The Expressiveness of Approximate Inference in Bayesian Neural Networks

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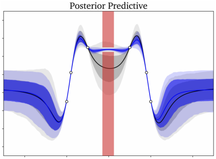
Why Bayesian neural networks?

Bayesian inference allows us to:

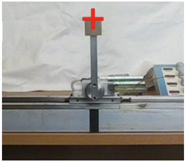
- Represent uncertainty.
- Encode prior beliefs.
- Trade off exploration and exploitation (RL, active learning, BayesOpt).
- Provide framework for continual learning.

BNNs aim to combine benefits of deep learning and Bayesian inference

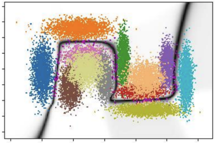
Filos et al. [2019]



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 $p(\mathcal{D}|\theta) \coloneqq \prod_{n=1}^{N} p(y_n|x_n, \theta) = \prod_{n=1}^{N} p(y_n|f_\theta(x_n))$.
- Prior $p(\theta)$.

Conventional training

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

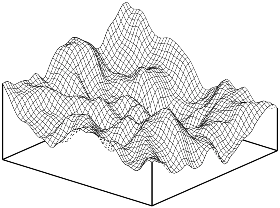
Bayesian inference

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

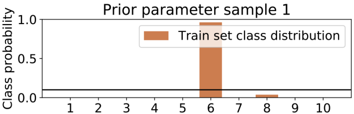
Bayesian approach not without its challenges!

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

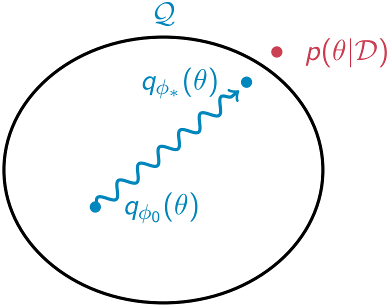
We focus on **approximating family methods**, which assume some tractable parametric form:

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

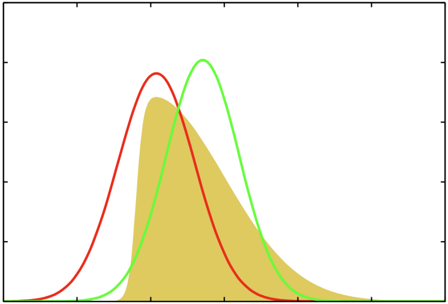
- $\mathcal{Q}$ is the **approximating family**, e.g. set of Gaussian distributions over θ.
- ϕ are parameters, e.g. mean and covariance matrix.
- Approximate inference amounts to choosing ϕ.
- E.g. Laplace approximation, expectation propagation, variational inference (VI).

Variational inference recap

- Choose $q \in \mathcal{Q}$ that minimises $\mathrm{KL}(q_\phi(\theta) \| p(\theta|\mathcal{D}))$.
- In practice optimise ELBO: $\mathbb{E}_{q_\phi(\theta)}[\log p(\mathcal{D}|\theta)] - \mathrm{KL}(q_\phi(\theta) \| p(\theta))$
- 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 $\mathcal{Q}$ available.

- Mean-field/fully-factorised Gaussian $\mathcal{Q}_{MF}$ [Denker and LeCun, 1990, Hinton and Van Camp, 1993]:

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

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

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

- Monte Carlo Dropout, $\mathcal{Q}_{DO}$ [Gal and Ghahramani, 2016].

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

  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 $\mathcal{Q}_{MF}$ vs $\mathcal{Q}_{FC}$:

> *"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 $\mathcal{Q}_{MF}$:

> *"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 $\mathcal{Q}_{MF}$ or $\mathcal{Q}_{DO}$ preferred. Can we justify this choice?

Criteria for success

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

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

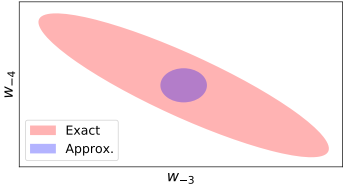
Here, 'good approximation' usually defined in **function space**:

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

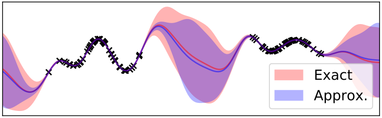
Example: weight space vs function space

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

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



MFVI overconfident in weight space as expected.



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

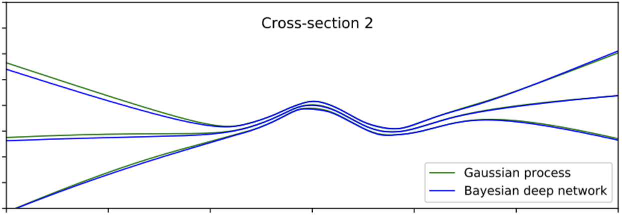
- Weight-space behaviour **doesn’t immediately carry over** to function-space.
- What about for BNNs?

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].

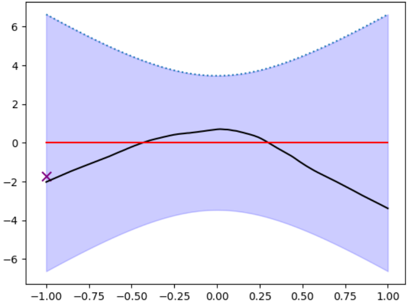
- We use both HMC and GP as references.
- GP expected to be qualitatively suggestive of exact posterior.

How does MFVI compare with GP?

Bayesian optimisation on toy dataset, using

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

Here's how the **GP** does:



GP BayesOpt using upper confidence bounds: iteration 1

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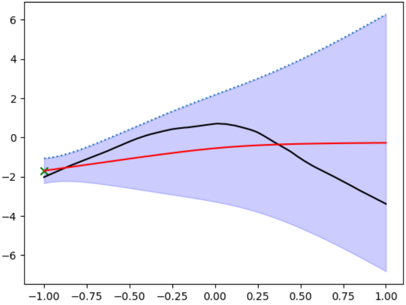

GP BayesOpt using upper confidence bounds: iteration 2

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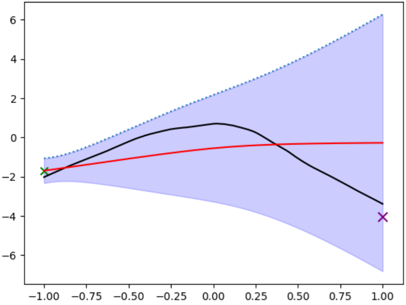

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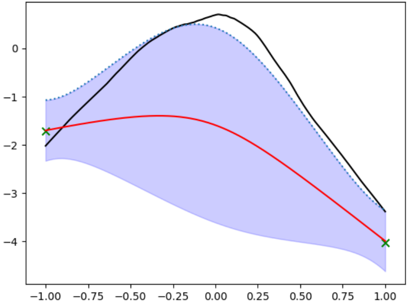

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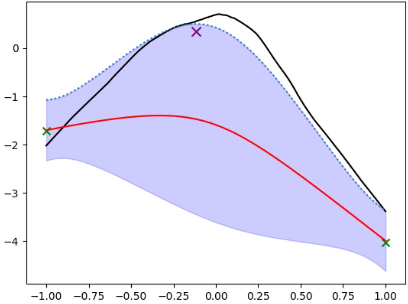

GP BayesOpt using upper confidence bounds: iteration 3

How does MFVI compare with GP?

Bayesian optimisation on toy dataset, using

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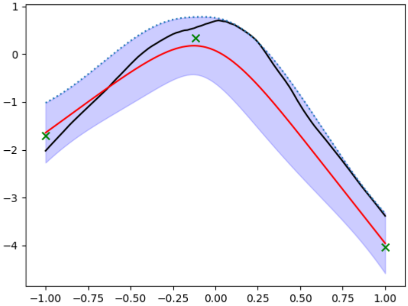
Here's how the **GP** does:



GP BayesOpt using upper confidence bounds: iteration 3

How does MFVI compare with GP?

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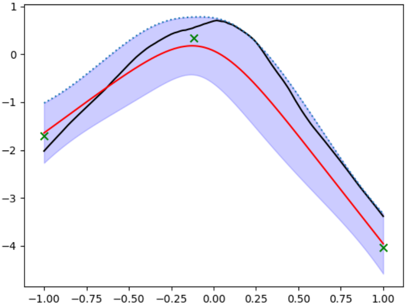
2. the equivalent infinite-width GP

GP finds optimum in 3 iterations.



GP BayesOpt using upper confidence bounds: iteration 3

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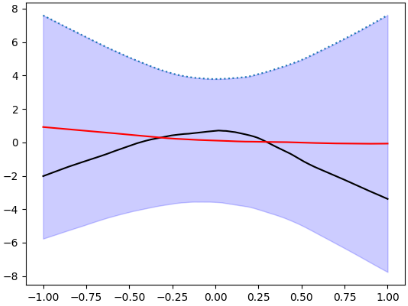

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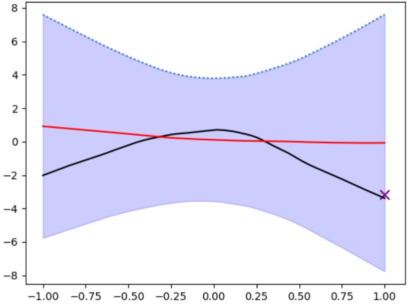

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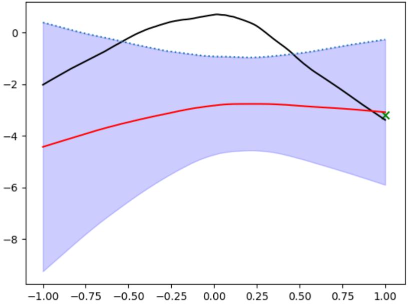

MFVI BayesOpt using upper confidence bounds: iteration 2

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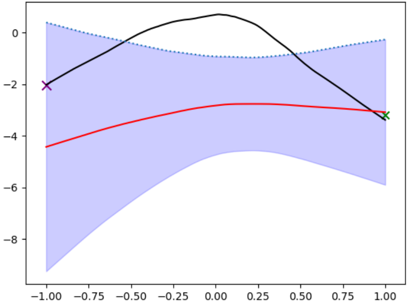

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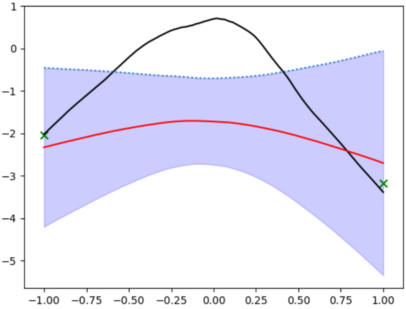

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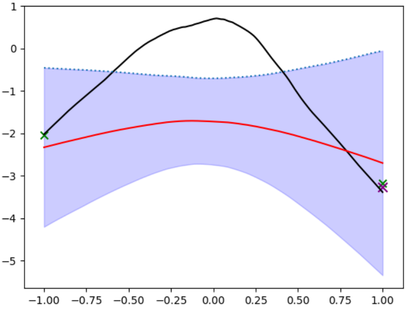

MFVI BayesOpt using upper confidence bounds: iteration 3

How does MFVI compare with GP?

Bayesian optimisation on toy dataset, using

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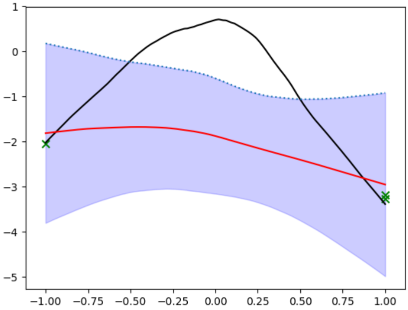


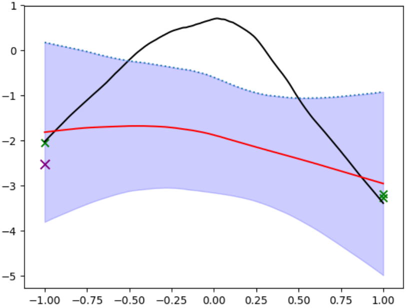
MFVI BayesOpt using upper confidence bounds: iteration 4

How does MFVI compare with GP?

Bayesian optimisation on toy dataset, using

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

Here's how the **MFVI BNN** does:



MFVI BayesOpt using upper confidence bounds: iteration 4

How does MFVI compare with GP?

Bayesian optimisation on toy dataset, using

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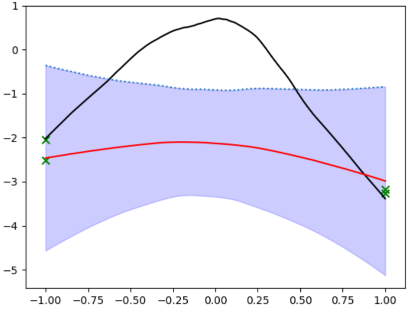
2. the equivalent infinite-width GP

Here's how the **MFVI BNN** does:



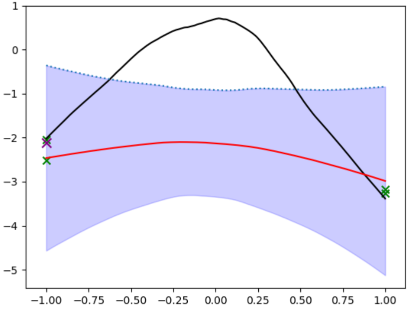
MFVI BayesOpt using upper confidence bounds: iteration 5

How does MFVI compare with GP?

Bayesian optimisation on toy dataset, using

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

Here's how the **MFVI BNN** does:



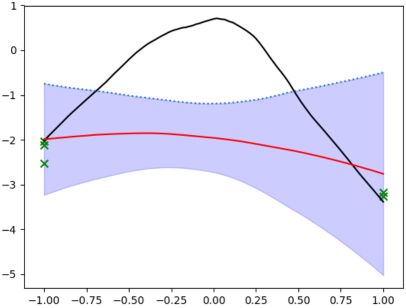
MFVI BayesOpt using upper confidence bounds: iteration 5

How does MFVI compare with GP?

Bayesian optimisation on toy dataset, using

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

Here's how the **MFVI BNN** does:



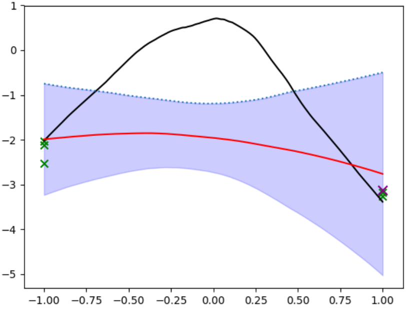
MFVI BayesOpt using upper confidence bounds: iteration 6

How does MFVI compare with GP?

Bayesian optimisation on toy dataset, using

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

Here's how the **MFVI BNN** does:



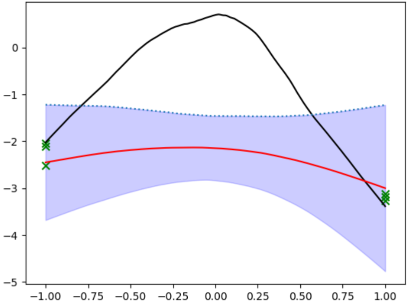
MFVI BayesOpt using upper confidence bounds: iteration 6

How does MFVI compare with GP?

Bayesian optimisation on toy dataset, using

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

Here's how the **MFVI BNN** does:



MFVI BayesOpt using upper confidence bounds: iteration 7

How does MFVI compare with GP?

Bayesian optimisation on toy dataset, using

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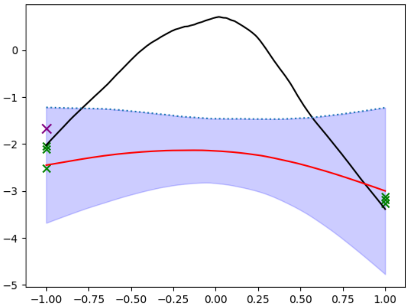
2. the equivalent infinite-width GP

Here's how the **MFVI BNN** does:



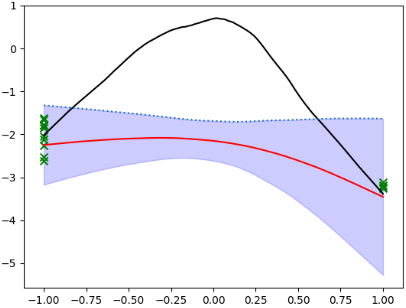
MFVI BayesOpt using upper confidence bounds: iteration 7

How does MFVI compare with GP?

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?



MFVI BayesOpt using upper confidence bounds: iteration 15

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:

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

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

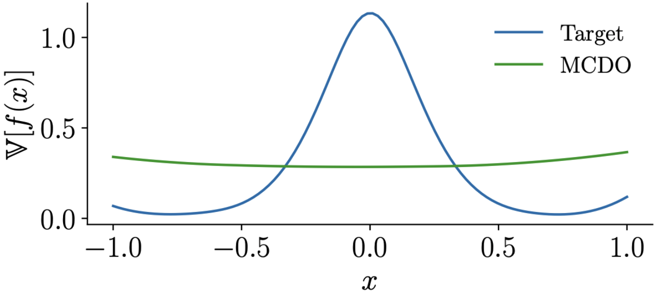
- As the input weights are deterministic,

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

- $a_i(x)$ is an affine function of x, and ϕ^2 is convex, so $\phi\left(a_i(x)\right)^2$ is convex in x.
- $\mathbb{V}[f(x)]$ 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 $\mathcal{Q}_{MF}$?

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

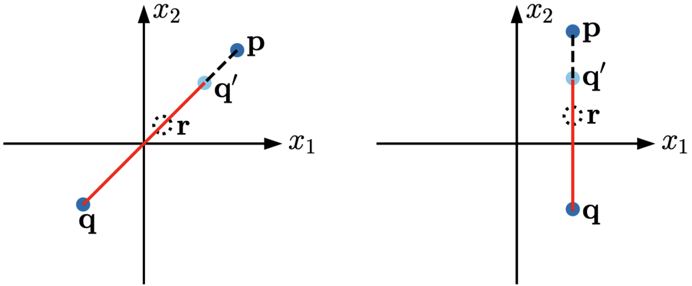
Theorem 2 (F., B., Li & Turner 2020).

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

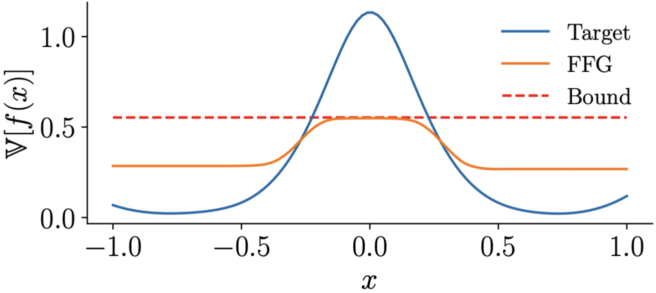


2 example line segments in BNN input space where theorem 2 applies.

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

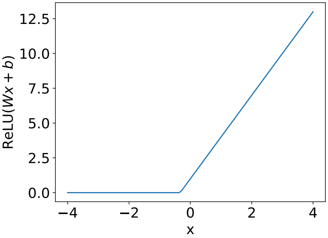
Proof more involved than dropout case.

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

Intuition:

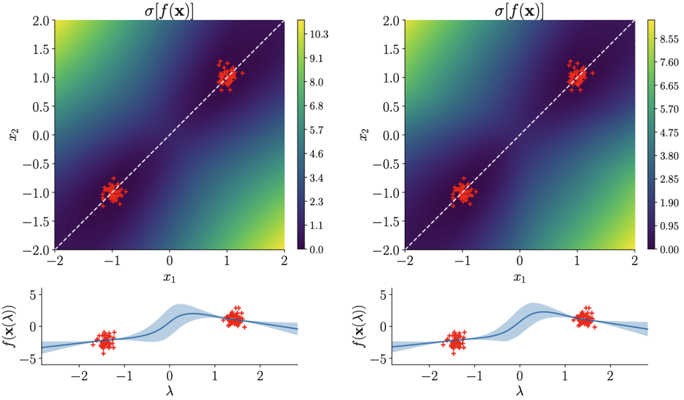
$$\text{Mean field} \implies \text{Variance of sum} = \text{Sum of variances}$$

But variance of each neuron is half bowl shaped:



So variance of any sum is approximately bowl-shaped.

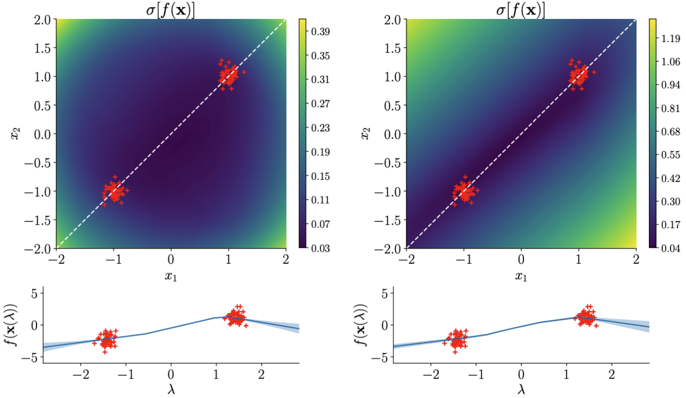
What about an actual inference task?



(a) Infinite-width limit GP (b) HMC

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

What about an actual inference task?



(c) MFVI (d) MCDO

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

Back to the criteria

1. The approximating family **must contain good approximations** to the posterior. ✗
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 $\mathcal{Q}_{MF}$ or $\mathcal{Q}_{DO}$ 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.

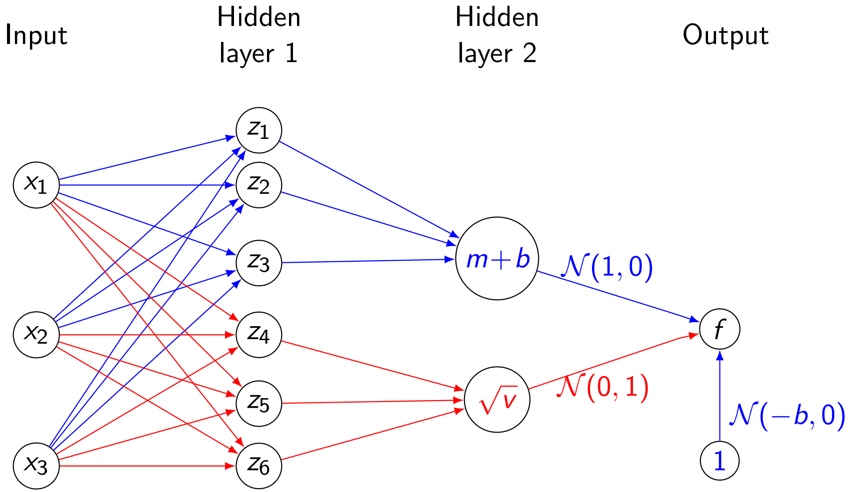
What about **deeper networks**?

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 $\mathcal{Q}_{DO}$ if dropout is *not* applied to input layer.

Construction for mean-field $\mathcal{Q}_{MF}$

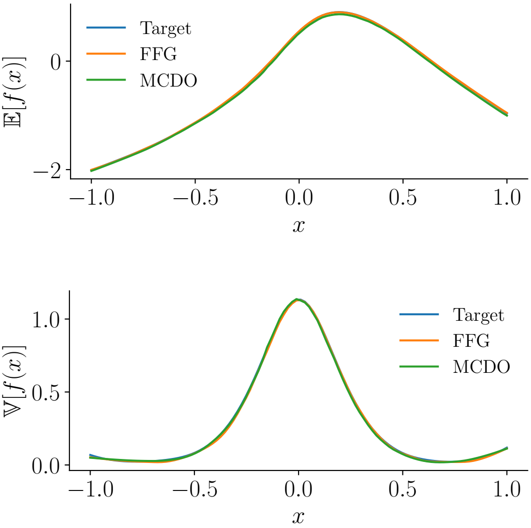


with $b = \min_{x \in A} m(x)$.

So $f \approx 1 \cdot \phi(m+b) + \gamma \cdot \phi(\sqrt{v}) - b \approx m + \gamma\sqrt{v}, \quad \gamma \sim \mathcal{N}(0,1)$.

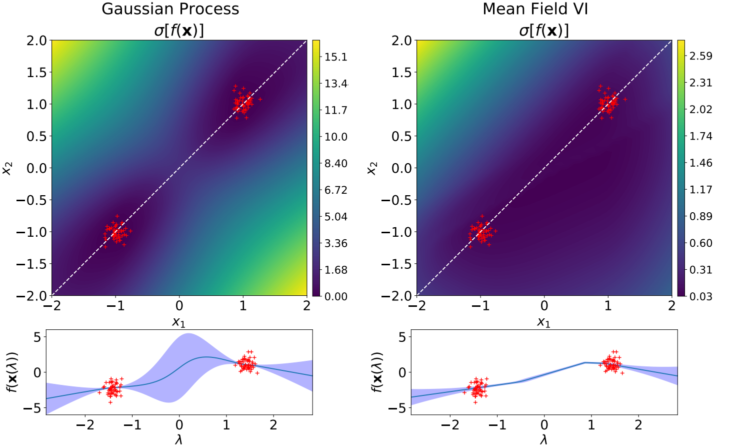
Numerical verification of Theorem 3

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



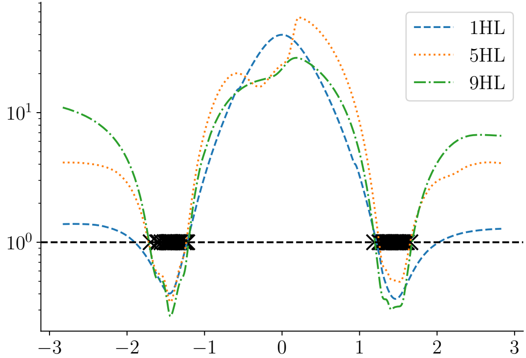
Variational Inference in Deep Nets

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



Variational Inference in Deep Nets

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

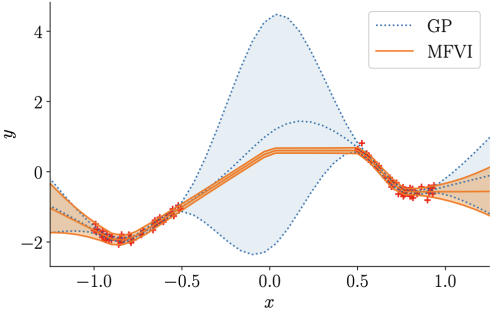


Overconfidence ratio $(\mathbb{V}_{GP}[f]/\mathbb{V}_{MFVI}[f])^{1/2}$ between two clusters of data.

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 $\mathcal{Q}_{DO}, \mathcal{Q}_{MF}$:

Criteria for success

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

Active learning case study

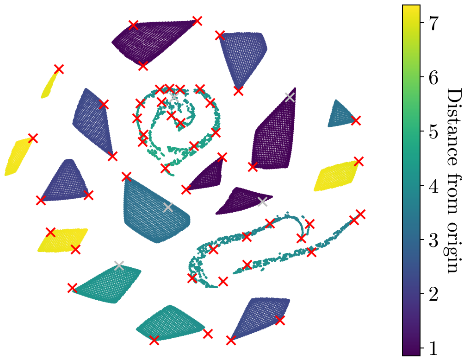
- Goal is to select informative data points to label.
- Common heuristic: Select points with high predictive variance.
- How do issues with uncertainty estimation affect performance?
- We consider a dataset where we observe active learning **fails**.
- Naval regression dataset, $N = 11934$, $D = 14$.

Table 1: Test RMSEs after 50^{th} 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	0.94 ± 0.11	0.31 ± 0.02
MFVI Random	0.15 ± 0.01	0.32 ± 0.01

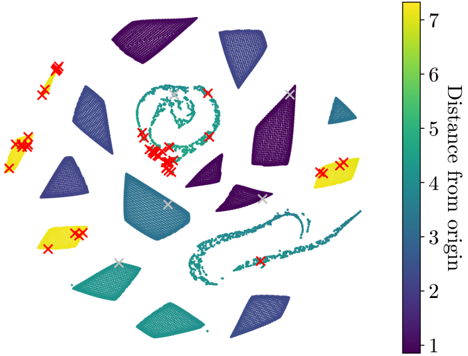
Can in-between uncertainty explain why active learning fails to improve over random for MFVI?

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 $\neq$ accurate posterior inference.

Conclusions

- Approximate inference with $\mathcal{Q}_{MF}$ and $\mathcal{Q}_{DO}$ 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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