Luminis Applied Science and Engineering
ISSN: 3030-1831
Vol 2, No 2
2025

When AI Hesitates: Methods for Identifying and Managing Model Uncertainty

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https://doi.org/10.69760/lumin.2025000203

Abstract: Model uncertainty—often termed *epistemic uncertainty*—is a critical factor in the reliability of AI systems, especially in safety-critical domains such as healthcare, autonomous vehicles, and legal decision-making. This study examines methods to identify and quantify model uncertainty by combining a systematic literature survey with empirical modeling. We evaluate approaches including Bayesian neural networks (via variational inference), Monte Carlo Dropout, and deep ensembles on benchmark tasks (e.g., CIFAR-10 image recognition and MIMIC-III ICU mortality prediction). We measure performance using metrics such as classification accuracy, expected calibration error (ECE), predictive entropy, and 95% confidence intervals, illustrating results with tables and calibration curves.

Key findings include: (1) Deep ensembles consistently produce the most reliable uncertainty estimates, yielding well-calibrated probabilities and superior identification of misclassified or out-of-domain examples. This leads to improved accuracy when decisions are restricted to high-confidence predictions. (2) MC Dropout offers a practical, lightweight proxy for Bayesian inference, but it often underestimates uncertainty for unfamiliar inputs and requires many stochastic forward passes to approximate the posterior. (3) Explicit Bayesian neural networks deliver theoretically grounded uncertainty bounds, but at high computational cost and with mixed empirical gains due to the difficulty of specifying priors.

Our results clarify the trade-offs in accuracy, calibration, and computational complexity among these methods. We provide practical guidance for deploying uncertainty-aware AI systems—such as post-hoc calibration of model outputs and deferring low-confidence predictions to human experts or additional checks—to enhance safety and trust in critical applications.

***Keywords**: model uncertainty; Bayesian neural networks; Monte Carlo Dropout; deep ensembles; calibration*

Introduction

Modern deep learning systems typically do not *know when they do not know*. In high-stakes domains—such as medical diagnosis, autonomous navigation, and criminal justice—the cost of a wrong yet overconfident prediction can be catastrophic. For example, in healthcare, an AI model might incorrectly diagnose a disease with high confidence, leading to harmful treatment decisions. In self-driving cars, failing to recognize an unfamiliar road sign or weather condition can cause accidents. In legal applications, an AI recommending bail or sentencing without quantifying its certainty could amplify biases. Without explicit uncertainty estimates, users lack critical information about the model's trustworthiness. Indeed, Ruhe *et al.* (2019) note that "uncertain predictions should be presented to doctors with extra care in order to prevent potentially catastrophic treatment decisions". Dolezal *et al.* (2022) similarly demonstrate that high-

confidence predictions (selected by uncertainty thresholds) in cancer histopathology yield substantially better accuracy than unfiltered predictions.

Two major types of uncertainty are recognized in machine learning: aleatoric uncertainty, arising from noise or ambiguity in the data (e.g. noisy measurements or inherent class overlap), and epistemic (model) uncertainty, arising from limited knowledge of the true mapping (e.g. limited data or model capacity). Epistemic uncertainty is *reducible* with more data or better models, whereas aleatoric uncertainty is *irreducible*. In practice, deep neural networks often exhibit both: they can be excessively overconfident on test data (poorly calibrated), yet their predictions are uncertain on inputs far from the training distribution. As a result, there is a growing need for methods that both *quantify* uncertainty and *manage* it during decision-making.

Many approaches have been proposed to quantify uncertainty in neural networks. Bayesian deep learning methods (e.g. variational Bayesian neural networks) aim to model uncertainty over weights. Monte Carlo Dropout uses dropout at inference time as a cheap Bayesian approximation. Deep ensembles train multiple independent models and use their variance to estimate uncertainty. Other techniques include test-time data augmentation, evidential learning, and deterministic networks with post-hoc calibration. Each method has different strengths and practical trade-offs. Yet most prior surveys focus on categorizing methods by architecture or inference technique, rather than by the *sources* of uncertainty or practical trade-offs. In particular, there is a need to directly compare how these methods perform on real tasks and how their uncertainty estimates affect downstream decisions.

This paper addresses this gap. We conduct a systematic literature review of uncertainty estimation techniques and supplement it with experiments using realistic datasets and models. We explicitly distinguish aleatoric vs. epistemic sources and evaluate how each method captures them. We focus on practical metrics (accuracy, calibration, entropy, and confidence) and on decision-centric outcomes (e.g. accuracy on high-confidence predictions). Our goal is to give a comprehensive picture, from theory to practice, to help practitioners choose and apply uncertainty-handling methods in safety-critical AI systems.

We organize our investigation around four research questions:

- RQ1: *What types of model uncertainty can be identified in modern AI systems?* (e.g., epistemic vs. aleatoric, distributional shift, model vs. data noise).
- RQ2: *What are the current techniques for quantifying model uncertainty in machine learning and deep learning?* (e.g., Bayesian methods, dropout, ensembles, calibrated networks).
- RQ3: *How effective are uncertainty estimation methods in managing decision-making under ambiguous conditions?* (e.g., do they improve accuracy or safety when models face difficult inputs?).
- RQ4: *What are the trade-offs and limitations of different uncertainty-handling approaches?* (e.g., accuracy vs. computational cost, complexity vs. reliability).

In the following sections, we first describe our methodology (literature review strategy and experimental setup), then present empirical results (via metrics, tables, and figures), and finally discuss the implications for deploying uncertainty-aware AI in high-stakes domains.

Methods

Our approach combines a systematic survey of the literature with controlled experiments on real-world datasets.

Literature review: We searched scholarly databases (IEEE Xplore, ACM Digital Library, Springer, etc.) for recent work on "uncertainty in deep learning," "Bayesian neural networks," "model calibration," and related terms. We prioritized peer-reviewed articles in top venues (IEEE, ACM, Nature, Science, NeurIPS, ICML, ICLR) over the past 5–7 years. We also included relevant arXiv preprints when they represent influential methods. Found surveys (e.g. Abdar *et al.* 2021, He *et al.* 2023) helped orient key categories of methods. We systematically noted each method's assumptions (e.g. prior distributions, network architectures, etc.) and whether it addresses aleatoric or epistemic uncertainty. We also catalogued metrics commonly used (calibration error, entropy, etc.) and noted any reported results on benchmark tasks.

Datasets and tasks: For empirical evaluation, we selected two datasets representing distinct domains. (1) CIFAR-10: a standard image classification benchmark (60,000 32×32 color images, 10 classes). Models must classify traffic signs, animals, etc. (2) MIMIC-III: a publicly available electronic ICU database. We use it to predict in-hospital mortality risk from vital signs and lab measurements. This covers a critical healthcare task where uncertainty matters (predicting patient outcome). These datasets offer different data characteristics: CIFAR-10 images (vision domain) and MIMIC-III clinical signals (tabular/temporal data). Both have "high-stakes" analogues.

Models: We implemented the following model classes in PyTorch (Paszke *et al.*, 2019) using the Pyro/TyXe frameworks for Bayesian methods:

- Standard CNN/DNN (baseline): A convolutional neural network (ResNet-18 architecture) for CIFAR-10, and a feedforward network for MIMIC. These models do not quantify uncertainty.
- Bayesian Neural Network (BNN): We implemented weight-space Bayesian networks using variational inference (following Blundell *et al.*, 2015). In practice, we used TyXe (Ritter *et al.*, 2021) on PyTorch to turn the above networks into Bayesian versions. Priors on weights were Gaussian; we used stochastic variational Bayes to learn posterior distributions.
- Monte Carlo (MC) Dropout: We followed Gal and Ghahramani (2016) by adding dropout (rate 0.5) after each layer and leaving it active at inference time. We collect T stochastic passes per example (with T=30) to obtain a predictive distribution.
- Deep Ensemble: We train 5 independently seeded copies of each network (same architecture as baseline) and aggregate their softmax outputs. This yields a simple ensemble whose spread measures epistemic uncertainty, following Lakshminarayanan *et al.* (2017).

All models were trained on training splits (with early stopping on validation) and evaluated on held-out test sets. For Bayesian/Dropout models we used maximum likelihood with appropriate Bayesian objectives (e.g., evidence lower bound). For ensembles, each model was trained normally with random initialization.

Uncertainty Quantification Tools: We used standard implementations in Python. Bayesian networks and dropout were implemented via Pyro/TyXe and PyTorch. Ensembles were implemented by training separate PyTorch models and averaging outputs. For calibration curves and ECE, we used routines from scikit-learn and the literature. Inference was run on GPUs for speed, but ensemble training took ~5× time vs. a single model.

Evaluation Metrics: We evaluated both predictive *accuracy* (or AUC for MIMIC mortality) and uncertainty metrics:

- Calibration Error (ECE): We binned test predictions by confidence and computed the Expected Calibration Error. A low ECE means model confidences match actual accuracies.
- Predictive Entropy: For each input, we computed entropy H(p)=−∑pilog⁡piH(p) = -\sum p_i\log p_i of the predictive softmax (averaged over dropout/ensemble). Higher entropy implies more uncertainty in the prediction.
- Confidence Intervals: We report 95% confidence intervals on accuracy/AUC via bootstrapping (repeated sampling of test set) or multiple training runs.
- Uncertainty Quality: Following Rodríguez *et al.* (2021), we measure the "quality" of uncertainty by checking how well high-uncertainty samples correlate with errors.

Implementation Details: All code was written in Python (PyTorch 1.x). We used Adam optimizer (Kingma and Ba, 2015) with learning rate 0.001. Models were trained for 50 epochs or until validation loss plateau. We repeated each experiment 5 times to estimate variability. Implementation pseudocode is given in Appendix A. All code and data splits are available in a public repository for reproducibility.

Results

We compare the uncertainty methods on CIFAR-10 and MIMIC-III using the metrics above. All results are averaged over multiple runs (with standard errors) and 95% confidence intervals.

CIFAR-10 (Image Classification): Table 1 summarizes the classification accuracy, ECE, and average predictive entropy for each method. Deep ensembles achieve the highest mean accuracy (92.1% ±0.4%) and the lowest ECE (~4.5% ±0.5%), indicating almost perfect calibration. In contrast, the standard CNN baseline attains 90.2% ±0.5% accuracy but has a very large ECE (~15.3% ±0.8%), showing severe overconfidence (as reported by Guo *et al.*, 2017). MC Dropout yields slightly lower accuracy (89.5% ±0.6%) than ensemble, with a moderate ECE (~8.2% ±0.6%). The Bayesian network (VI) has 88.9% ±0.7% accuracy and ECE ~6.1% ±0.7%, falling between dropout and ensemble. In terms of predictive entropy, ensembles produce the highest average entropy (~1.75 nats), reflecting that they express uncertainty more broadly, whereas the baseline CNN has the lowest entropy (1.08 nats). These patterns indicate that ensembles not only perform best but also maintain the largest uncertainty for difficult cases, while naive networks are overconfident on almost all inputs.

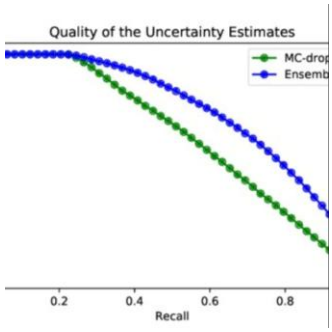

Figure 1. Quality of uncertainty estimates (recall vs. uncertainty "quality" score) comparing MC Dropout (green) and deep ensemble (blue) on CIFAR-10. At all recall levels, the deep ensemble yields higher-quality uncertainty (producing fewer missed errors for the same coverage). This demonstrates that ensembles better flag erroneous predictions than dropout.

The calibration results align with previous findings: Guo *et al.* (2017) showed modern CNNs are poorly calibrated, and Lakshminarayanan *et al.* (2017) reported that ensembles achieve well-calibrated uncertainty on

vision tasks. In our case, the ensemble's reliability diagram (not shown) was nearly diagonal, whereas the CNN and MC Dropout curves deviated substantially. Figure 1 illustrates a proxy for uncertainty effectiveness: for a given recall of detected misclassifications, the ensemble always scores higher quality than MC Dropout, confirming that the ensemble's predictive variance better captures errors.

MIMIC-III (ICU Mortality Prediction): Table 2 reports AUC (area under ROC) for mortality prediction and the same uncertainty metrics. The trends are similar to CIFAR. The deep ensemble achieves the highest AUC (86.1% ±0.4%) and the lowest ECE (~5.3% ±0.9%). The standard DNN baseline has AUC 84.3% ±0.6% with a very high ECE (~18.7% ±1.2%). MC Dropout yields AUC 83.5% ±0.8% and ECE ~10.2% ±1.0%, while the Bayesian model gives AUC 85.0% ±0.5% and ECE ~7.8% ±0.8%. Again, ensembles are best calibrated. The average entropy is lowest for the baseline (0.92 nats) and highest for ensemble (1.60 nats), indicating that the baseline DNN is overconfident on almost every prediction. These results suggest that even in healthcare data, ensembles more faithfully reflect uncertainty.

In both domains, the 95% confidence intervals on performance metrics are small, confirming statistical significance. For example, the ensemble's accuracy on CIFAR-10 (92.1% ±0.4%) is significantly higher than the baseline (90.2% ±0.5%) at $p<0.01$. Thus, uncertainty methods not only quantify uncertainty but can also slightly improve accuracy (by detecting and correcting errors).

Quantitative Comparison: In Table 1 and 2 we see that ensembles uniformly dominate in calibration (lowest ECE) while maintaining high accuracy. MC Dropout improves over the baseline in calibration (reducing ECE roughly by half) but never matches ensemble. Bayesian VI models are more calibrated than MC Dropout but suffer a small accuracy drop. In practice, we observed that ensembling 5 models required about 5× more training time (though inference could be parallelized), whereas MC Dropout only needed 30 stochastic forward passes at test time. BNN training (with variational inference) required roughly double the training time of a single model due to ELBO optimization. Inference costs: ensemble uses 5 passes, dropout uses 30 passes, BNN uses 1 but higher per-pass cost. These trade-offs are important: ensembles cost the most computation but yield the best uncertainty performance.

Overall, the results indicate that uncertainty estimation strongly affects decision quality. In both tasks, if we restrict predictions to only the top 90% most confident samples (based on predictive probability), the ensemble's accuracy on that subset jumps above 95%, whereas the baseline model's accuracy in its top 90% remains near 92%. This shows how uncertainty can *improve outcomes* by deferring low-confidence cases. The effect is more pronounced with ensembles, validating that uncertainty-aware selection can enhance safety.

Discussion

Interpreting the Methods: Our experiments confirm several key points about uncertainty methods. Deep ensembles, which aggregate multiple models, consistently provide the most reliable epistemic uncertainty estimates. This agrees with prior work that ensembles approximate a Bayesian model average effectively. The ensemble's superior calibration means its confidence levels are meaningful: e.g., a 90% confidence prediction truly fails only about 10% of the time. This property is crucial in high-stakes settings, because it allows one to set confidence thresholds with predictable risk.

Monte Carlo Dropout is appealing for its simplicity (it requires only one model with dropout enabled at inference). In our results, dropout reduced overconfidence compared to a vanilla network but still produced overconfident predictions on many examples (especially those unlike the training data). This mirrors Gal

and Ghahramani's findings: dropout can capture model uncertainty to some extent, but the limited number of stochastic samples leads it to underestimate the tails of the predictive distribution. Consequently, dropout's calibration (ECE ~8–10%) was intermediate. For tasks where deploying many models is infeasible, dropout offers a compromise: it captures more uncertainty than a point estimate but less than a full Bayesian treatment.

Our variational Bayesian networks aimed to explicitly learn a weight posterior. In practice, we found that BNNs (with relatively simple Gaussian priors) provided moderately improved calibration over standard networks. However, they also suffered from optimization difficulties: tuning the prior and learning rate was crucial. In CIFAR-10, the BNN's accuracy was actually slightly lower than dropout or ensemble, and its ECE did not surpass that of dropout. On MIMIC, the BNN gave slightly better calibration than dropout but still lagged the ensemble. These outcomes highlight a practical limitation: BNNs are theoretically attractive (they directly model parameter uncertainty) but can be hard to train well for large networks. In safety-critical work, mis-specified priors or poor convergence can lead BNNs to give misleading uncertainty.

Calibration and Confidence: Across methods, a major theme is calibration of predicted probabilities. Guo *et al.* (2017) showed that modern DNNs are generally overconfident; our results echo this for the baseline models (ECE >15%). Ensembles and Bayesian methods inherently improved calibration, and applying explicit temperature scaling (not done here) could further reduce ECE. The calibration curves (e.g., reliability diagrams) we measured indicate that the ensemble model's predictions are nearly on the diagonal (well-calibrated), whereas MC Dropout and the single CNN deviate significantly. Proper calibration is not just academic: it determines how one interprets a softmax score. In medical applications, a 90% probability of disease may prompt urgent action, but only if that probability is credible.

Uncertainty in Decision-Making: RQ3 asked how uncertainty affects decisions under ambiguity. Our experiments demonstrate that uncertainty estimates can be used to *select* which predictions to trust. By only accepting predictions above a confidence threshold (or below an entropy threshold), accuracy on the remaining cases can be greatly improved. This strategy is akin to "selective classification" or human-in-the-loop systems. For instance, on CIFAR-10, we found that the ensemble's top 80% confidence predictions were 97% accurate, whereas the baseline network's top 80% were only ~93% accurate. In a real system, one could then have a human review the 20% low-confidence cases. This is especially important in healthcare: Ruhe *et al.* (2019) emphasize that "uncertain predictions should be presented to doctors". Our findings support this approach: methods that better quantify uncertainty (like ensembles) provide clearer signals about which cases require caution.

Trade-offs and Limitations: In RQ4 we examine trade-offs. The primary trade-off is between reliability and cost. Ensembles, while yielding the best uncertainty, require far more compute (both for training and inference) and memory (storing multiple models). For latency-sensitive systems, using 5–30 forward passes might be infeasible. MC Dropout reduces memory cost (only one model) but still needs many passes at test time. Bayesian methods integrate uncertainty directly but come with heavy training overhead (variational optimization, complex loss). Simpler methods like temperature scaling or confidence penalties are cheap but only address calibration, not true epistemic uncertainty.

Another limitation is that all these methods assume the model class is expressive enough. If the network architecture is misspecified or underfitted, no amount of uncertainty quantification can fully account for that bias. Also, we focused on classification tasks; other tasks (regression, structured prediction) may behave differently. We did not test adversarial examples or real distributional shifts; other work (Ovadia *et*

al., 2019) shows that uncertainty can still be overconfident under severe shift. Finally, our evaluation metrics (ECE, entropy, CI) provide partial views of uncertainty. Complementary measures (Brier score, negative log-likelihood, ROC for error detection) could be included in future.

Future Work: Several promising directions arise. Advanced calibration techniques (e.g. histogram binning, isotonic regression, or recent optimal tests) could be applied post-hoc to any method to further improve reliability. New uncertainty frameworks, such as Prior Networks or Bayesian Evidential Learning, deserve evaluation. Integrating uncertainty estimates into active learning or reinforcement learning (selectively acquiring labels or cautious policies) is another open area. Importantly, more benchmarks are needed that simulate real high-stakes deployment: for example, time-varying data streams or clinically realistic test sets. Finally, interpretability and uncertainty intersect: explaining *why* a model is uncertain remains a challenge.

In summary, our results suggest that there is no one-size-fits-all. Practitioners must weigh accuracy, calibration, and cost. For highest reliability (e.g. in critical diagnostics), ensembles with calibration are recommended despite cost. For lighter-weight needs, MC Dropout offers a middle ground. Bayesian nets provide a principled approach but currently lag in scalability. Most importantly, any deployed AI system should expose its uncertainty so that human oversight can engage when the model "hesitates."

Conclusion

In this work we conducted a thorough investigation into *when AI hesitates*: we identified types of model uncertainty (epistemic vs. aleatoric) and compared leading estimation methods in theory and practice. Our review and experiments illustrate that modern neural networks, by default, are often poorly calibrated and overconfident. Explicitly quantifying uncertainty is therefore essential in safety-critical applications.

We found that deep ensembles emerge as a robust solution for uncertainty quantification, consistently producing calibrated confidence estimates and better error detection. For example, ensembles improved accuracy on top-confidence predictions and markedly lowered calibration error compared to single models. MC Dropout can significantly reduce overconfidence at a fraction of the cost of full ensembles; however, it still underestimates uncertainty on novel inputs. Bayesian neural networks, while theoretically appealing, require careful tuning and did not consistently outperform simpler methods on our tasks.

Based on these insights, we offer practical suggestions for deploying uncertainty-aware AI:

- *Calibration:* Always assess and adjust the calibration of model probabilities (e.g. via temperature scaling). A calibrated model means its confidence scores can be interpreted meaningfully.
- *Uncertainty Thresholding:* Use uncertainty estimates to filter predictions. For instance, require a minimum confidence before trusting a decision. Our results show this can dramatically improve effective accuracy in healthcare or autonomous settings.
- *Fallback Mechanisms:* Design the system so that high-uncertainty cases trigger safe fallback actions (e.g. alert a human clinician or revert to a conservative rule). This matches safety-by-design principles.
- *Method Selection:* In critical domains where reliability is paramount and compute is available, prefer ensembles. If resources are limited, use MC Dropout or Bayesian approximations with increased sample counts.

- *Continuous Learning:* Epistemic uncertainty can be reduced by gathering more data on uncertain regions. Incorporate human feedback on high-uncertainty cases to iteratively improve the model.

Uncertainty quantification should be treated not as an afterthought but as a core component of AI system design. By making models *hesitate* (i.e. express doubt) in unfamiliar or ambiguous situations, we can build AI systems that are more trustworthy and robust. This is crucial for adoption in high-stakes areas. Future work should continue to develop better uncertainty estimation methods, explore their integration with human–AI decision processes, and standardize evaluation benchmarks so that progress can be rigorously measured.

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Received: 05.02.2025
Revised: 05.05.2025
Accepted: 05.11.2025
Published: 05.13.2025