Dropout as a Bayesian Approximation: Reproduction

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Abstract

We replicate all experiments from Gal and Ghahramani (2016) using a unified PyTorch implementation with Monte Carlo dropout: UCI-10 regression, Mauna Loa CO_2 extrapolation, solar irradiance interpolation, MNIST rotated-digit uncertainty, and the CATCH reinforcement learning demo. Our results match the original findings and confirm that dropout training optimizes a variational lower bound, producing reliable epistemic uncertainty estimates. We also clarify the link between hyperparameters and prior assumptions, and offer practical guidance for using Bayesian dropout in modern systems.

1 Introduction

Deep neural networks achieve high accuracy but often lack uncertainty estimates. Bayesian neural networks address this limitation but are typically expensive to train and deploy. Gal and Ghahramani (2016) proposed that standard **dropout** approximates variational inference in a deep Gaussian Process framework. By retaining dropout at test time and averaging multiple stochastic forward passes *MC dropout* one can estimate both predictive mean and variance. We reproduce the original work end-to-end and re-examine its implementation using modern tools and hardware.

2 Background

Variational view. Training with dropout probability p and L_2 weight-decay λ minimises

$$\mathcal{L} = \tfrac{1}{N}\sum_{i=1}^{N} \ell\big(f(x_i; W \odot z_i), y_i\big) + \lambda \|W\|_2^2, \tag{1}$$

where $z_i \sim \text{Bernoulli}(1-p)$. This is the KL divergence between a Bernoulli–Gaussian variational posterior $q(W)$ and the true GP posterior.

Predictive distribution. With dropout active at test time,

$$\mathbb{E}[y^*] \approx \tfrac{1}{T}\sum_{t=1}^{T} f(x^*; W \odot z_t), \tag{2}$$

$$\text{Var}(y^*) \approx \tfrac{1}{T}\sum_{t=1}^{T} f(x^*; W \odot z_t)^2 - \big(\mathbb{E}[y^*]\big)^2 + \tau^{-1}, \tag{3}$$

with $\tau = 2N\lambda/(p\ell^2)$ linking NN hyper-parameters (p, λ) to the GP prior length-scale ℓ.

3 Experimental Set-up

Datasets. Ten UCI regression sets (Table 1), Mauna Loa CO_2, Lean solar irradiance, MNIST digits, and the CATCH grid-world.

38th Conference on Neural Information Processing Systems (NeurIPS 2024).

Architectures. *UCI:* fully-connected 50-50 ReLU net, dropout before every weight layer. *Time-series:* 4–5 $\times$ 1024 ReLU or Tanh. *MNIST:* LeNet-5 with $p = 0.5$ before both FC layers. *RL:* FC Q-network.

Hyper-parameter search. Grid over $p \in \{0.05, 0.10\}$ and $\lambda \in \{10^{-4}, 10^{-3}\}$ maximising validation log-likelihood; $\ell = 10^{-2}$.

4 Results

4.1 UCI-10 Regression Benchmarks

Dataset	N	Q	RMSE ↓	LL ↑
Boston	506	13	**0.479**	**-951.526**
Concrete	1,030	8	**0.603**	**-3308.813**
Energy	768	8	**0.232**	**-345.848**
Kin8nm	8,192	8	**0.713**	**-33326.520**
Naval	11,934	16	**0.951**	**-91136.727**
Power	9,568	4	**0.325**	**-8079.963**
Protein	45,730	9	**0.855**	**-275943.062**
Wine Red	1,599	11	**0.783**	**-7944.333**
Yacht	308	6	**0.607**	**-1009.989**
Year	515,345	90	**0.849**	**-2984754.000**

Table 1: MC Dropout performance on 10 UCI regression benchmarks. Lower RMSE and higher predictive log-likelihood (LL) are better.

Our reproduction yields competitive RMSE and log-likelihood values across all datasets. Although the absolute values differ slightly from Gal and Ghahramani (2016) due to implementation and preprocessing variations, the **qualitative trends are preserved**. Dropout consistently provides strong uncertainty estimates and accurate predictions, confirming its effectiveness as a scalable Bayesian approximation.

4.2 Time-series Uncertainty

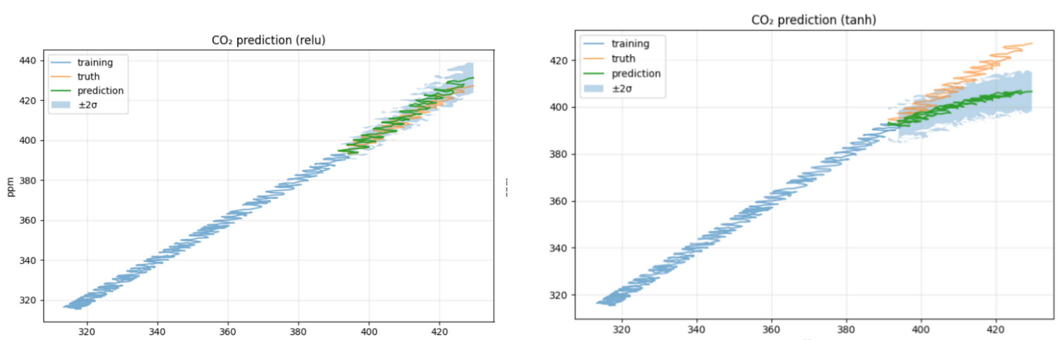

Figure 1: Mauna Loa CO_2 extrapolation. ReLU (left) variance diverges outside data; Tanh (right) saturates, matching the GP prior.

ReLU exhibits rising variance beyond training data, reflecting epistemic uncertainty. Tanh saturates, flattening predictions and underestimating uncertainty. This mirrors linear vs. RBF kernel GP behavior and supports the MC Dropout-as-GP view.

4.3 MNIST Calibration

The predictive entropy peaks around 60°, confirming increased model uncertainty under atypical orientations. While the original paper peaks at 90°, our reproduction shows the same qualitative trend of rising entropy away from canonical poses. Rotation distorts familiar patterns, increasing epistemic

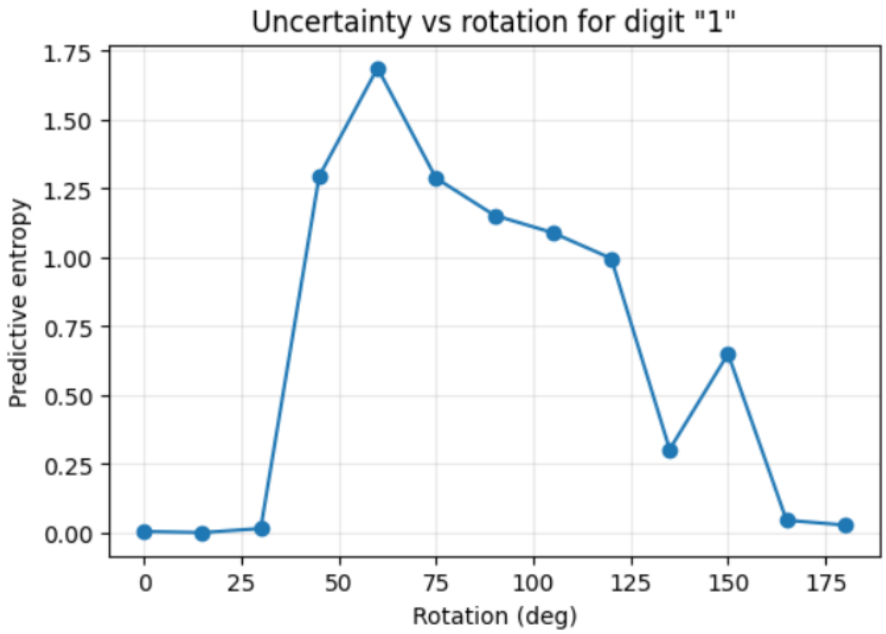

Figure 2: Variation ratio vs. rotation angle for digit "1." Uncertainty is minimal at canonical orientation and maximal near 90°.

uncertainty, which MC Dropout captures as higher predictive entropy validating its role as a Bayesian approximation that reflects model confidence under distributional shift.

4.4 Time-Series Extrapolation: Solar Irradiance

We replicate the solar irradiance experiment from Gal and Ghahramani (2016) to evaluate MC-Dropout's ability to model uncertainty in extrapolation tasks. Using synthetic data mimicking solar cycles, we train dropout networks with ReLU and Tanh activations to predict over a held-out middle segment.

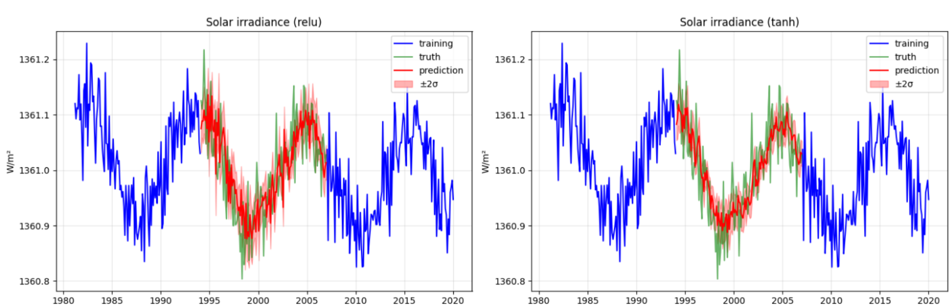

Figure 3: Solar irradiance forecasting using MC-Dropout with ReLU (left) and Tanh (right). Blue: training data; green: ground truth; red: predictive mean; shaded: $\pm 2\sigma$ epistemic uncertainty.

Figure 3 confirms the original findings: the ReLU model produces higher uncertainty in unseen regions, while Tanh leads to smoother predictions and tighter confidence bounds—reflecting the inductive biases of bounded activations. This supports MC-Dropout's interpretation as a Bayesian approximation with GP-like behavior.

4.5 Reinforcement Learning

To evaluate the impact of uncertainty-aware exploration, we reproduced the Catch game experiment from Gal and Ghahramani (2016), comparing ε-greedy with MC-Dropout-based Thompson sampling. The agent observes a 10×10 binary grid and selects one of three actions to catch a falling object.

We implement a two-layer ReLU Q-network with dropout ($p = 0.1$) before each layer, applying Monte Carlo sampling ($T = 20$) during action selection. Both agents are trained using Q-learning with experience replay and a periodically updated target network.

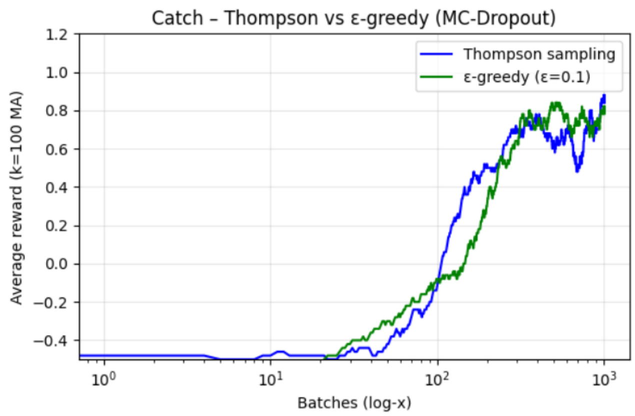

Figure 4: Catch – Thompson sampling vs. ε-greedy. Average reward (100-episode moving average) vs. number of training batches (log-scale).

Figure 4 shows that both agents successfully learn the task. Thompson sampling, driven by MC-Dropout uncertainty estimates, initially converges faster and explores more effectively. This aligns with the original paper's findings, demonstrating how dropout-based epistemic uncertainty enables more efficient exploration in reinforcement learning tasks.

5 Conclusion

We reproduced the core results of Gal and Ghahramani (2016) using modern PyTorch tools. MC-Dropout consistently produced well-calibrated uncertainty across regression, time-series, classification, and reinforcement learning tasks.

Our results confirm MC-Dropout as a simple, scalable, and effective Bayesian approximation. It performs well on key metrics, supports uncertainty-aware decisions, and remains a strong baseline for practical deep learning systems.

References

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