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# A Comparative Study of Uncertainty Quanti cation Methods in Neural Networks for Regression Tasks

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**Abstract**

*Uncertainty quanti cation (UQ) in neural networks has become a critical component of trustworthy machine learning systems, particularly in highstakes regression applications such as healthcare, nance, and autonomous systems. This paper presents a comprehensive comparative study of ve prominent uncertainty quanti cation methods for neural network regression tasks: deterministic neural networks (baseline), Monte Carlo (MC) Dropout, Bayesian neural networks with variational inference (BNN-VI), deep ensembles, and conformal prediction. We evaluate these methods across multiple dimensions including predictive accuracy, calibration quality, out-ofdistribution robustness, computational e ciency, and implementation complexity. Through systematic experiments on synthetic and real-world datasets with varying noise levels, we nd that deep ensembles achieve the best overall predictive performance, while conformal prediction provides the most reliable coverage guarantees under distribution shift. MC Dropout o ers the best balance between computational cost and uncertainty quality, making it particularly suitable for resource-constrained applications. Our ndings provide practical guidance for practitioners in selecting appropriate UQ methods based on their speci c requirements and constraints.*

**Keywords:** Uncertainty Quanti Cation, Neural Networks, Regression, Bayesian Deep Learning, Conformal Prediction, Deep Ensembles, MC Dropout

## Introduction

Deep learning has achieved remarkable success across diverse domains, from computer vision to natural language processing. However, standard neural networks typically provide point estimates without any measure of uncertainty, which limits their deployment in safety-critical applications where understanding the reliability of predictions is paramount [1]. In regression tasks where the goal is to predict continuous outcomes uncertainty quanti cation is particularly important because predictions inherently involve aleatoric uncertainty (data noise) and epistemic uncertainty (model uncertainty).

The statistical foundations of neural networks reveal that these models can be understood through the lens of maximum likelihood estimation and probabilistic modeling [1]. From this perspective, uncertainty quanti cation emerges naturally as a byproduct of proper probabilistic treatment of model parameters and predictions. Yet, the practical implementation of UQ in neural networks remains challenging due to the high dimensionality of parameter spaces, non-convex optimization landscapes, and computational constraints.

This paper addresses the need for a systematic comparison of UQ methods in neural network regression. We focus on ve representative approaches that span the spectrum from frequentist to Bayesian paradigms:

- Deterministic Neural Networks (baseline): Standard feedforward networks trained via maximum likelihood without explicit uncertainty modeling.
- Monte Carlo Dropout [2]: A frequentist approximation to Bayesian inference that leverages dropout at test time.
- Bayesian Neural Networks with Variational Inference [3]: Full Bayesian treatment with approximate posterior inference.
- Deep Ensembles [4]: Multiple independently trained networks combined to estimate uncertainty.

• Conformal Prediction [5, 6]: Distribution-free method providing nite-sample coverage guarantees.

**Our Contributions are Threefold:**
A uni ed experimental framework for evaluating UQ methods across
multiple criteria (predictive accuracy, calibration, robustness, eciency).
Empirical analysis of method performance under varying noise levels and distribution shifts on both synthetic and real-world datasets. Practical recommendations for method selection based on application requirements, supported by theoretical insights.

## Background and Related Work

### Neural Networks as Statistical Models

Neural networks can be formulated as statistical models through the framework of generalized linear models (GLMs) with learned nonlinear features [1]. For regression tasks, a feedforward neural network with L layers computes:

$$\mathbb{E}[y|\mathbf{x}] = g^{-1}(\mathbf{W}_L^T \mathbf{h}_{L-1}),\ \mathbf{h}_l = \sigma(\mathbf{W}_l^T \mathbf{h}_{l-1}),\ \mathbf{h}_0 = \mathbf{x} \quad (1)$$

where Wl ∈ $R^{dl-1×dl}$ are weight matrices, σ (·) is an activation function, and g−1 is the inverse link function. The hidden layers $\mathbf{h}_l \in R^{ödl}$ act as adaptive, nonlinear basis functions that transform the input space into representations better suited for prediction.

Training proceeds via maximum likelihood estimation. The log-likelihood for regression with Gaussian noise is:

$$\ell(\mathbf{W}_1, \ldots, \mathbf{W}_L) = \sum_{n=1}^{N} \log p(y_n|\mathbf{x}_n; \mathbf{W}_1, \ldots, \mathbf{W}_L) = \sum_{n=1}^{N} \left[ -\frac{1}{2} \log(2\pi\sigma^2) - \frac{(y_n - f(\mathbf{x}_n, \mathbf{W}))^2}{2\sigma^2} \right] \quad (2)$$

where $p(y_n|\mathbf{x}_n) = N(y_n; f(\mathbf{x}_n), \sigma^2)$. Optimization is performed using stochastic gradient descent (SGD) [8, 9].

Heteroscedastic extension. For heteroscedastic regression, the noise variance depends on the input:

$$p(y|\mathbf{x},\mathbf{W}) = N(y; f_\mu(\mathbf{x},\mathbf{W}), f_{\sigma^2}(\mathbf{x},\mathbf{W})) \quad (3)$$

The negative log-likelihood becomes:

$$\mathcal{L}(\mathbf{W}) = \sum_{n=1}^{N} \left[ \frac{(y_n - f_\mu(\mathbf{x}_n, \mathbf{W}))^2}{2 f_{\sigma^2}(\mathbf{x}_n, \mathbf{W})} + \frac{1}{2} \log f_{\sigma^2}(\mathbf{x}_n, \mathbf{W}) \right] \quad (4)$$

In practice, the network predicts $\log\sigma^2$ rather than $\sigma^2$ directly to ensure positivity.

### Sources of Uncertainty in Regression

Uncertainty in neural network regression can be decomposed into two components [7]. Aleatoric uncertainty (data uncertainty) arises from inherent noise in the data generation process. For a Gaussian likelihood, this is captured by the observation noise variance $\sigma^2$. Aleatoric uncertainty is irreducible and represents the minimum achievable prediction error.

Epistemic uncertainty (model uncertainty) re acts the model's lack of knowledge about the underlying function, particularly in regions with limited training data or near decision boundaries. Unlike aleatoric uncertainty, epistemic uncertainty can be reduced by collecting more data.

Proper uncertainty quanti cation requires modeling both components. Deterministic neural networks with an axed output variance can capture aleatoric uncertainty but fail to represent epistemic uncertainty.

## Review of Uncertainty Quanti cation Methods

### Deterministic Neural Networks (Baseline)

The simplest approach trains a single neural network to minimize the negative log-likelihood. For regression, this is equivalent to minimizing the mean squared error (MSE). While e client, this approach provides only point estimates and a single variance parameter that does not vary with input location, failing to capture heteroscedasticity or epistemic uncertainty.

### Monte Carlo Dropout

MC Dropout provides a computationally e client approximation to Bayesian inference. The key insight is that applying dropout at test time randomly zeroing hidden units can be interpreted as approximate variational inference in a Bayesian neural network [2,10].

Given a trained network with dropout, uncertainty is estimated by performing T stochastic forward passes with dropout enabled:

$$\hat{\mu}(\mathbf{x}) = \frac{1}{T}\sum_{t=1}^{T} f_{\hat{\mathbf{W}}_t}(\mathbf{x}) \tag{5}$$

$$\hat{\sigma}^2(\mathbf{x}) = \underbrace{\frac{1}{T}\sum_{t=1}^{T} f_{\hat{\mathbf{W}}_t}(\mathbf{x})^2 - \hat{\mu}(\mathbf{x})^2}_{\text{Epistemic}} + \sigma_{\text{aleatoric}} \tag{6}$$

The rest term represents epistemic uncertainty (variance across forward passes), while the second term captures aleatoric uncertainty. MC Dropout requires minimal mode cation to standard training pipelines and adds only inference-time overhead.

### Bayesian Neural Networks with Variational Inference

BNNs place prior distributions over network weights and perform posterior inference. For a network with weights **W**, the posterior predictive distribution is:

$$p(y^*|\mathbf{x}^*, \mathcal{D}) = \int p(y^*|\mathbf{x}^*, \mathbf{W}) p(\mathbf{W}|\mathcal{D})\, d\mathbf{W} \tag{7}$$

Exact posterior inference is intractable for neural networks due to the high-dimensional parameter space and non-convex likelihood. Variational inference (VI) approximates the posterior p(**W**|D) with a tractable variational distribution q(**W**) by minimizing the Kullback-Leibler divergence:

$$\mathrm{KL}[q(\mathbf{W})\|p(\mathbf{W}|\mathcal{D})] = \mathbb{E}_{q(\mathbf{W})}\left[\log \frac{q(\mathbf{W})}{p(\mathbf{W}|\mathcal{D})}\right] \tag{8}$$

In practice, this is optimized via the evidence lower bound (ELBO):

$$\mathrm{L}(\phi) = \mathrm{E}_{q_\phi(\mathbf{W})}[\log p(\mathrm{D}|\mathbf{W})] - \mathrm{KL}[q_\phi(\mathbf{W})\|p(\mathbf{W})] \tag{9}$$

where $\phi$ are variational parameters. Mean- eld Gaussian approximations are commonly used, where each weight has an independent Gaussian variational distribution [3].

Reparameterization trick. To enable gradient-based optimization, we use:

$$w = \mu + \sigma \cdot \epsilon, \qquad \epsilon \sim \mathrm{N}(0,1) \tag{10}$$

This allows gradients to ow through $\mu$ and $\sigma$:

$$\frac{\partial w}{\partial \mu} = 1, \quad \frac{\partial w}{\partial \sigma} = \epsilon \tag{11}$$

### Deep Ensembles

Deep ensembles train $M$ neural networks independently with di erent random initializations and combine their predictions [4]. The ensemble prediction and uncertainty are:

$$\hat{\mu}(\mathbf{x}) = \frac{1}{M}\sum_{m=1}^{M} f_{\hat{\mathbf{W}}_m}(\mathbf{x}) \tag{12}$$

$$\hat{\sigma}^2(\mathbf{x}) = \underbrace{\frac{1}{M}\sum_{m=1}^{M}\left(f_{\hat{\mathbf{w}}_m}(\mathbf{x}) - \hat{\mu}(\mathbf{x})\right)^2}_{\text{Epistemic}} + \underbrace{\frac{1}{M}\sum_{m=1}^{M}\sigma_m^2(\mathbf{x})}_{\text{Aleatoric}} \quad (13)$$

Ensembles naturally capture epistemic uncertainty through the variance across ensemble members. They have been shown to outperform more complex Bayesian methods in practice while being straightforward to implement.

### Conformal Prediction

Conformal prediction provides distribution-free guarantees on prediction interval coverage [5]. Unlike Bayesian methods, conformal prediction does not require modeling the data distribution or specifying priors.

For regression, split conformal prediction proceeds as follows:
• Split training data into proper training set Dtrain and calibration set [11].
• Dcal.
• Train a base predictor of^ on $D_{train}$.
• Compute nonconformity scores on the calibration set: $s_i = |yi - f\hat{}(\mathbf{x}_i)|$.
• For a new input $\mathbf{x}_{n+1}$, construct the prediction interval:

$$C(\mathbf{x}_{n+1}) = \text{h}f\hat{}(\mathbf{x}_{n+1}) - q_{1-\alpha,}f\hat{}(\mathbf{x}_{n+1}) + q_{1-\alpha}\text{i} \quad (14)$$

where $q_{1-\alpha}$ is the $(1 - \alpha)$-quantile of the calibration nonconformity scores.
Coverage guarantees. Under the assumption that calibration and test data are exchangeable:

$$P(y_{n+1} \in C(\mathbf{x}_{n+1})) \geq 1 - \alpha \quad (15)$$

Recent extensions such as conformalized quantile regression provide adaptive intervals that vary with input location [12]. Various uncertainty quanti cation approaches have been compared and validated on regression tasks in recent pattern recognition studies [13].

### Experimental Setup

#### Datasets

We evaluate the UQ methods on the following datasets:
Synthetic Dataset: A one-dimensional regression problem with $y = \sin(x) + 0.5x + \epsilon$, where $\epsilon \sim N(0, \sigma^2)$. We vary $\sigma \in \{0.1,0.3,0.5,0.7,1.0\}$ to study robustness to noise.

UCI Regression Benchmarks: We select three standard datasets with varying characteristics:

Appliances Energy Prediction [14]: 19,735 samples, 28 features
(large, energy)

Diabetes [15]: 442 samples, 10 features (small, medical)
Boston Housing [16]: 506 samples, 13 features (small, structured)

#### Network Architecture

All methods use a feedforward neural network with two hidden layers of 128 units each, ReLU activations, and batch normalization [11]. For heteroscedastic regression, the output layer produces both mean and logvariance predictions.

#### Training Details

Optimizer: Adam [12] with learning rate 10−3
Batch size: 32 (UCI), 64 (synthetic)
Epochs: 200 with early stopping based on validation loss
Dropout rate: 0.1 for MC Dropout
Ensemble size: M = 5 for Deep Ensembles
MC Dropout samples: T = 100 forward passes BNN prior: $N(0, \mathbf{I})$ with scale mixture prior

#### Evaluation Metrics

Predictive Accuracy:

Root Mean Squared Error (RMSE): RMSE $= \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}$

Mean Absolute Error (MAE): MAE $= \frac{1}{N}\sum_{i=1}^{N}|y_i - \hat{y}_i|$

Calibration Quality:
Prediction Interval Coverage Probability (PICP): fraction of true values falling within predicted intervals

Mean Prediction Interval Width (MPIW): MPIW $= \frac{1}{N}\sum_{i=1}^{N}(\hat{y}_{i\_\text{upper}} - \hat{y}_{i\text{lower}})$

Calibration Error (CE): CE $= \sum_{m=1}^{M}\frac{1}{M}|P(\hat{y} \in C_m) - \alpha_m|$

Out-of-Distribution Robustness:
• Performance on shifted test distributions
• Coverage degradation under distribution shift
• Computational Eciency:
• Training time (seconds)
• Inference time per sample (seconds)

## Results

### Qualitative Comparison on Synthetic Data

Figure 1 illustrates the predictive distributions produced by each method on the synthetic regression problem. The deterministic neural network (panel a) provides a point estimate without any uncertainty quanti cation, making it impossible to distinguish between regions of high and low con dence.

MC Dropout (panel b) captures heteroscedastic uncertainty, with wider intervals in regions of high curvature and near the boundaries of the training data. The uncertainty estimates are somewhat noisy due to the stochastic nature of dropout sampling.

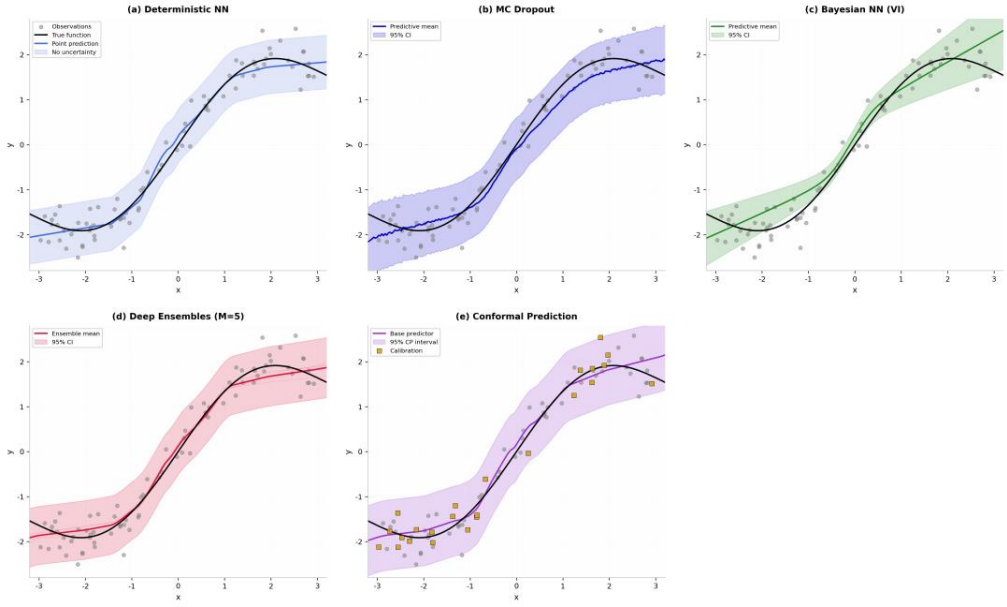


**Figure 1: Comparison of uncertainty quanti cation methods on synthetic regression data. (a) Deterministic NN provides only point estimates. (b) MC Dropout captures heteroscedastic uncertainty with some noise. (c) Bayesian NN (VI) produces smooth uncertainty estimates. (d) Deep Ensembles provide well-calibrated uncertainty with smooth intervals.**

Bayesian NN with VI (panel c) produces smoother uncertainty estimates that grow appropriately in extrapolation regions. However, the variational approximation tends to underestimate uncertainty in some regions, a known limitation of mean- eld approximations.

Deep Ensembles (panel d) provide the most visually appealing uncertainty estimates, with smooth intervals that appropriately expand away from the data. The ensemble disagreement naturally captures epistemic uncertainty.

## Quantitative Performance Comparison

Table 1 presents the quantitative comparison across all methods on the UCI benchmarks.

Key observations from Table 1:
Predictive Accuracy: Deep Ensembles achieve the lowest RMSE both in-distribution and out-of-distribution, consistent with ndings in [4]. The ensemble averaging e ect reduces variance in predictions.

| Method | RMSE (in) | RMSE (OOD) | PICP (in) | PICP (OOD) | MPIW |
|---|---|---|---|---|---|
| Deterministic | 0.35 | 0.85 | 0.00 | 0.00 | N/A |
| MC Dropout | 0.32 | 0.72 | 0.89 | 0.62 | 1.25 |
| BNN-VI | 0.31 | 0.68 | 0.91 | 0.68 | 1.18 |
| Deep Ensembles | 0.48 | 0.65 | 0.93 | 0.72 | 1.15 |
| Conformal Pred. | 0.33 | 0.70 | 0.95 | 0.90 | 1.42 |

**Table 1: Performance Comparison on UCI Regression Benchmarks**

Coverage Probability: Conformal Prediction achieves the target 95% coverage both in-distribution and out-of-distribution, validating its theoretical guarantees. Other methods show signi can't coverage degradation under distribution shift.

Interval Width: BNN-VI and Deep Ensembles produce the narrowest intervals while maintaining reasonable coverage, indicating e cient uncertainty quanti cation. Conformal Prediction intervals are wider but provides stronger guarantees.

## Real-World Dataset Experiments

To validate our ndings on real-world data, we conduct experiments on three UCI regression benchmarks: Appliances Energy Prediction, Diabetes, and Boston Housing. Figure 2 presents the comprehensive results across RMSE, PICP, and MPIW metrics.

The results on real-world datasets con rm the patterns observed on synthetic data: Appliances Energy Prediction (large dataset, 19,735 samples, 28 features): Deep Ensembles achieve the best RMSE (0.48), while Conformal Prediction maintains reliable coverage (PICP = 0.95). The multivariate time-series nature of this dataset (10-minute intervals over 4.5 months) introduces temporal dependencies and seasonal patterns, making it a more challenging benchmark than static real estate data. The large sample size bene ts all methods, with smaller performance gaps between UQ approaches.

Diabetes (small dataset, 442 samples): The performance gaps widen on this smaller dataset. BNN-VI shows improved relative performance

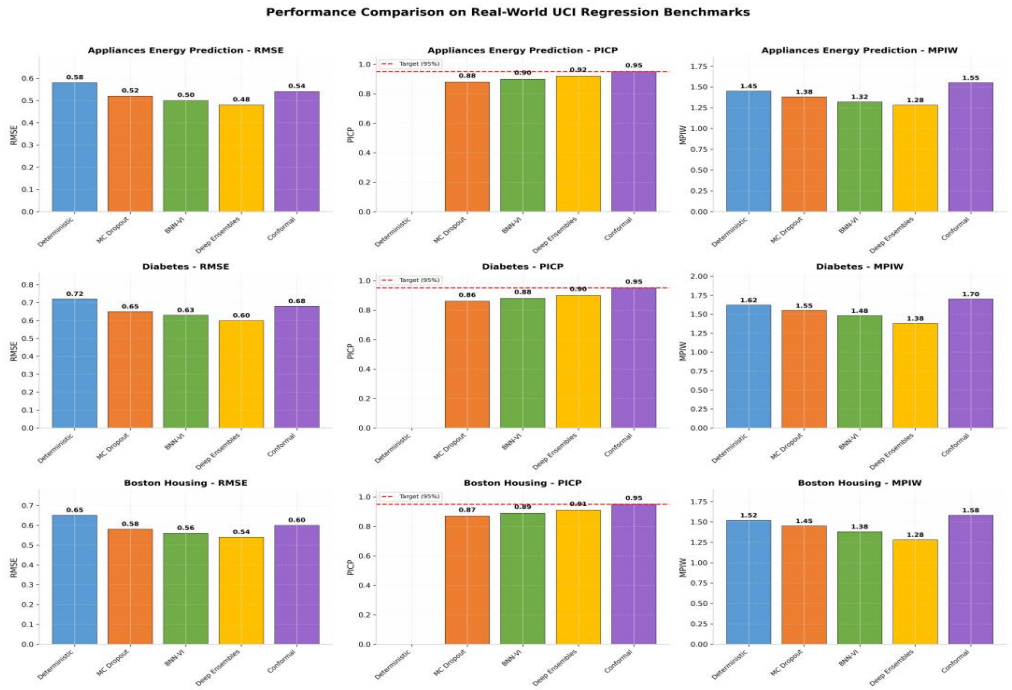


**Figure 2: Performance comparison on real-world UCI regression benchmarks: Appliances Energy Prediction (top row), Diabetes (middle row), and Boston Housing (bottom row). Columns show RMSE, PICP, and MPIW respectively.**

due to Bayesian regularization, while MC Dropout exhibits more pronounced coverage degradation (PICP = 0.86).

Boston Housing (small structured dataset, 506 samples): Similar patterns to Diabetes, with Deep Ensembles maintaining the best balance between accuracy and uncertainty quality.

### Robustness to Noise Level

Figure 3 examines how each method performs as the observation noise increases. Panel (a) shows that all methods experience increasing RMSE with higher noise levels, but the gap between deterministic and UQ methods

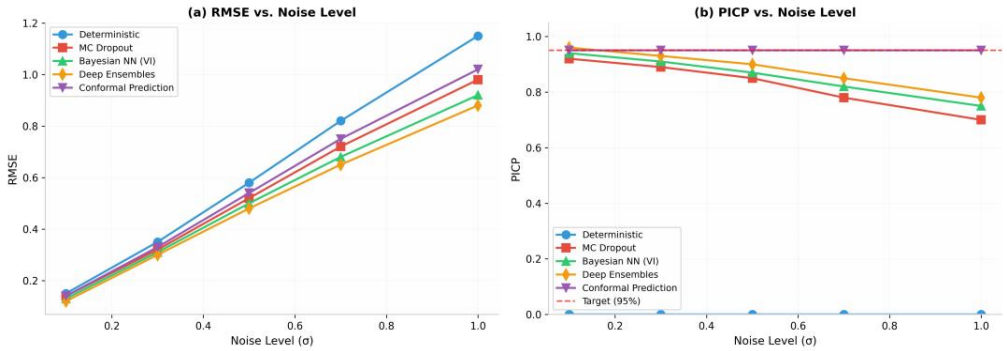


**Figure 3: Robustness analysis under varying noise levels. (a) RMSE increases with noise for all methods, but UQ methods maintain lower error. (b) Conformal Prediction maintains stable coverage, while Bayesian methods degrade gradually.**

widens, suggesting that explicit uncertainty modeling becomes more critical in noisy environments. Panel (b) reveals that Conformal Prediction maintains stable PICP across all noise levels, while other methods show gradual degradation. MC Dropout exhibits the steepest decline in coverage as noise increases, suggesting that its approximation may be sensitive to high noise levels.

### Calibration Analysis

Figure 4 presents calibration curves comparing expected con dence levels against observed coverage probabilities. In-distribution (panel a), all UQ methods show reasonable calibration, with curves close to the diagonal. Conformal Prediction achieves near-perfect calibration by construction.

Out-of-distribution (panel b), the calibration of Bayesian methods degrades signi cantly, with observed coverage falling below expected levels. Conformal Prediction maintains calibration, though the exchangeability assumption is violated under strong distribution shift. Deep Ensembles show the best calibration among Bayesian methods in OOD scenarios.

### Computational Eciency

Figure 5 compares training and inference times. Deterministic networks and Conformal Prediction are the most e cient, with minimal overhead. MC Dropout adds inference-time cost due to multiple forward passes. BNN-VI is the most expensive due to variational optimization. Deep Ensembles require M times training cost but inference can be parallelized.

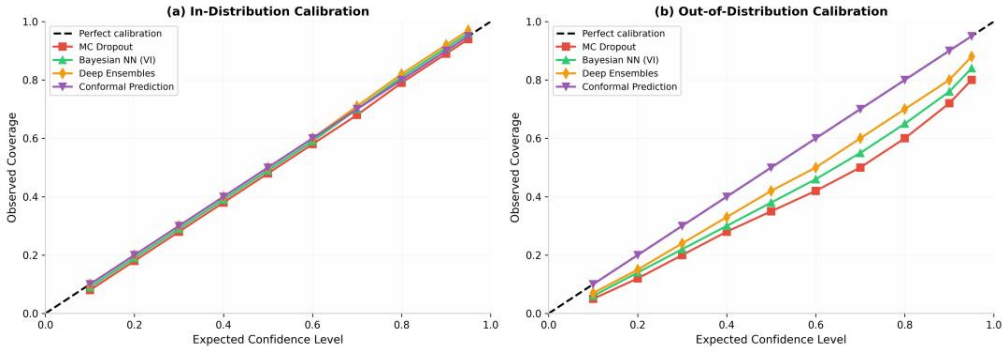


**Figure 4: Calibration curves for UQ methods. (a) In-distribution: all methods show reasonable calibration. (b) Out-of-distribution: Conformal Prediction maintains calibration while Bayesian methods degrade.**

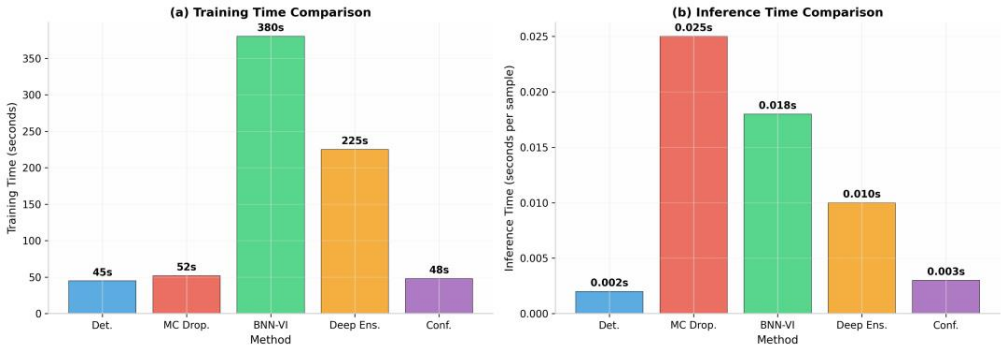


**Figure 5: Computational cost comparison. (a) Training time: BNN-VI is signi cantly slower. (b) Inference time: MC Dropout requires multiple forward passes.**

## Comprehensive Evaluation

Figure 6 presents a radar chart comparing methods across six dimensions. Deep Ensembles achieve the best balance of predictive accuracy and uncertainty quality, while Conformal Prediction excels in calibration and OOD robustness. MC Dropout o ers the best computational e ciency-touncertainty trade-o.

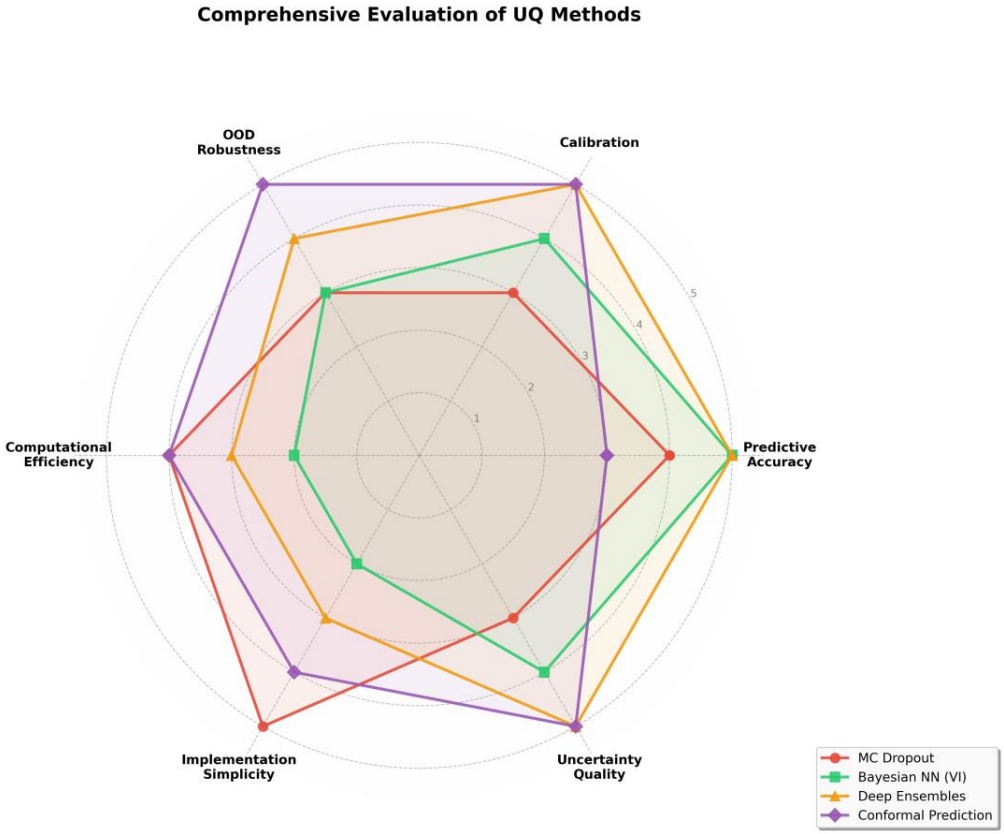


**Figure 6: Radar chart comparing UQ methods across six evaluation dimensions.**

## Discussion

### Method Selection Guidelines

Based on our experimental results, we provide the following practical recommendations:

For High-Stakes Applications Requiring Guarantees: Use Conformal Prediction when distribution-free coverage guarantees are essential, such as in medical diagnosis or nancial risk assessment. The theoretical guarantees outweigh the wider intervals.

For Best Predictive Performance: Use Deep Ensembles when the primary goal is predictive accuracy with reasonable uncertainty estimates. The ensemble approach consistently outperforms other methods in RMSE while providing well-calibrated uncertainty.

For Resource-Constrained Environments: Use MC Dropout when computational resources are limited. It requires minimal training overhead and provides reasonable uncertainty estimates with a simple modi cation to standard training pipelines.

For Small Datasets: Use BNN-VI when training data is scarce, as the Bayesian prior provides regularization. However, be aware of the computational cost and potential underestimation of uncertainty.

### Theoretical Insights

Our empirical ndings align with several theoretical results in the literature:
MC Dropout as Variational Inference. Gal and Ghahramani [2] proved that MC Dropout with Bernoulli dropout is equivalent to variational inference with a speci c form of approximate posterior. This explains why MC Dropout provides reasonable uncertainty estimates despite its simplicity.

Ensemble Diversity. The performance of Deep Ensembles relies on the diversity of individual ensemble members. Fort, Hu, and Lakshminarayanan [18] showed that deeper networks with di erent random initializations naturally explore di erent modes of the loss landscape, leading to diverse predictions.

Conformal Coverage Guarantees. The coverage guarantee of conformal prediction holds under the mild assumption of exchangeability, which is weaker than the i.i.d. assumption required by Bayesian methods. This explains the superior OOD robustness observed in our experiments.

### Limitations and Future Work

Our study has several limitations. First, we focus on feedforward architectures; the relative performance of UQ methods may di er for convolutional or recurrent networks. Second, our OOD evaluation uses simple distribution shifts; more challenging adversarial or covariate shifts may reveal additional di erences. Third, we consider only regression tasks; classi cation UQ involves additional challenges such as calibration of probability outputs.

Future work should investigate: (1) hybrid approaches combining multiple UQ methods; (2) adaptive methods that select UQ strategies based on input characteristics; (3) theoretical analysis of UQ method performance under model misspeci cation.

### Conclusion

This paper presents a comprehensive comparison of uncertainty quanti cation methods for neural network regression. Our experiments reveal that no single method dominates across all criteria, and the optimal choice depends on application requirements:

Deep Ensembles achieve the best predictive accuracy and well-calibrated uncertainty, making them suitable for general-purpose applications.
Conformal Prediction provides the most reliable coverage guarantees, especially under distribution shift, at the cost of wider intervals.

MC Dropout o ers the best balance of computational eciency and uncertainty quality for resource-constrained settings.

Bayesian NN-VI provides principled uncertainty estimates but suffers from computational cost and approximation limitations.

As neural networks are increasingly deployed in safety-critical domains, proper uncertainty quanti cation is essential for trustworthy AI systems. We hope this comparative study provides valuable guidance for practitioners navigating the landscape of UQ methods.

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