The Expressiveness of Approximate Inference in Bayesian Neural Networks

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Why Bayesian neural networks?

Bayesian inference allows us to:

- Represent uncertainty.
- Encode prior beliefs.
- Trade off exploration and exploitation (RL, active learning, BayesOpt).
- Provide framework for continual learning.

BNNs aim to combine benefits of deep learning and Bayesian inference



Posterior Predictive





Filos et al. [2019]

Yang et al. [2020]

Deisenroth and Rasmussen [2011]

Pan et al. [2020]

Bayesian neural networks

Probabilistic model:

- Input x, weights θ , neural network f_{θ} .
- Likelihood $p(\mathcal{D}|\theta) := \prod_{n=1}^{N} p(y_n|x_n, \theta) = \prod_{n=1}^{N} p(y_n|f_{\theta}(x_n)).$
- Prior $p(\theta)$.

Conventional training

Optimise: $\theta_{MAP} = \arg \max_{\theta} [\log p(\mathcal{D}|\theta) + \log p(\theta)].$

Predict: $p(y_*|x_*, \theta_{MAP})$.

Bayesian inference

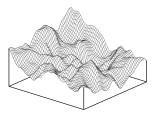
Bayes' theorem: $p(\theta|\mathcal{D}) \propto p(\mathcal{D}|\theta)p(\theta)$.

Predict: $p(y_*|x_*, \mathcal{D}) = \mathbb{E}_{p(\theta|\mathcal{D})}[p(y_*|x_*, \theta)].$

Bayesian approach not without its challenges!

First main challenge — the prior

- 1 How can we specify a good prior?
 - Model mismatch can lead to poor predictions.
 - Often factorised Gaussian for convenience.
 - Prior sampling can yield insights:



BNN sample from Neal [1995]



Typical prior predictive from Wenzel et al. [2020]

Second main challenge — the posterior

- 2 How can we perform good inference?
 - Need to approximate high-dimensional integral.
 - Difficult to verify if approximation has succeeded.
 - Is performance due to the model or to the approximation?

These two challenges are linked.

- Often priors are chosen by evaluating the posteriors they induce. "Ye priors shall be known by their posteriors" [Good, 1983].
- Lack of reliable inference hampers prior evaluation.

This talk will focus on **analysing approximate inference**.

Approximate inference

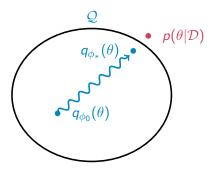
We focus on approximating family methods, which assume some tractable parametric form:

$$\mathbb{E}_{p(\theta|\mathcal{D})}\left[p(y_*|\mathsf{x}_*,\theta)\right] \approx \mathbb{E}_{q_{\phi}(\theta)}\left[p(y_*|\mathsf{x}_*,\theta)\right], \quad q_{\phi}(\theta) \in \mathcal{Q}.$$

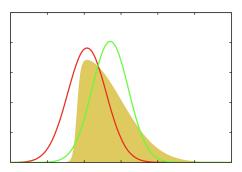
- Q is the approximating family, e.g. set of Gaussian distributions over θ .
- ullet ϕ are parameters, e.g. mean and covariance matrix.
- Approximate inference amounts to choosing ϕ .
- E.g. Laplace approximation, expectation propagation, variational inference (VI).

Variational inference recap

- Choose $q \in \mathcal{Q}$ that minimises $\mathrm{KL}(q_{\phi}(\theta) || p(\theta | \mathcal{D}))$.
- In practice optimise ELBO: $\mathbb{E}_{q_{\phi}(\theta)} \left[\log p(\mathcal{D}|\theta) \right] \mathrm{KL}(q_{\phi}(\theta) \| p(\theta))$
- Converts integration into optimisation.
- If $p(\theta|\mathcal{D}) \in \mathcal{Q}$, then $q_{\phi_*}(\theta) = p(\theta|\mathcal{D})$.



Examples of approximating family methods



Exact posterior, Laplace, variational inference. From Bishop [2006].

Laplace and VI here share the same Gaussian \mathcal{Q} , but choose ϕ differently.

Approximating families

Many choices for Q available.

 Mean-field/fully-factorised Gaussian Q_{MF} [Denker and LeCun, 1990, Hinton and Van Camp, 1993]:

$$q_{\phi}(heta) = \prod_i \mathcal{N}(heta_i; \mu_i, \sigma_i^2).$$

• Full-covariance Gaussian \mathcal{Q}_{FC} [MacKay, 1992, Barber and Bishop, 1998]:

$$q_{\phi}(\theta) = \mathcal{N}(\theta; \mu, \Sigma).$$

• Monte Carlo Dropout, Q_{DO} [Gal and Ghahramani, 2016].

$$\widehat{\mathsf{W}} = \mathsf{W}\operatorname{diag}(\boldsymbol{\epsilon}),$$

where ϵ is a vector of Bernoulli random variables.

Choosing approximating families

How should we choose the approximating family? This is an old question.

MacKay on **Laplace** with Q_{MF} vs Q_{FC} :

"The diagonal approximation is no good because of the strong posterior correlations in the parameters." — MacKay [1992]

Hinton & van Camp's response on **VI** with Q_{MF} :

"It is not clear how much is lost by ignoring the off-diagonal terms... because in this case the [variational] learning will try to force the noise in the weights to be independent."

— Hinton and Van Camp [1993]

In modern BNNs Q_{MF} or Q_{DO} preferred. Can we justify this choice?

Criteria for success

For an approximating family method to succeed, it must satisfy **two criteria**:

- The approximating family must contain good approximations to the posterior.
- 2 The method must then select a good approximate posterior within this family.

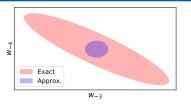
Here, 'good approximation' usually defined in function space:

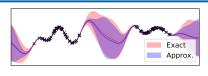
- We often don't care about the weights θ !
- Interested in predictive $\mathbb{E}_{p(\theta|\mathcal{D})}[p(y_*|x_*,\theta)]$.
- Can make assessing impact of approximations less straightforward.

Example: weight space vs function space

Mean-field VI on Bayesian linear regression with RBF features:

$$y(x) = \sum_{i=-10}^{10} w_i \psi_i(x), \quad \psi_i(x) = \exp(-(x-i)^2), \quad w_i \sim \mathcal{N}(0,1)$$





But predictions in function space quite accurate! Note "in-between" uncertainty.

MFVI overconfident in weight space as expected.

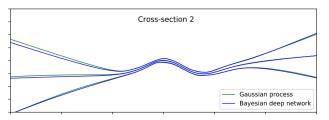
- Weight-space behaviour doesn't immediately carry over to function-space.
- What about for BNNs?

References for the exact posterior

Need good reference to assess inference.

- Exact inference impossible.
- Hamiltonian Monte Carlo possible, but slow, and hard to diagnose.

Deep BNNs approach Gaussian processes as width increases [Matthews et al., 2018, Hron et al., 2020].

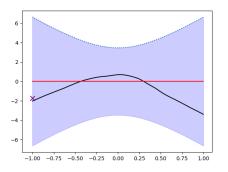


3 hidden-layer, width 50 BNN vs. GP. From Matthews et al. [2018].

- We use both HMC and GP as references.
- GP expected to be qualitatively suggestive of exact posterior.

Bayesian optimisation on toy dataset, using

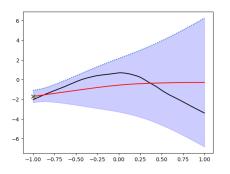
- 1 single hidden layer MFVI
- 2 the equivalent infinite-width GP



GP BayesOpt using upper confidence bounds: iteration 1

Bayesian optimisation on toy dataset, using

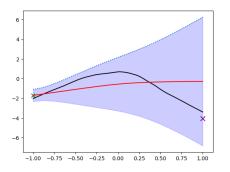
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GP BayesOpt using upper confidence bounds: iteration 2

Bayesian optimisation on toy dataset, using

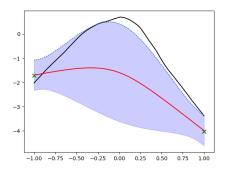
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GP BayesOpt using upper confidence bounds: iteration 2

Bayesian optimisation on toy dataset, using

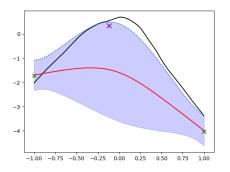
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GP BayesOpt using upper confidence bounds: iteration 2

Bayesian optimisation on toy dataset, using

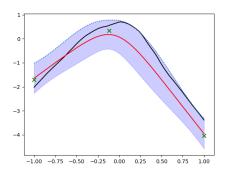
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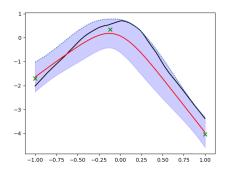


GP BayesOpt using upper confidence bounds: iteration 3

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GP finds optimum in 3 iterations.

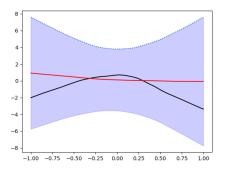


GP BayesOpt using upper confidence bounds: iteration 3

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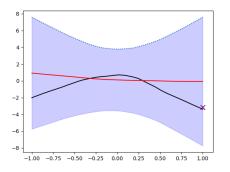
Here's how the MFVI BNN does:



Bayesian optimisation on toy dataset, using

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- 2 the equivalent infinite-width GP

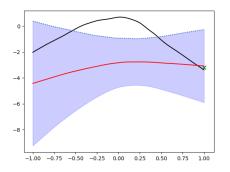
Here's how the MFVI BNN does:



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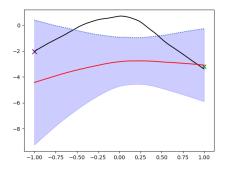
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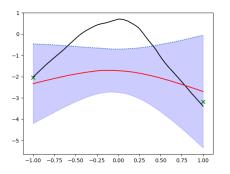
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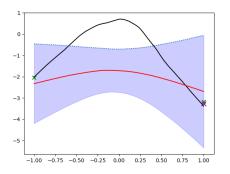
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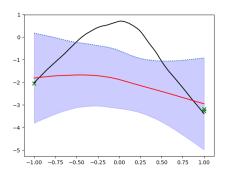
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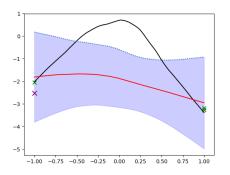
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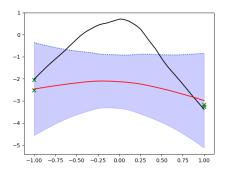
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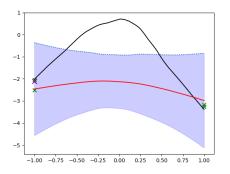
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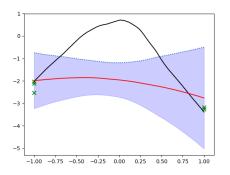
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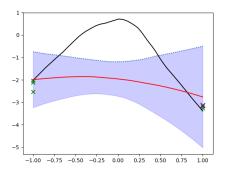
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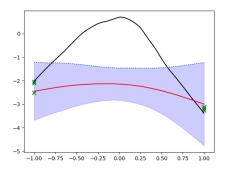
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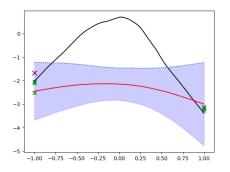
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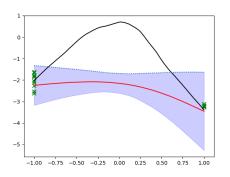
Here's how the MFVI BNN does:



Bayesian optimisation on toy dataset, using

- 1 single hidden layer MFVI
- 2 the equivalent infinite-width GP

MFVI still can't find optimum after 15 iterations! Why?



1HL Dropout BNNs \rightarrow convex predictive variance

Let $\mathbb{V}[f(x)] := \mathbb{E}[(f_{\theta}(x) - \mathbb{E}[f_{\theta}(x)])^2]$ be predictive variance at x.

Theorem 1 (F., B., Li & Turner 2020).

For any single hidden layer network with ReLU nonlinearities and a distribution of weights in \mathcal{Q}_{DO} , if dropout is not applied to the input layer, $\mathbb{V}[f(x)]$ is convex in x.

- 1HL dropout networks with ReLU activations can't have in-between uncertainty!
- A weaker statement is true if input layer is also dropped out.

Proof sketch of theorem 1

Dropout applied independently to each neuron, so:

$$\mathbb{V}[f(x)] = \mathbb{V}\left[\sum_{i=1}^{H} w_i \phi\left(a_i(x)\right) + b\right]$$
 (1)

$$=\sum_{i=1}^{H} \mathbb{V}\left[w_{i}\phi\left(a_{i}(x)\right)\right] + \mathbb{V}[b]$$
 (2)

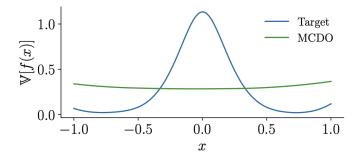
As the input weights are deterministic,

$$\mathbb{V}\left[w_i\phi\left(a_i(x)\right)\right] = \mathbb{V}\left[w_i\right]\phi\left(a_i(x)\right)^2$$

- $a_i(x)$ is an affine function of x, and ϕ^2 is convex, so $\phi(a_i(x))^2$ is convex in x.
- V[f(x)] is a positive linear combination of convex functions!

Numerical verification of theorem 1

- Obtain reference predictive variance function from a GP.
- Perform gradient descent to **directly minimise** $(\mathbb{V}_{\text{dropout}}[f(x)] \mathbb{V}_{\text{target}}[f(x)])^2$ on a grid.



MC dropout predictive variance can't match target variance **even when explicitly trained to**, due to theorem 1.

What about mean-field Q_{MF} ?

- In dropout proof, we used that the bottom layer was deterministic.
- Does a similar result hold for mean-field Gaussian Q_{MF} , where bottom layer is stochastic?

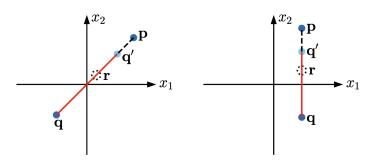
Theorem 2 (F., B., Li & Turner 2020).

There exist line segments in input space, \overrightarrow{pq} , such that for any single hidden layer network with ReLU nonlinearities and a distribution of weights in \mathcal{Q}_{MF} , for all $r \in \overrightarrow{pq}$,

$$\mathbb{V}[f(r)] \leq \mathbb{V}[f(p)] + \mathbb{V}[f(q)].$$

Constraint is weaker than convexity in theorem 1, but still implies a lack of in-between uncertainty!

Line segments of bounded variance

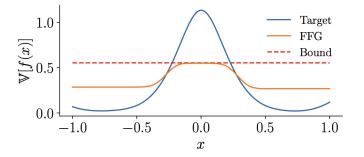


2 example line segments in BNN input space where theorem 2 applies.

- $\mathbb{V}[f(r)] \leq \mathbb{V}[f(p)] + \mathbb{V}[f(p)]$ on the red line segment.
- If input is 1-dimensional, applies to any line segment crossing origin.
- Empirically find in-between uncertainly lacking on random line segments.
- Could be symptomatic of more general pathologies.

Numerical verification of theorem 2

- Obtain reference predictive variance function from a GP.
- Perform gradient descent to **directly minimise** $(\mathbb{V}_{\text{mean-field}}[f(x)] \mathbb{V}_{\text{target}}[f(x)])^2$ on a grid.



Fully-factorised Gaussian (FFG) BNN predictive variance can't match target variance **even when explicitly trained to**, due to theorem 2.

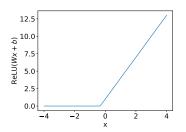
Intuition for theorem 2

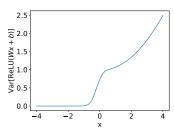
Proof more involved than dropout case.

- Single hidden layer NNs are universal function approximators.
- Surprising that variance of a mean-field BNN is not universal!
 Intuition:

Mean field \implies Variance of sum = Sum of variances

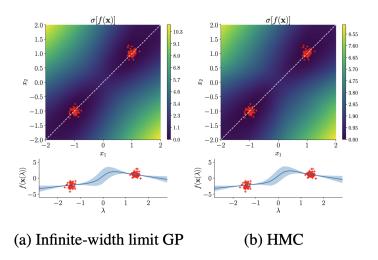
But variance of each neuron is half bowl shaped:





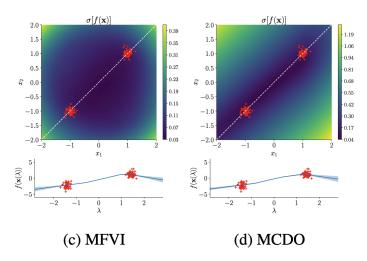
So variance of any sum is approximately bowl-shaped.

What about an actual inference task?



References for exact predictive show plenty of in-between uncertainty.

What about an actual inference task?



- VI with Q_{MF} or Q_{DO} loses in-between uncertainty.
- In this case, approximate inference, rather than the model, responsible for overconfidence!

Back to the criteria

- The approximating family must contain good approximations to the posterior. X
- 2 The method must then select a good approximate posterior within this family.

If in-between uncertainty desired, the first criterion is not satisfied for Q_{MF} or Q_{DO} with one hidden layer.

Hence cannot be fixed by:

- Choosing a better prior.
- Using a better optimiser.
- Using a tempered posterior, e.g., Wenzel et al. [2020].
- Minimising a different divergence.
- Etc.

What about deeper networks?

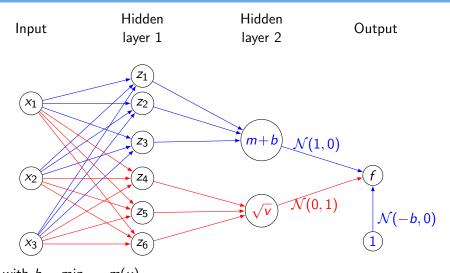
Deep networks can have in-between uncertainty

Theorem 3 (F., B., Li & Turner 2020).

Let $A \subset \mathbb{R}^d$ be compact, and $m: A \to \mathbb{R}, v: A \to \mathbb{R}_+$ be both continuous. For any $\epsilon > 0$, there exists a sufficiently wide 2HL ReLU network f, s.t. we can find a distribution in \mathcal{Q} with $\|\mathbb{E}[f] - m\|_{\infty} < \epsilon$ and $\|\mathbb{V}[f] - v\|_{\infty} < \epsilon$; where $\mathcal{Q} \in \{\mathcal{Q}_{DO}, \mathcal{Q}_{MF}\}$.

- Universality theorem for first two moments of marginal of predictive distribution of random networks.
- Just because these networks exist doesn't mean they are easy to find with conventional approximate Bayesian inference (e.g. VI).
- N.B. Only applies to Q_{DO} if dropout is *not* applied to input layer.

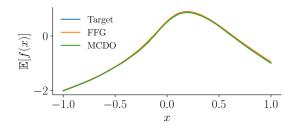
Construction for mean-field Q_{MF}

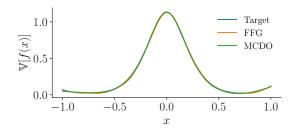


with $b = \min_{x \in A} m(x)$. So $f \approx 1 \cdot \phi(m+b) + \gamma \cdot \phi(\sqrt{v}) - b \approx m + \gamma \sqrt{v}$, $\gamma \sim \mathcal{N}(0,1)$.

Numerical verification of Theorem 3

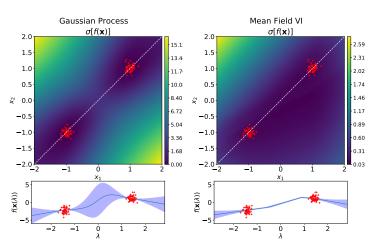
Try to fit mean and variance function from before, but with 2HL net:





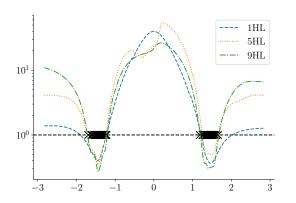
Variational Inference in Deep Nets

Does theorem 3 imply good uncertainty quantification with VI in deep BNNs?



Variational Inference in Deep Nets

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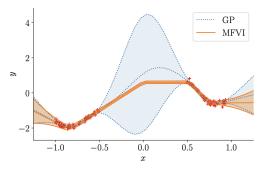


Overconfidence ratio $(\mathbb{V}_{GP}[f]/\mathbb{V}_{MFVI}[f])^{1/2}$ between two clusters of data.

Effect of initialisation

Is this behaviour due to the objective, the optimiser, or something else?

- Initialise 2HL BNN by matching GP mean and variance.
- Then optimise mixture of ELBO and squared error objective.
- Gradually move to just optimising ELBO.



BNN that starts with in-between uncertainty loses it once ELBO optimisation converges!

Limitations of Theorem 3

- Unclear how wide is "sufficiently wide".
- Only tells us about one-dimensional marginal distributions.
- Only tells us about first and second moments.
- Doesn't tell us how to find these 'good' approximate posteriors.

For in-between uncertainty in **VI** in deep BNNs with Q_{DO}, Q_{MF} :

Criteria for success

- The approximating family must contain good approximations to the posterior. ✓
- 2 The method must then select a good approximate posterior within this family. X

Active learning case study

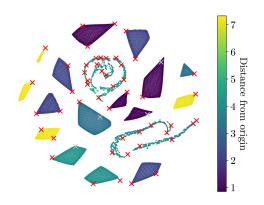
- Goal is to select informative data points to label.
- Common heuristic: Select points with high predictive variance.
- How do issues with uncertainty estimation affect performance?
- We consider a dataset where we observe active learning fails.
- Naval regression dataset, N = 11934, D = 14.

Table 1: Test RMSEs after 50th iteration of active learning.

	1 HL	4 HL
NN-GP Active	0.04 ± 0.00	0.05 ± 0.00
NN-GP Random	0.12 ± 0.01	0.16 ± 0.01
MFVI Active	$\textbf{0.94} \pm \textbf{0.11}$	0.31 ± 0.02
MFVI Random	0.15 ± 0.01	0.32 ± 0.01

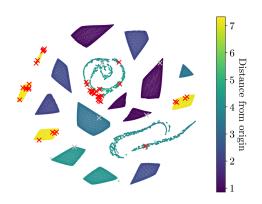
Can in-between uncertainty explain why active learning fails to improve over random for MFVI?

t-SNE plot of 1HL NN-GP acquisitions



- Points chosen at 'corners' of clusters.
- Every cluster sampled.

t-SNE plot of 1HL MFVI acquisitions



- 'Outermost' clusters favoured.
- 'In-between' clusters ignored.
- Effect lessens somewhat in deeper networks, but:
 - Approximate inference still much worse than exact NN-GP.
 - Struggles to outperform random.

Limitations and follow-up work

Limitations:

- Theorems don't explain empirical behaviour of deep BNNs.
- When is in-between uncertainty actually important?
- Focus on regression, not classification.
- Very difficult to find reliable references for the true posterior in big networks.

Subsequent work (Farquhar et al. [2020]), claims \mathcal{Q}_{MF} less restrictive in deeper nets. However:

- We observe lack of in-between uncertainty in deep nets trained with VI.
- Some conclusions rely on performance of methods on benchmarks such as ImageNet ≠ accurate posterior inference.

Conclusions

- Approximate inference with Q_{MF} and Q_{DO} in BNNs can lose qualitative features of the exact predictive.
- In 1HL BNNs, in-between uncertainty is provably absent.
- In deeper BNNs, in-between uncertainty is empirically lost.
- In-between uncertainty can mean the difference between outperforming random baseline and not, in active learning.
- Further work is needed to understand exact vs. approximate inference in, e.g. large convolutional networks.

Thanks for listening!

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