Uncertainty in Bayesian Neural Networks

Javier Antorán, Xiping Liu, Efstratios Markou, Xianrui Zheng; {ja666, xl445, em626, xz396}@cam.ac.uk

Why be Bayesian?

- Weight uncertainty: knowing what we don't know.
- Balance modelling capacity and simplicity.

Approximate Inference Methods

The posterior over \(w\) is intractable for neural nets. We consider the following approximations.

- Bayes by Backprop [1]
  \[
  \text{ELBO} \approx \mathbb{L}[\mu, \sigma] = \frac{1}{N} \sum N \left[ \log p(y|x,w) - \log q(w|\mu, \sigma) - \log p(w) \right]
  \]
  where \(w = \mu + \sigma \odot \epsilon\), \(\epsilon \sim \mathcal{N}(0, I)\).

- MC Dropout [3]
  \[
  \text{ELBO} \approx \mathbb{L}[\mu] = \log p(y|x, w) - \lambda |\mu|^2
  \]
  \(w = \mathbf{m} \odot \mathbf{z}; \quad \mathbf{z} \sim \text{Bernoulli}(p_{\text{drop}})\).

- Stochastic Gradient Langevin Dynamics [4]
  \[
  \Delta w(t) = \epsilon(t) \cdot \frac{\partial}{\partial w} \log p(y|x, w(t)) + \frac{N_D}{\text{batch size}} \sum \log p(y_n|x_n, w(t)) + \eta(t)
  \]
  \(\eta(t) \sim \mathcal{N}(0, \epsilon(t)M)\).

Uncertainty Decomposition

Uncertainty caused by noise, or aleatoric uncertainty, can be quantified as \(E_{\epsilon} p(\epsilon|x, w)\) or \(H_{\epsilon} = H(\epsilon|x)\). Model or epistemic uncertainty can be measured as \(\text{Var}_w p(y|x, w)\) or \(H_w = H(y|x) - H_{\epsilon}\) [2].

Homoscedastic Regression

- MAP Ensemble
- BBP Gaussian
- MC dropout
- SGLD
- GP Ground truth

Figure: Toy homoscedastic regression task. Data is generated by a GP with a RBF kernel \((\ell = 1, \sigma_n = 0.3)\). We use a single-output FC network with one hidden layer of 200 ReLU units to predict the regression mean \(\mu(x)\). A fixed \(\log \sigma\) is learnt separately.

Heteroscedastic Regression

- MAP Ensemble
- BBP Gaussian
- MC dropout
- SGLD
- GP Ground truth

Figure: Toy heteroscedastic regression task. Data is generated by a GP with a RBF kernel \((\ell = 1, \sigma_n = 0.3 \cdot |x + 2|)\). We use a two-head network with 200 ReLU units to predict the regression mean \(\mu(x)\) and log-standard deviation \(\log \sigma(x)\).

MNIST Classification

<table>
<thead>
<tr>
<th>Model</th>
<th>MAP</th>
<th>MAP Ensemble</th>
<th>BBP</th>
<th>BBP GMM</th>
<th>BBP Local Reparam</th>
<th>MC Dropout</th>
<th>SGLD</th>
<th>P-SGLD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Log Likelihood</td>
<td>-572.90</td>
<td>-496.54</td>
<td>-1100.29</td>
<td>-1008.28</td>
<td>-892.85</td>
<td>-1086.43</td>
<td>-435.458</td>
<td>-828.29</td>
</tr>
<tr>
<td>Error %</td>
<td>1.58</td>
<td>1.53</td>
<td>2.60</td>
<td>2.38</td>
<td>2.28</td>
<td>2.61</td>
<td>1.37</td>
<td>1.76</td>
</tr>
</tbody>
</table>

Table: MNIST test results for methods under consideration. We approximate \(E_{\epsilon} p(y|x, w)\) with 100 MC samples. We use a FC network with two 1200 unit ReLU layers. If unspecified, the prior is Gaussian. P-SGLD uses RMSprop preconditioning.

Figure: Comparison of each method’s decomposed predictive entropy on ood samples: rotated MNIST digits. \(t\) is the correct class.

Discussion

Bayesian methods produced plausible uncertainties on the homoscedastic task. They underestimate epistemic uncertainty on the heteroscedastic task. Additional experiments on real datasets are needed. BBP underfits MNIST, resulting in a large aleatoric uncertainty. SGLD methods provide better epistemic uncertainty on ood samples through a less localised posterior approximation; the samples of \(w\) explain the data in diverse ways. Weight distributions reflect this.

Method performance varies across tasks and metric being evaluated. There is no clear best method. Optimising BBP hyperparameters is difficult.

References