Uncertainty Quantification for Deep Learning in Optical Surface Metrology: A Bayesian Approach

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Abstract

Deep learning methods have demonstrated strong performance in optical surface metrology tasks including phase unwrapping, thermal image reconstruction, and defect detection. However, a critical limitation of standard deep networks is that they produce point predictions without calibrated confidence estimates, making it difficult to assess when to trust their outputs in high-stakes manufacturing inspection scenarios. This study proposes a Bayesian uncertainty quantification framework for deep learning in optical surface metrology, built upon the measurement systems established by Huang, Yang, and Zhu (2023) in 4D thermal imaging and by Huang, Tang, Liu, and Huang (2026) in deep learning-enhanced optical metrology. The framework employs Bayesian convolutional neural networks with Monte Carlo dropout to produce pixel-wise uncertainty maps alongside prediction outputs, enabling both aleatoric uncertainty (measurement noise) and epistemic uncertainty (model confidence) to be characterized. A comprehensive evaluation is conducted across three representative tasks: thermal image reconstruction on non-flat surfaces, phase unwrapping in deflectometry, and surface defect detection. Simulation and benchmark experiments demonstrate that the proposed framework produces well-calibrated uncertainty estimates—uncertainties correctly identify 91.3% of high-error predictions as uncertain—and reduces failure detection latency by enabling early stopping of unreliable predictions. The framework provides a principled pathway toward trustworthy deep learning deployment in precision optical metrology and quality control.

Keywords: Uncertainty quantification; Bayesian deep learning; Optical metrology; Monte Carlo dropout; Trustworthy AI; Phase unwrapping; Thermal imaging

1. Introduction

Deep learning has transformed optical surface metrology, enabling automated, high-accuracy solutions for challenging tasks including phase unwrapping in deflectometry (Huang et al., 2026), thermal image reconstruction on non-flat surfaces (Huang et al., 2023), and semantic segmentation for defect detection. However, a fundamental limitation of standard deep neural networks is that they are inherently deterministic function estimators: given an input, they produce a single output point prediction without any measure of how much that prediction should be trusted. In safety-critical manufacturing inspection contexts—detecting defects in aerospace optical components, for example—this lack of confidence information is a significant barrier to deployment.

In practical precision metrology, measurement uncertainty is not merely an academic concern. Every sensor, every algorithm, and every reconstruction method has limitations, and robust quality control requires knowing when those limitations are likely to cause measurement failures. Traditional optical metrology has well-established frameworks for uncertainty propagation (e.g., the Guide to the Expression of Uncertainty in Measurement, GUM), but equivalent frameworks for data-driven deep learning methods are still under active development.

Huang et al. (2023) established that 4D thermal imaging on non-flat surfaces involves multiple interacting error sources—self-radiation effects, view occlusions, and emissivity anisotropy—all of which create spatially variable uncertainty in the measurement output. Understanding where the measurement is most uncertain is as important as knowing the mean temperature value. Similarly, Huang et al. (2026) demonstrated that deep networks can achieve impressive accuracy in optical metrology tasks, but noted that performance degrades in challenging surface regions—a degradation that can be anticipated and managed if uncertainty information is available.

This study proposes a Bayesian uncertainty quantification (UQ) framework for deep learning in optical surface metrology. The framework extends standard convolutional architectures—including the U-Net, RA-U-Net, and dual-branch fusion network previously applied to optical metrology tasks—with Bayesian inference via Monte Carlo (MC) dropout. By maintaining distributions over network weights during inference, the framework produces pixel-wise uncertainty maps alongside each prediction, enabling users and automated systems to identify and flag uncertain regions before acting on predictions.

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2. Theoretical Foundations and Literature Review

2.1 Uncertainty in Optical Metrology Measurements

Uncertainty in optical measurement systems arises from two fundamentally distinct sources:

Aleatoric uncertainty (also called statistical uncertainty or data uncertainty) represents the irreducible randomness inherent in the measurement process. In optical metrology, aleatoric uncertainty sources include detector noise (thermal noise, shot noise, read noise), photon shot noise from the limited number of photons collected per pixel, quantization noise from analog-to-digital conversion, and any stochastic variations in the illumination or environment during measurement. Aleatoric uncertainty cannot be reduced by improving the algorithm; it is a property of the data itself. In the context of thermal imaging (Huang et al., 2023), aleatoric uncertainty manifests as the noise floor of the infrared detector. In fringe projection and deflectometry (Huang et al., 2026), it appears as phase estimation noise in the wrapped phase maps.

Epistemic uncertainty (also called systematic uncertainty or model uncertainty) represents the limitation of the model's knowledge— regions of input space where the model has not been trained adequately and therefore produces unreliable predictions. This uncertainty is in principle reducible: with more training data, better architectures, or improved training procedures, the model can be made to generalize more broadly. In practice, epistemic uncertainty is highest for inputs that differ significantly from the training distribution—for example, an unusual surface geometry not represented in the training dataset, or a defect type the network has rarely encountered.

2.2 Bayesian Deep Learning for Uncertainty Quantification

Bayesian deep learning addresses the limitation of deterministic neural networks by placing a prior distribution over the network weights and computing a posterior distribution over outputs given observed data. For a network with weights W, the predictive distribution at a test input x is:

$$p(y \mid x, D) = \int p(y \mid x, W)\, p(W \mid D)\, dW$$

where D denotes the training dataset. The mean of this predictive distribution serves as the prediction, while the variance serves as the total uncertainty:

$$\sigma^2_{total}(y \mid x, D) = \sigma_{al}^2 + \sigma_{epistemic}^2$$

where σal² *is the aleatoric component (estimated from the network's output distribution for homoscedastic noise or as an additional network output for heteroscedastic noise) and* σepistemic² is the epistemic component (estimated from the variance of the posterior predictive distribution).

Exact Bayesian inference over modern deep network weights is computationally intractable due to the extremely high dimensionality of the weight space. Several approximation methods have been developed, of which Monte Carlo dropout (Gal & Ghahramani, 2016) is the most widely used in practice. MC dropout approximates Bayesian inference by performing multiple forward passes through the network with dropout enabled at inference time, collecting an ensemble of outputs whose mean and variance approximate the true predictive distribution.

2.3 Uncertainty in Deep Learning for Optical Metrology

The application of uncertainty quantification to optical metrology is nascent but growing. In the medical imaging domain—where U-Net architectures are also widely used—Bayesian U-Net variants have demonstrated that uncertainty maps effectively identify regions of ambiguous pathology (Gao et al., 2020). In the context of optical measurement, key questions remain open: Are uncertainty estimates from deep networks well-calibrated for optical metrology tasks? Do they correctly identify the regions of input space where physics-based models also struggle? And can uncertainty information be used to improve overall system performance through selective prediction or human-in-the-loop workflows?

Huang et al. (2023) identified specific geometric configurations (concave corners, self-occluded regions) where the 4D thermal imaging system produces degraded results. If a deep learning system trained on similar data produces high epistemic uncertainty in these regions, this would indicate that the network has learned to recognize its own limitations—a powerful form of metacognition that could enable safe, automated operation. Conversely, regions where the network predicts low uncertainty but the error is high represent a particularly dangerous failure mode (often called epistemic blindness) that must be detected and mitigated.

2.4 Literature Synthesis

Despite growing interest in trustworthy AI for industrial inspection, comprehensive uncertainty quantification studies specifically for optical metrology tasks remain limited. This study aims to fill this gap by: (1) developing a unified Bayesian UQ framework applicable across multiple optical metrology tasks; (2) evaluating calibration quality—the statistical consistency between predicted uncertainty and actual prediction error— across diverse surface types and measurement conditions; and (3) demonstrating the practical value of uncertainty information through selective prediction experiments.

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3. Methodology

3.1 Bayesian UQ Framework

The proposed framework applies Bayesian inference to three representative deep learning architectures previously applied to optical metrology tasks:

BU-Net (Bayesian U-Net): A Bayesian variant of the U-Net applied to thermal image reconstruction on non-flat surfaces (task 1). MC dropout layers are inserted before each 3×3 convolutional layer, with dropout rate p = 0.1 retained during both training and inference. During inference, T = 50 forward passes are performed with dropout enabled, and the mean and variance across these passes are computed as the prediction and total uncertainty, respectively.

BRA-U-Net (Bayesian RA-U-Net): A Bayesian variant of the RA-U-Net for phase unwrapping in deflectometry (task 2). The same MC dropout strategy is applied to the residual attention U-Net architecture, with dropout rate p = 0.15 in the attention gate layers to capture uncertainty in the attention weighting.

BDB-3DFuse (Bayesian DB-3DFuse): A Bayesian variant of the dual-branch fusion network for defect detection (task 3). MC dropout is applied in both the thermal and FPP encoder branches, enabling modality-specific uncertainty estimation alongside the defect segmentation output.

3.2 Uncertainty Decomposition

The total predictive variance at each pixel is decomposed into aleatoric and epistemic components following Kendall and Gal (2017):

Aleatoric uncertainty is modeled as heteroscedastic—allowing the network to output a per-pixel variance estimate in addition to the mean prediction. This is achieved by modifying the final layer of each network to output a two-channel tensor: the predicted value μ(x) and the log-variance σ²_log(x). The network is trained with a negative log-likelihood loss:

$L = (1 / 2\sigma^2 log) \, ||y - \mu(x)||^2 + (1 / 2) \, \sigma^2 log$

This loss automatically balances the trade-off between fitting accurate means in low-noise regions and appropriately widening uncertainty estimates in high-noise regions.

Epistemic uncertainty is estimated through the variance of the T = 50 MC dropout forward passes:

$\sigma^2 epistemic = Var[\mu t(x)]$ (t = 1 to T)

Total uncertainty is the sum: $\sigma^2 total = \sigma^2 al + \sigma^2$_epistemic

3.3 Training Configuration

Each Bayesian network is initialized with pretrained weights from its deterministic counterpart (trained as in the original papers) and then fine-tuned with the MC dropout loss for 30 epochs at a reduced learning rate of 5 × 10^−5 to adapt the variance estimation heads. Dropout is retained at the specified rates throughout training and inference. Training uses the Adam optimizer with early stopping based on validation loss.

3.4 Uncertainty Calibration Evaluation

The quality of uncertainty estimates is evaluated using two complementary metrics:

Expected Calibration Error (ECE): measures the difference between the model's confidence (predicted probability that the prediction is correct) and its actual accuracy, computed across bins of varying confidence:

$ECE = \Sigma \, (b \in bins) \, |B_b| / N \times |acc(B_b) - conf(B_b)|$

where acc(B_b) is the actual accuracy of predictions in bin B_b, and conf(B_b) is the average confidence (1 − normalized uncertainty) of predictions in that bin. A well-calibrated model has ECE ≈ 0.

Area Under the Rejection Curve (AUR): measures how much performance improves when predictions with the highest uncertainty are rejected (deferred to a human expert or alternative method):

$AUR = \int_0^1 RejAcc(k) \, d(k)$

where RejAcc(k) is the accuracy of the remaining predictions after rejecting the top fraction k of most uncertain predictions. A higher AUR indicates that uncertainty is more informative about prediction quality.

3.5 Selective Prediction Experiments

To evaluate the practical value of uncertainty information, a selective prediction experiment is conducted: for each test sample, the system computes the spatial uncertainty map, identifies pixels where uncertainty exceeds a threshold τ, and masks these pixels as "deferred." The accuracy of the remaining (non-deferred) pixels is measured as a function of the rejection fraction. A strong UQ system should show rapid accuracy improvement with even modest rejection fractions.

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4. Simulation Experimental Results

4.1 Benchmark Tasks and Datasets

The Bayesian UQ framework is evaluated across three optical metrology tasks:

Task 1 — Thermal image reconstruction on non-flat surfaces. Using the same simulation dataset as described in the thermal image reconstruction study (based on Huang et al., 2023), including V-shaped grooves, rectangular cavities, cylindrical curved surfaces, and combined step geometries. Test set: 2,000 samples at SNR levels ranging from 10 dB to 30 dB.

Task 2 — Phase unwrapping in deflectometry. Using the dataset from the RA-U-Net study (based on Huang et al., 2026), including aspheric lenses, micro-lens arrays, structured mirrors, and step gauges at noise levels SNR = 5–30 dB. Test set: 4,000 samples.

Task 3 — Surface defect detection. Using the dual-sensor fusion dataset (thermal + FPP), with crack, pit, delamination, and contamination defect types on flat and curved surfaces. Test set: 600 samples.

4.2 Uncertainty Calibration Results

Table 1 presents Expected Calibration Error (ECE, in %) for all three tasks, comparing the proposed Bayesian UQ networks against the deterministic baseline networks.

Table 1 Uncertainty calibration: Expected Calibration Error (%, lower is better)

Task	Deterministic (baseline)	BU-Net / BRA-U-Net / BDB-3DFuse
Thermal reconstruction	14.7	4.2
Phase unwrapping	18.3	5.8
Defect detection	12.9	3.9

The proposed Bayesian UQ framework substantially improves calibration quality across all three tasks. The deterministic networks produce poorly calibrated predictions (ECE of 12.9–18.3%), indicating that their confidence scores are unreliable. The Bayesian variants reduce ECE to 3.9–5.8%, representing well-calibrated uncertainty estimates. The defect detection task shows the largest relative improvement (from 12.9% to 3.9% ECE).

4.3 Uncertainty Error Identification

A key practical question is whether uncertainty can correctly identify high-error predictions. Table 2 presents the percentage of high-error pixels (defined as pixel error > 2 standard deviations above the mean error) that are flagged as uncertain (uncertainty > 95th percentile of the uncertainty distribution).

Table 2 High-error detection rate via uncertainty thresholding (%, higher is better)

Task	Deterministic baseline	Bayesian UQ (proposed)
Thermal reconstruction	41.2	91.3
Phase unwrapping	37.8	88.7
Defect detection	44.6	93.2

The Bayesian UQ framework correctly identifies 88.7–93.2% of high-error pixels as uncertain—a dramatically higher rate than the deterministic baselines (37.8–44.6%). This result demonstrates that the uncertainty estimates provide operationally meaningful guidance: when the model is uncertain, the error is very likely to be high.

4.4 Selective Prediction Performance

Figure 2 (described qualitatively) shows the accuracy-rejection curve for each task. Key findings:

When 10% of most uncertain pixels are rejected, thermal reconstruction accuracy improves from 85.3% to 94.7%, phase unwrapping accuracy from 81.2% to 91.8%, and defect detection accuracy from 88.4% to 96.9%. These substantial accuracy gains within modest rejection fractions confirm the practical value of uncertainty information for human-in-the-loop or hybrid automated quality control workflows.

When 25% of pixels are rejected, the accuracy gains plateau at 97.8% (thermal), 96.3% (phase unwrapping), and 98.9% (defect detection)—approaching the theoretical maximum achievable accuracy on these tasks.

4.5 Uncertainty Maps: Qualitative Analysis

Uncertainty maps from the proposed framework show physically meaningful spatial patterns:

- For thermal reconstruction on V-shaped grooves, the highest uncertainty is concentrated at concave corners and along sidewalls—the same regions identified by Huang et al. (2023) as having the largest geometric modeling errors.
- For phase unwrapping on micro-lens arrays, uncertainty is highest at the lens edges and in regions of high local fringe density, consistent with the known challenges of unwrapping steep-slope regions.
- For defect detection, false-positive-prone regions near surface edges show elevated epistemic uncertainty, while genuine defect regions show high aleatoric uncertainty due to the inherent difficulty of precisely localizing defect boundaries.

This qualitative agreement between learned uncertainty and known physical challenges provides strong evidence that the Bayesian network has learned physically meaningful representations of its own limitations.

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5. Discussion

5.1 Practical Implications for Optical Metrology

The results have significant practical implications for deploying deep learning in precision optical metrology. Quality control workflows can use uncertainty maps to implement selective prediction: automated decisions are made for pixels where the model is confident, while uncertain pixels are flagged for human expert review or alternative measurement methods. The experiments demonstrate that rejecting just 10–15% of most uncertain pixels yields accuracy improvements of 8–10 percentage points—without any change to the underlying model or hardware.

The high-error detection rates (> 88%) achieved by the uncertainty thresholding approach are particularly valuable for safety-critical applications. Rather than relying on a single accuracy metric that masks the distribution of errors, engineers can now know not just what the measurement is, but how much to trust it at each individual pixel.

5.2 Relationship to Prior Work

This work extends both foundational references. From Huang et al. (2023), it takes the empirical observation that certain geometric configurations (concave regions, occlusion zones) systematically produce larger measurement errors, and formalizes this observation as spatially variable epistemic uncertainty that can be automatically learned by Bayesian networks. From Huang et al. (2026), it adopts the principle that deep networks can learn useful representations of complex optical measurement data, and extends this to the task of uncertainty estimation—the network's representation of its own limitations rather than just the physical quantity being measured.

5.3 Limitations

Several important limitations should be noted. First, the current framework requires multiple ($T = 50$) forward passes during inference, increasing computational cost by approximately 50× compared to a single deterministic pass. While this is acceptable for offline inspection workflows, it poses challenges for real-time inline inspection at high throughput. Future work should explore single-pass uncertainty estimation through network architectures designed for efficient uncertainty approximation. Second, the calibration experiments are conducted on simulation data. Real-world calibration may be influenced by distribution shift between simulation and reality—a challenge that can be addressed through domain adaptation techniques. Third, the current framework models only spatial uncertainty (pixel-wise). Global, image-level uncertainty—for out-of-distribution input detection when an entire sample is unlike anything in the training set—remains an open research problem.

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6. Conclusion

This paper proposes a Bayesian uncertainty quantification framework for deep learning in optical surface metrology, extending three representative network architectures (U-Net, RA-U-Net, and DB-3DFuse) with Monte Carlo dropout to produce spatially resolved uncertainty maps alongside predictions.

Comprehensive evaluation across three tasks—thermal image reconstruction, phase unwrapping, and defect detection—demonstrates that the proposed framework produces well-calibrated uncertainty estimates with Expected Calibration Errors of 3.9–5.8%, compared to 12.9–18.3% for deterministic baselines. The uncertainty thresholding approach correctly identifies 88.7–93.2% of high-error predictions as uncertain, and selective prediction experiments show that rejecting just 10% of most uncertain pixels improves accuracy by 8–10 percentage points.

The key contributions are: (1) a unified Bayesian UQ framework applicable across diverse optical metrology tasks and network architectures; (2) demonstration that uncertainty estimates correspond to physically meaningful failure modes identified in prior work; and (3) evidence that uncertainty information enables practically significant improvements in downstream prediction quality through selective prediction.

This work provides a principled foundation for trustworthy deep learning deployment in precision optical metrology and manufacturing quality control, where calibrated uncertainty is essential for safe, reliable automated decision-making.

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