structured data collection with supervised ML modelling and bootstrap-based uncertainty estimation to deliver uncertainty-aware predictions for CMM measurement outcomes on both prismatic and freeform artefacts.
The approach supports uncertainty-informed inspection planning and provides a pathway toward metrologically trustworthy virtual validation and digital metrology workflows. [8,9]

2. Materials and methods

2.1 Measured artefact and geometry definition

The experimental investigation was conducted using a precision-calibrated spherical artefact (ball bearing sphere, *$Ø_{sph}$ = (107.943±0.003) mm, Sphericity = (4.5±3.0) µm*), selected due to its well-defined geometry, rotational symmetry, and widespread use as a reference feature in coordinate metrology. The sphere can be seen in Figure 1.

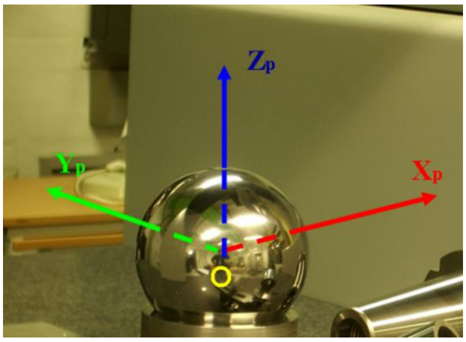

Figure 1: Ball bearing sphere [10]

The sphere provides a controlled yet non-trivial surface for studying the influence of measurement strategy, sampling, and alignment on CMM measurement outcomes while avoiding confounding effects associated with mixed geometries (e.g., cones or cylinders).
The calibrated diameter and sphericity of the artefact were taken as traceable reference values. All measurement deviations were evaluated relative to a nominal CAD model constructed using the calibrated sphere parameters. The sphere centre was used as the primary datum for alignment and evaluation, ensuring repeatability and minimizing datum-related ambiguity.

2.2 Coordinate measuring system and probing configuration

All measurements were performed using a tactile coordinate measuring machine operating in a temperature-controlled environment at (20.0 ± 0.5) °C. A touch-trigger probing system equipped with a ruby stylus of constant ball diameter was employed throughout the experimental campaign to isolate the effects of strategy-related parameters from probe size variability.
Two probe configurations were considered: a single vertical probing direction and a multi-directional probing configuration, allowing assessment of probing orientation effects while maintaining identical tip geometry. Measurement speed (10 mm/s), approach distance (2 mm), and probing force (100 mN) were kept constant across all experiments to reflect an industrially realistic but controlled measurement setup.
All measurements were performed using a ZEISS high-accuracy bridge-type Coordinate Measuring Machine (CMM) installed in a temperature-controlled metrology laboratory at (20.0 ± 0.5) °C. The CMM is designed for high-precision dimensional inspection and offers a maximum permissible error (MPE) of (2.0 + L/500) µm, where L is the measured length expressed in millimetres, ensuring traceable and stable measurement performance. The machine was equipped with a tactile probing system and calibrated according to the manufacturer's specifications prior to the experimental campaign.

2.3 Design of Experiments (DOE)

A full-factorial Design of Experiments was adopted to systematically investigate the influence of key measurement process parameters on spherical CMM measurements. Four factors were selected, each at two levels. Table 1 represents the input variables and their levels. Figures 2 to 4 represent different levels for input variables.

Table 1: DOE factors and levels

Factor	Level 1	Level 2
Sample density (A)	ISO/TS 16610-49	Reduced
Measurement strategy (B)	Transversal	Longitudinal
Probe Configuration (C)	3 mm Star Probe –y, +y, -x, +x	3 mm single probe -z
Alignment (D)	Repeated	Single

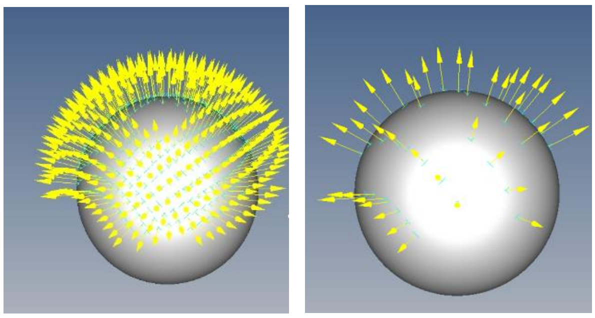

Figure 2: Sampling density, ISO16610-49 (left), and reduced 1/8 (right) [10]

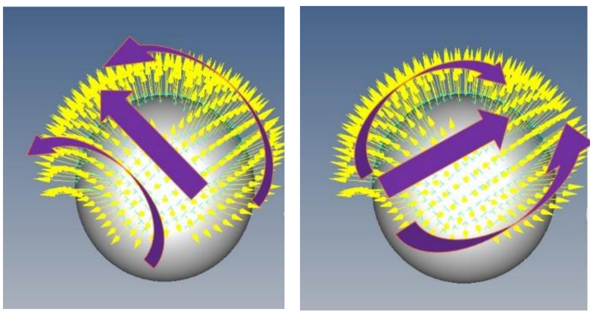

Figure 3: Measurement strategy, Transversal (left), and Longitudinal (right) [10]

The full factorial design resulted in 16 factor combinations. Each experimental condition was repeated three times to quantify measurement repeatability and enable statistical analysis. The experimental runs were randomized to mitigate systematic temporal effects.

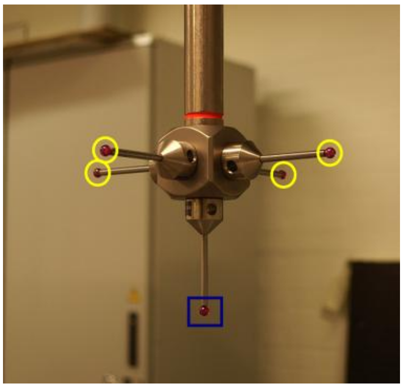

Figure 4: Probe configuration, Star probe (yellow), and a single probe (blue) [10]

2.4 Bootstrap sampling and GUM

Uncertainty associated with the machine learning–based predictions was quantified using a non-parametric bootstrap approach integrated with the Guide to the Expression of Uncertainty in Measurement (GUM). In this study, 1000 bootstrapped datasets were generated based on the original 16-datapoints dataset by resampling the original DOE-based measurement data with replacement. Figure 5 represents a scheme of how bootstrapping with resampling works.

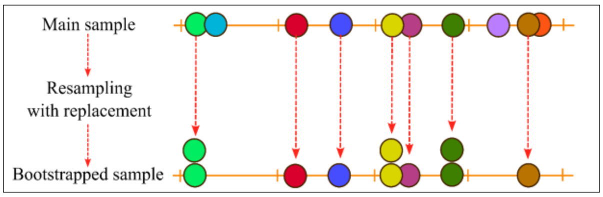

Figure 5: A scheme of bootstrap with resampling

The ML model was retrained for each dataset, producing an ensemble of predictions for sphere diameter deviation and form error. The standard uncertainty was estimated as the standard deviation of the bootstrap prediction distribution, while the expanded uncertainty was obtained using a coverage factor of K=2, in accordance with GUM principles. This approach enables data-driven, GUM-compliant uncertainty estimation without analytical uncertainty propagation.
The proposed framework complements ISO 15530-3, which provides traceable but task-specific uncertainty evaluation requiring dedicated experiments. In contrast, the present approach combines traceable data, interpretable models, and GUM-consistent bootstrap uncertainty to enable scalable estimation across multiple measurement configurations.
The resulting uncertainty should be interpreted as a task-specific uncertainty of model-based predictions, supporting virtual inspection and uncertainty-informed decision-making in digital-twin-based CMM environments.

2.5 Machine learning prediction model

To predict the sphere diameter and form error, regression models were employed as an interpretable white-box machine learning approach to predict CMM measurement outcomes. Polynomial and linear regression models were tried on both the outputs of diameter and form error. Based on the prediction results, due to the overfitting of the polynomial model, the linear regression model is used for the form error. But since the polynomial regression model showed a higher prediction accuracy, without overfitting, for the diameter, it was chosen as the prediction model. The models express the measurand as an explicit analytical function of the input factors, enabling direct interpretation of parameter effects and their coupled influences.
Unlike black-box models, regression models provide a closed-form prediction equation that can be readily integrated with bootstrap resampling and propagated through the GUM framework for uncertainty evaluation. This transparency makes the approach particularly suitable for metrological applications requiring traceable and physically interpretable models.

2.6 Output variables and objectives

The primary output variables are Geometric deviation metrics, including diameter deviation and local form error relative to the calibrated reference.
These outputs served a dual purpose. First, they enabled the identification of the most influential measurement parameters and interactions affecting spherical CMM measurements. Second, they formed the dataset for training supervised machine learning models and for subsequent bootstrap-based uncertainty quantification, supporting uncertainty-aware prediction of CMM measurement outcomes as proposed in the data-driven framework.

3. Results and discussion

As mentioned in the methods section, a machine learning model was trained for each resample, resulting in an ensemble of prediction models. The standard deviations of the regression coefficients obtained from the bootstrap ensemble were propagated through the measurement model using the GUM framework. This procedure enables the transformation of statistical model variability into a metrologically interpretable uncertainty statement for both investigated output quantities.
The adopted approach ensures that the uncertainty associated with model training, parameter estimation, and experimental variability is consistently transferred to the predicted measurand.

3.1 Uncertainty of diameter prediction

A machine learning model was trained on diameter data (assisted with the bootstrapped dataset). The following prediction regression equation was obtained for the diameter prediction:

$$\textit{Diameter} = 107.94 + 0.0035\times A + 0.0023\times B + 0.0029\times C - 0.0007\times D - 0.0040\times A^2 - 0.0057\times AB - 0.0014\times AC + 0.0016\times AD - 0.0008\times B^2 - 0.0008\times BC + 0.0007\times BD + 0.0005\times C^2 - 0.0001\times CD$$

The GUM-based uncertainty results, including the effective degrees of freedom and expanded uncertainty for diameter prediction, are summarized in Table 2.

Table2: GUM-based uncertainty results for diameter

Description	Symbol	value
Combined variance of y	$u^2(y)$	1.2×10^{-3} mm^2
Standard uncertainty	u(y)	3.4×10^{-2} mm
Effective degree of freedom	v(y)	69
Coverage factor	k	2.0
Expanded uncertainty	U(y)	0.068 mm

For the sample configuration of 1-1-2-2, the predicted diameter value is 107.911. So, the relative expanded uncertainty becomes 0.1%. Among the input variables, measurement strategy (B) and workpiece alignment (D) have a greater effect on the uncertainty of prediction compared to the other two factors of point density (A) and probe configuration (C).

3.2 Uncertainty of form error prediction

A similar bootstrap-based uncertainty analysis was conducted for the prediction of spherical form error.
For the spherical form error, the regression model obtained from the full dataset is:

$$\textit{Form error} = 47.125 - 21.075\times A - 3.750\times B + 0.150\times C + 2.750\times D$$

The GUM-based uncertainty results, including the effective degrees of freedom and expanded uncertainty for form error prediction, are summarized in Table 3.

Table 3: GUM-based uncertainty results for form error

Description	Symbol	value
Combined variance of y	$u^2(y)$	4.5 µm^2
Standard uncertainty	u(y)	2.1 µm
Effective degree of freedom	v(y)	69
Coverage factor	k	2.0
Expanded uncertainty	U(y)	4.2 µm

For the sample configuration of 1-1-2-2, the predicted value of the form error is calculated to be 28 µm. So, the corresponding relative expanded uncertainty is calculated to be equal to 15%, significantly higher than for the diameter.
The uncertainty budget reveals that form error prediction is substantially more sensitive to coefficient variability, particularly those associated with sampling density (A) and measurement strategy (B). The larger regression coefficients amplify the propagated uncertainty, resulting in a wider coverage interval.
The ensemble predictions revealed a wider variability compared to diameter estimation, reflecting the higher sensitivity of form measurements to probing strategy and alignment. The framework successfully quantified this variability through the bootstrap-derived uncertainty bands, allowing discrimination between more and less robust measurement configurations. The results highlight that form error uncertainty is particularly influenced by sampling density and probe configuration, underlining the importance of strategy selection when measuring freeform or quasi-freeform surfaces.

3.3 Consistency with GUM principles

For both diameter and form error, the bootstrap-derived prediction distributions enabled GUM-compliant uncertainty reporting, with standard uncertainty obtained from the ensemble spread and expanded uncertainty derived using an appropriate coverage factor. The results confirm that the proposed framework provides stable and repeatable uncertainty estimates without relying on analytical uncertainty propagation or geometry-specific calibrated artefacts. This demonstrates the suitability of the approach for scalable uncertainty evaluation and supports its application within virtual metrology and digital-twin-based CMM workflows.

4. Conclusion

This work presented a data-driven framework for uncertainty-aware prediction in coordinate metrology, combining DOE-based experimental design, supervised machine learning, bootstrap resampling, and GUM-compliant uncertainty propagation.
The results demonstrate that:

- Sphere diameter predictions exhibited low relative expanded uncertainty (0.1%), confirming its robustness as a global geometrical parameter.
- Form error predictions showed significantly higher uncertainty (15%), reflecting their intrinsic sensitivity to sampling density, measurement strategy, alignment configuration, and, in general, a more challenging measuring task.
- The propagated uncertainty values are consistent with known CMM behaviour and physical metrology principles.

The integration of bootstrap resampling with GUM propagation enables the translation of statistical model variability into traceable metrological uncertainty statements. Unlike conventional ISO 15530-3 approaches, the proposed framework does not require geometry-specific calibrated artefacts for each new measurement configuration. Instead, it leverages experimentally acquired datasets to generate scalable uncertainty predictions.
The methodology bridges DOE-based metrology and modern data-driven modelling, providing a structured pathway toward uncertainty-aware virtual CMM validation and digital metrological twins. By quantifying prediction reliability, the framework supports uncertainty-informed measurement planning and adaptive inspection strategies.

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