

Bayesian Ensembling: Unified Framework for Bayesian Model Selection

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Abstract

We develop a unified library for Bayesian model selection and ensembling, integrating multiple Bayesian inference methods under a single interface. The library provides modular components for model ensembling through posterior sampling, making Bayesian methods accessible for deep learning tasks.

1 Motivation

Bayesian methods provide principled uncertainty estimation but suffer from fragmented implementations across multiple libraries. Our project unifies these approaches into a single framework focused on model ensembling, where each algorithm defines strategies to sample models from posterior distributions.

2 Planned Algorithms

2.1 Core Methods

- **Practical Variational Inference (ELBO):** With local reparameterization trick and pruning heuristic
- **Scalable Laplace Approximation:** Kronecker-factored Hessian for efficient posterior approximation
- **Variational Rényi Bound:** Generalization of ELBO using Rényi divergence for flexible inference
- **Probabilistic Backpropagation:** Moment propagation with Gaussian posterior approximations

2.2 Baseline Comparisons

- Hamiltonian Monte Carlo (HMC)
- Monte Carlo Dropout

3 Library Design

- **Unified API:** Single interface for all Bayesian ensembling methods
- **Model Agnostic:** Works with MLP architectures
- **Posterior Sampling:** Each algorithm provides different sampling strategies
- **Hyperparameter Tuning:** Built-in optimization for method-specific parameters

4 Planned Figures

4.1 Headline Figure: Unified Bayesian Ensembling Framework

Description: A conceptual diagram showing the unified architecture:

- **Input Layer:** MLP model architectures
- **Inference Layer:** Parallel Bayesian methods (ELBO, Laplace, Rényi, HMC, MC Dropout) generating posterior samples
- **Aggregation Layer:** Weighted combination of samples based on posterior probabilities
- **Output Layer:** Final ensemble predictions with uncertainty quantification

4.2 Figure 2: Method Comparison Scatter Plot

Description: Performance comparison of all implemented methods:

- **X-axis:** Prediction Performance (task-specific metric)
- **Y-axis:** Expected Calibration Error (ECE)
- **Point colors:** Different Bayesian methods
- **Point size:** Training time or computational cost
- **Highlight:** Optimal Pareto front showing best performance-calibration trade-offs

4.3 Figure 3: Library Architecture Diagram

Description: Technical architecture of the unified library:

- **Core API Layer:** Unified interface for users
- **Method Abstraction Layer:** Common interface for all Bayesian algorithms
- **Implementation Layer:** Specific implementations of each method
- **Evaluation Module:** Standardized metrics and benchmarking tools

5 Experimental Plan

- **Datasets:** UCI benchmarks and synthetic datasets
- **Models:** MLP architectures of varying complexity
- **Metrics:** Performance metrics, calibration error, computational efficiency
- **Implementation:** Building on existing PyTorch implementations