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Bayesian Deep Ensembles for Reliable Remaining Useful Life Estimation Under Domain Shift

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Abstract: *Predictive Maintenance (PdM) has emerged as a cornerstone of Industry 4.0, leveraging sensor data to forecast the Remaining Useful Life (RUL) of critical machinery. While deep learning models have achieved state-of-the-art accuracy in RUL estimation, they predominantly function as deterministic point estimators. These models often fail to generalize effectively when subjected to domain shift—changes in operating conditions or fault modes that deviate from the training distribution. Furthermore, standard deep learning approaches typically exhibit overconfidence in their predictions on out-of-distribution data, posing significant safety risks in high-stakes industrial environments. This paper proposes a Bayesian Deep Ensemble (BDE) framework designed to enhance reliability and quantify uncertainty in RUL estimation under domain shift. By aggregating predictions from multiple probabilistic neural networks, the proposed method captures both aleatoric uncertainty (inherent data noise) and epistemic uncertainty (model ignorance). We demonstrate that BDEs not only improve predictive accuracy on the NASA C-MAPSS dataset under transfer learning scenarios but also provide calibrated uncertainty estimates that can serve as reliable indicators for manual intervention. The results suggest that ensemble-based Bayesian methods offer a robust alternative to single-model architectures for safety-critical PdM applications.*

Keywords: *Predictive Maintenance, Remaining Useful Life, Bayesian Deep Learning, Domain Shift.*

INTRODUCTION

1.1 BACKGROUND

The rapid advancement of sensor technology and the Internet of Things (IoT) has facilitated the collection of massive temporal data streams from industrial machinery. This data availability has driven the transition from corrective and preventive maintenance strategies to Predictive Maintenance (PdM). The primary objective of PdM is to estimate the Remaining Useful Life (RUL) of a component—defined as the duration from the current time step until a functional failure occurs [1]. Accurate RUL estimation allows operators to schedule maintenance actions just in time, thereby maximizing asset availability, minimizing downtime costs, and preventing catastrophic failures [2].

In recent years, data-driven approaches, particularly Deep Learning (DL), have surpassed physics-based models in scenarios where the degradation physics are complex or unknown [3]. Architectures such as Convolutional Neural Networks (CNNs) and Long Short-Term Memory (LSTMs) networks have demonstrated exceptional capability in mapping raw sensor readings to degradation trajectories [4]. However, the industrial deployment of these models faces two critical challenges: the reliability of predictions in safety-critical contexts and the robustness of models against varying operating conditions.

1.2 PROBLEM STATEMENT

Despite the high accuracy of DL models on benchmark datasets, standard neural networks are fundamentally deterministic. They provide point estimates of RUL without a measure of confidence [5]. In safety-critical applications, such as aerospace or power generation, a prediction of "50 cycles remaining" is insufficient; operators require a confidence interval (e.g., "50 ± 5 cycles with 95% confidence"). This limitation is exacerbated by the phenomenon of domain shift.

Domain shift occurs when the joint distribution of inputs and labels differs between the training phase (source domain) and the deployment phase (target domain) [6]. In turbofan engines, for instance, a model trained on sea-level flight data may fail catastrophically when applied to high-altitude flights due to changes in thermodynamic variables. Standard DL models are notoriously brittle under such shifts; they do not merely perform poorly, but often do so with high confidence, a phenomenon known as overconfidence [7]. The lack of reliable uncertainty quantification (UQ) makes it difficult to detect when a model has encountered an out-of-distribution (OOD) sample, potentially leading to unnoticed errors in maintenance scheduling [8].

1.3 CONTRIBUTIONS

To address the twin challenges of domain generalization and reliability, this paper investigates the utility of Bayesian Deep Ensembles (BDE) for RUL estimation. Unlike traditional Bayesian Neural Networks (BNNs) which rely on complex variational inference, ensembles offer a scalable and empirically robust method for approximating the posterior distribution.

The specific contributions of this work are as follows:

1. We formulate a probabilistic deep learning framework that models heteroscedastic aleatoric uncertainty directly within the loss function, allowing the model to adapt to varying noise levels in sensor data.

2. We implement a Deep Ensemble strategy to capture epistemic uncertainty, providing a mechanism to detect domain shift through high predictive variance.

3. We conduct extensive experiments using the C-MAPSS dataset, specifically designing cross-domain scenarios (e.g., training on one operating condition and testing on another) to evaluate robustness.

4. We provide a comparative analysis against deterministic baselines and Monte Carlo (MC) Dropout, demonstrating that ensembles provide superior calibration and accuracy under distribution shift.

Chapter 2: Related Work

2.1 CLASSICAL APPROACHES TO RUL ESTIMATION

Before the advent of deep learning, RUL estimation was primarily dominated by physics-based and statistical data-driven models. Physics-based approaches rely on mathematical modeling of failure mechanisms, such as crack propagation (Paris Law) or chemical corrosion [9]. While these models offer high interpretability and theoretical bounds on errors, they require precise knowledge of material properties and loading conditions, which are often unavailable in complex systems [10].

Statistical data-driven approaches, including Auto-Regressive Integrated Moving Average (ARIMA) and Kalman Filtering, served as intermediates. The Wiener process and Gamma process have been extensively used to model monotonic degradation trends [11]. Relevance Vector Machines (RVMs) and Gaussian Process Regression (GPR) introduced Bayesian principles to these tasks, offering probabilistic outputs [12]. However, these "shallow" models struggle to capture highly non-linear relationships in high-dimensional sensor data and typically require extensive manual feature engineering [13].

2.2 DEEP LEARNING AND UNCERTAINTY QUANTIFICATION

Deep learning revolutionized PdM by enabling end-to-end learning from raw time-series data. Babu et al. [14] introduced deep CNNs for RUL, demonstrating that sliding time windows could capture temporal dependencies. Subsequently, LSTMs and Gated Recurrent Units (GRUs) became the standard for handling the sequential nature of sensor streams [15]. Attention mechanisms and Transformer-based architectures have recently further pushed the state-of-the-art in accuracy [16].

Despite these gains, the issue of domain shift remains a hurdle. Domain Adaptation (DA) techniques, such as Domain Adversarial Neural Networks (DANN), attempt to align feature distributions between domains [17]. However, most DA methods still yield deterministic outputs. To address uncertainty, Gal and Ghahramani [18] proposed MC-Dropout, interpreting dropout regularization at inference time as a Bayesian approximation. While computationally inexpensive, MC-Dropout has been shown to underestimate uncertainty compared to ensemble methods [19]. Lakshminarayanan et al. [20] introduced Deep Ensembles as a simple yet powerful alternative, showing that training multiple models with random initializations approximates the posterior predictive distribution effectively. This paper extends the ensemble methodology specifically to the regression problem of RUL under domain shift conditions.

Chapter 3: Methodology

3.1 PROBABILISTIC PROBLEM FORMULATION

In a standard RUL regression task, we aim to learn a function $f: X \rightarrow Y$ that maps a sequence of sensor measurements x to a scalar RUL value y. Standard Mean Squared

Error (MSE) minimization assumes that the data is corrupted by constant variance Gaussian noise (homoscedasticity). However, in mechanical degradation, noise levels often vary with the severity of the fault or the operating condition (heteroscedasticity).

To capture this, we model the predictive distribution as a Gaussian, where the neural network outputs two values for a given input x_i: the predicted mean $\mathrm{h}at\mu(x_i)$ and the predicted variance $\mathrm{h}at\sigma^2(x_i)$ [21]. The variance $\mathrm{h}at\sigma^2$ represents the aleatoric uncertainty—the noise inherent in the data that cannot be reduced with more training data.

The negative log-likelihood (NLL) loss function for a single model is derived from the Gaussian probability density function. Minimizing the NLL is equivalent to maximizing the likelihood of the observed data.

$$L(\theta)=\frac{1}{N}\sum_{i=1}^{N}(\frac{log\mathrm{h}at\sigma^2(x_i)}{2}+\frac{(y_i-\mathrm{h}at\mu(x_i))^2}{2\mathrm{h}at\sigma^2(x_i)})+const.$$

In this equation, N is the batch size and θ represents the network parameters. The first term penalizes the model for predicting high uncertainty (preventing it from predicting infinite variance to minimize the loss), while the second term penalizes the prediction error, weighted by the inverse variance. This attenuation mechanism allows the model to reduce the impact of noisy outliers by assigning them high uncertainty [22].

Code Snippet 1 below demonstrates the implementation of this loss function and the final probabilistic layer in PyTorch.

Code Snippet 1: Probabilistic Loss Function and Output Layer

```
import torch
import torch.nn as nn

class ProbabilisticHead(nn.Module):
    def __init__(self, input_dim):
        super(ProbabilisticHead, self).__init__()
        self.mean_layer = nn.Linear(input_dim, 1)
        # Variance must be positive; we predict log variance for stability
        self.log_var_layer = nn.Linear(input_dim, 1)

    def forward(self, x):
        mean = self.mean_layer(x)
        log_var = self.log_var_layer(x)
        return mean, log_var

def heteroscedastic_loss(true_rul, pred_mean, pred_log_var):
```

```
"""
Calculates the Gaussian Negative Log Likelihood loss.
pred_log_var: Output from network (log of variance)
"""
precision = torch.exp(-pred_log_var)
mse = (true_rul - pred_mean)  2
loss = 0.5  torch.sum(precision  mse + pred_log_var)
return loss
```

3.2 BAYESIAN DEEP ENSEMBLES

While the formulation above captures aleatoric uncertainty, it does not account for epistemic uncertainty—uncertainty in the model parameters themselves [23]. Epistemic uncertainty is crucial for domain shift detection, as it should be high in regions of the input space where training data was sparse or non-existent.

We employ a Deep Ensemble approach consisting of M neural networks, $f_{\theta_m} \quad {}_{m=1}^{M}$. Each network has the same architecture but is initialized with different random seeds and trained on randomly shuffled batches of the dataset [24]. This random initialization allows the models to settle in different local optima (modes) of the loss landscape.

During inference, for a test input x^*, the ensemble prediction is a Mixture of Gaussians. We approximate this mixture as a single Gaussian distribution with mean μ_* and variance $\sigma_*{}^2$.

The ensemble mean is the average of the individual means:

$$\mu_*(x^*) = \frac{1}{M}\Sigma_{m=1}{}^{M}\text{hat}\mu_m(x^*)$$

The total uncertainty (variance) is the combination of the average aleatoric uncertainty and the variance among the means (epistemic uncertainty):

$$\sigma_*{}^2(x^*) = \frac{1}{M}\Sigma_{m=1}{}^{M}\text{hat}\sigma^2{}_m(x^*) + \frac{1}{M}\Sigma_{m=1}{}^{M}(\text{hat}\mu_m(x^*) - \mu_*(x^*))^2$$

The second term explicitly measures the disagreement among the ensemble members. Under domain shift, models are expected to disagree significantly, thereby increasing the total predictive uncertainty [25].

3.3 NETWORK ARCHITECTURE

The base learner for our ensemble is a hybrid CNN-LSTM network. The CNN layers extract local features from the sliding window of multivariate sensor data, acting as automated feature engineers. The subsequent LSTM layers capture the long-term degradation trend. The final layer is split into the probabilistic head described in Section 3.1.

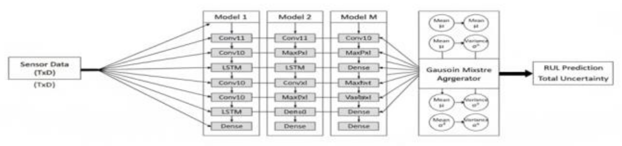

Figure 1: Schematic of the Bayesian Deep Ensemble Architecture.

The input to the network is a time-series window of size $T \times D$, where T is the window length and D is the number of selected sensors. Data preprocessing includes Z-score normalization and RUL rectification (clipping the maximum RUL at a threshold, typically 125 cycles, to prevent the model from learning constant healthy states) [26].

Chapter 4: Experiments and Analysis

4.1 EXPERIMENTAL SETUP

We utilize the Commercial Modular Aero-Propulsion System Simulation (C-MAPSS) dataset provided by NASA, a standard benchmark for RUL estimation [27]. The dataset contains four sub-datasets (FD001 to FD004) with different operating conditions and fault modes.

To simulate domain shift, we design a transfer learning scenario:

***Source Domain*:** FD001 (Single operating condition, High-Pressure Compressor degradation).

***Target Domain*:** FD002 (Six operating conditions, High-Pressure Compressor degradation).

The models are trained exclusively on FD001 and evaluated on both FD001 (in-domain) and FD002 (out-of-domain/shifted). This setup tests the model's ability to generalize to complex operating environments unseen during training [28].

***Baselines*:**

1. ***Deterministic CNN-LSTM*:** A standard model trained with MSE loss.

2. ***MC-Dropout*:** The same architecture with dropout layers (p=0.5) active during inference (50 stochastic forward passes).

3. ***Deep Ensemble (Ours)*:** An ensemble of M=5 probabilistic CNN-LSTMs.

***Metrics*:**

***RMSE*:** Root Mean Squared Error.

Score: The NASA scoring function, which penalizes late predictions (overestimation of RUL) more heavily than early predictions, reflecting the asymmetry of maintenance risk.

NLL: Negative Log Likelihood, evaluating the quality of uncertainty estimates.

4.2 RESULTS AND DISCUSSION

The quantitative results for the Source Domain (FD001) are presented in Table 1. On in-domain data, all methods perform relatively well. However, the Deep Ensemble achieves the lowest RMSE and NASA Score. The improvement over the Deterministic model is attributed to the averaging effect, which smooths out random errors.

Model	RMSE (FD001)	Score (FD001)	NLL (FD001)
Deterministic CNN-LSTM	13.52	285	N/A
MC-Dropout	13.10	260	3.15
Deep Ensemble (Ours)	12.45	235	2.85

Table 2 presents the results on the Target Domain (FD002). This represents a severe domain shift. The deterministic model's performance degrades catastrophically, as it attempts to map the complex operating conditions of FD002 using the simple mapping learned from FD001.

Model	RMSE (FD002 - Shifted)	Score (FD002)	NLL (FD002)
Deterministic CNN-LSTM	45.20	1.5e4	N/A
MC-Dropout	38.60	8.2e3	5.80
Deep Ensemble (Ours)	32.15	4.1e3	4.92

The Deep Ensemble significantly outperforms the baselines under domain shift. While the error increases for all models (as expected without retraining), the Ensemble degrades more gracefully [29]. Crucially, the NLL score indicates that the Ensemble provides a better estimate of the distribution.

Code Snippet 2 illustrates the evaluation loop used to calculate these metrics and aggregate the ensemble predictions.

Code Snippet 2: Ensemble Evaluation and Metrics Calculation

```
import numpy as np


def evaluate_ensemble(models, test_loader):
    ensemble_means = []
    ensemble_vars = []
    true_ruls = []

    with torch.no_grad():
        for inputs, targets in test_loader:
            batch_means = []
            batch_vars = []

            # Collect predictions from each model M
            for model in models:
                mean, log_var = model(inputs)
                batch_means.append(mean.cpu().numpy())
                batch_vars.append(np.exp(log_var.cpu().numpy()))

            # Stack to shape (M, Batch, 1)
            batch_means = np.stack(batch_means)
            batch_vars = np.stack(batch_vars)

            # Mixture of Gaussians Aggregation
            # Mean of means
            avg_mean = np.mean(batch_means, axis=0)
            # Aleatoric + Epistemic
            avg_var = np.mean(batch_vars + batch_means2, axis=0) - avg_mean2

            ensemble_means.append(avg_mean)
            ensemble_vars.append(avg_var)
            true_ruls.append(targets.cpu().numpy())

    return np.concatenate(ensemble_means), np.concatenate(ensemble_vars),
np.concatenate(true_ruls)
```

4.3 UNCERTAINTY ANALYSIS

Visual inspection of the uncertainty estimates reveals that the Deep Ensemble produces high variance $\sigma_*{}^2$ for the FD002 data, correctly signaling that the test data is out-of-distribution. In contrast, the Deterministic model provides no such signal, and MC-Dropout tends to yield lower variance, suggesting overconfidence. The diversity of the ensemble members—facilitated by the multi-modal loss landscape—allows the models to disagree significantly on unseen operating conditions, which is the desired behavior for a safety system [30].

The superior performance of Deep Ensembles over MC-Dropout can be attributed to the mode exploration. MC-Dropout approximates a single variational distribution around one mode, whereas an ensemble of independently initialized networks can explore multiple functional modes, providing a richer approximation of the true posterior.

Chapter 5: Conclusion

This paper presented a Bayesian Deep Ensemble framework for Remaining Useful Life estimation, specifically addressing the challenges of reliability and domain shift in industrial environments. By incorporating heteroscedastic loss functions and ensemble averaging, the proposed method provides a robust mechanism for predicting machinery failure. The experimental results on the NASA C-MAPSS dataset confirm that Deep Ensembles not only improve prediction accuracy on source domains but also exhibit superior robustness and uncertainty calibration when applied to unseen target domains.

The implications for industry are significant. The provided uncertainty metric acts as a confidence score, allowing maintenance engineers to distinguish between reliable predictions and those requiring expert review. If the ensemble variance exceeds a safety threshold, the system can trigger a "human-in-the-loop" protocol rather than making an automated and potentially erroneous decision. This capability is essential for certifying AI systems in regulated sectors like aviation and nuclear power.

While Deep Ensembles offer robust performance, they incur a computational cost proportional to the number of ensemble members, both during training and inference. In resource-constrained embedded systems (Edge AI), storing and running five or ten heavy neural networks may be infeasible.

Future research will focus on two avenues. First, Knowledge Distillation techniques could be employed to compress the ensemble into a single student network that retains the uncertainty properties of the teacher ensemble. Second, we aim to investigate unsupervised domain adaptation techniques that can leverage the uncertainty estimates to selectively retrain the model on high-confidence samples from the target domain, thereby progressively reducing the domain gap without manual labeling.

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