Function-space Inference with Sparse Implicit Processes

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Estimating the uncertainty of the predictions

Modern *ML* (*e.g.* NNs) $\rightarrow$ **point-wise predictions**

Info. on the **uncertainty of the predictions** $\rightarrow$ **Bayesian formulation**

$$\text{Posterior dist.} \qquad p(\mathbf{w}|\mathcal{D}) = p(\mathbf{w})p(\mathcal{D}|\mathbf{w})/p(\mathcal{D})$$

$$\text{Predictive dist.} \qquad p(y|\mathcal{D}, x) = \int p(y|\mathbf{w}, x)\, p(\mathbf{w}|\mathcal{D})\, \mathrm{d}\mathbf{w}$$

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$p(\mathcal{D})$ intractable! $\Rightarrow$ *approximate solutions* s.a. *MCMC*-based techinques, *VI*, *EP*, *AVB*, etc.

$\Rightarrow$ Inference with finite set of parameters (*e.g.* neurons in BNNs)

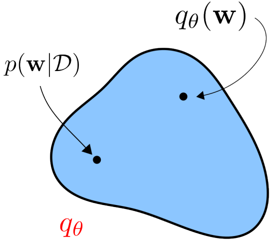
Variational Inference

VI $\rightarrow$ Parametric q to **approximate** target (intractable) posterior p

Evidence Lower Bound (ELBO):

$$\mathcal{L} = \sum_{i=1}^{N} \mathbb{E}_q[\log p(\mathbf{y}_i|\mathbf{W}, \mathbf{x}_i)] - \text{KL}(q|\text{prior})$$

- Monte Carlo and mini-batches!
- Closed-form solution if p and q are Gaussian!



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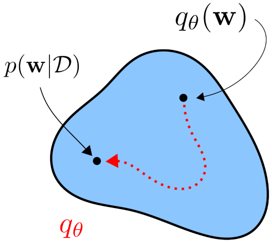

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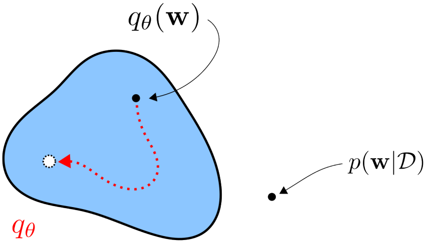

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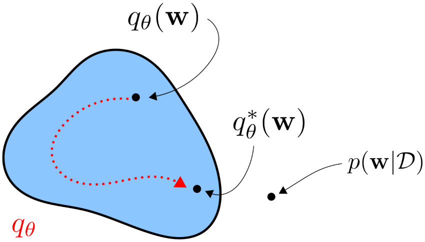

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More flexible inference model ⇒ Implicit model for weights

Implicit distribution: Samples available, but not the p.d.f.

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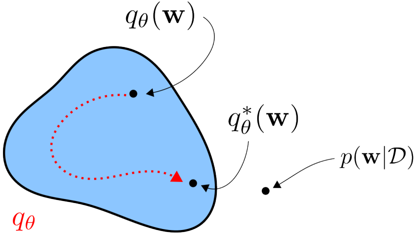

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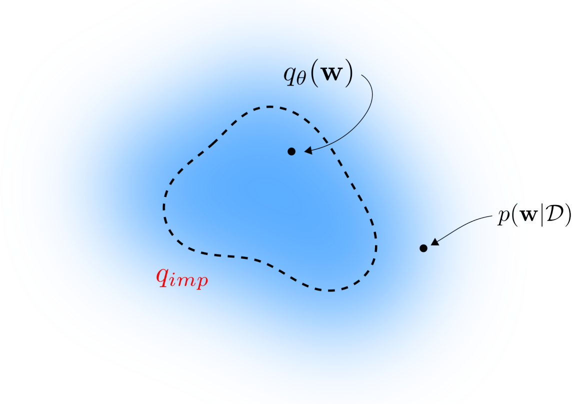

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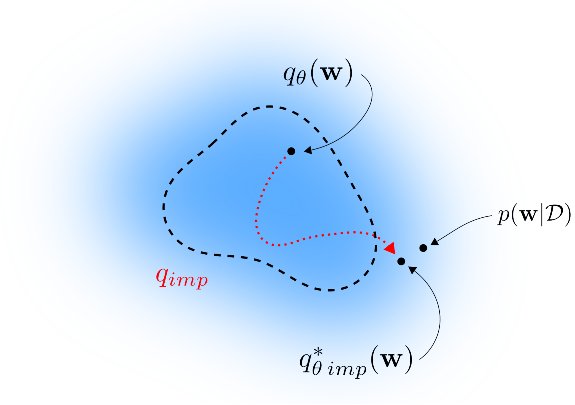

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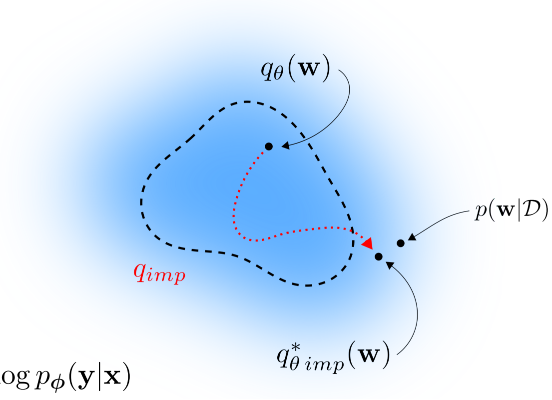

ML training → $\mathbb{E}_{p_{\mathcal{D}}(\mathbf{x})} \log p_{\boldsymbol{\phi}}(\mathbf{y}|\mathbf{x})$

$$\max_{\boldsymbol{\theta},\boldsymbol{\phi}} \mathbb{E}_{p_{\mathcal{D}}(\mathbf{x})}\Big[\underbrace{-\mathrm{KL}(q_{\boldsymbol{\theta}}(\mathbf{w})||p(\mathbf{w}))}_{\mathbb{E}_{q_{\boldsymbol{\theta}}(\mathbf{w})}[\log p(\mathbf{w}) - \log q_{\boldsymbol{\theta}}(\mathbf{w})]} + \mathbb{E}_{q_{\boldsymbol{\theta}}(\mathbf{w})} \log p_{\boldsymbol{\phi}}(\mathbf{y}|\mathbf{x},\mathbf{w})\Big]$$

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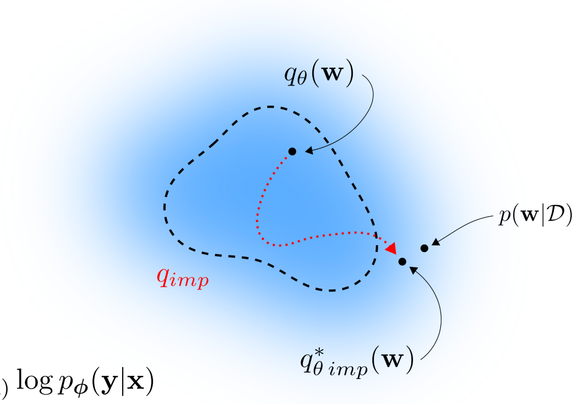

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[Mescheder et. al., 2017]

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Regular approximate Bayesian inference ⇒ **parameter space**

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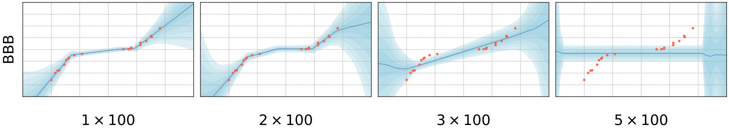

[Sun et al., 2019]

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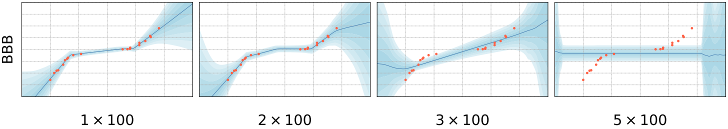

Function-space is challenging but with **benefitial**:

1. Avoids issues related to the original inference problem space
2. Better predictions and uncertainty estimates
3. More flexible priors than GPs

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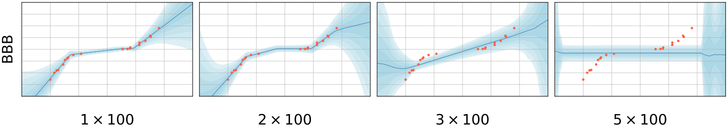

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Implicit Processes ⇒ generalization for the prior and posterior formulation in function-space

[Sun et al., 2019]

Implicit Processes

Collection of random variables $f(\cdot)$, such that any finite collection $(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n))$ has joint distribution defined by the generative process:

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Bayesian neural networks: $\theta \Rightarrow$ means and variances of $\mathbf{W}$

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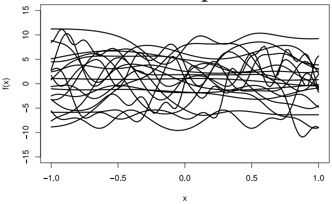
Neural sampler: $\theta \Rightarrow$ weights of non-linear function $g_\theta(\cdot, \cdot)$.

Prior samples



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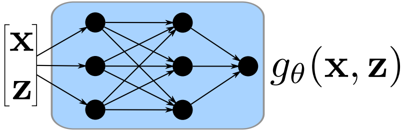

Learning under Implicit Process Priors

Goals:

1. Find flexible approximations to the exact posterior distribution
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Previous approaches:

1. Variational Implicit Process (**VIP**, Ma et al., 2019)
   - ▶ IP prior and GP approximation for the predictions
   - ⊘ Only provides GP-like predictions (Normally distributed)
2. Functional Bayesian Neural Network (**FBNN**, Sun et al., 2019)
   - ▶ IP prior & posterior, trained using Stein Gradient Estimator
   - ⊘ SGE approach cannot train the prior parameters

Inference with IPs and inducing points

Implicit process $f(\mathbf{x}) = h_\phi(\mathbf{x}, \boldsymbol{\epsilon})$ as approximate implicit posterior of the IP prior ($\sim$*FBNNs*, *full IP-based model*)

Approximate Inference via functional VI (*f-ELBO*):

$$\mathcal{L}(q) = \sum_{i=1}^{N} \mathbb{E}_q[\log p(y_i|f(\mathbf{x}_i))] - \mathrm{KL}(q|\mathrm{prior})\,.$$

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2. Intractable conditional posterior
   - Partial Monte Carlo GP approximation for the conditional $p(\mathbf{f}|\mathbf{u})$ in the posterior ($\sim$*VIPs*)

Training the system

Final posterior approximation (with implicit $q_\phi(\mathbf{u})$):

$$q(\mathbf{f}, \mathbf{u}) = p_\theta(\mathbf{f}|\mathbf{u})q_\phi(\mathbf{u})$$

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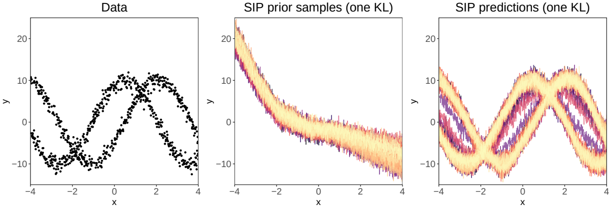
KL-divergence **intractable** (**implicit** q and p) $\Rightarrow$ classifier (DNN)

$$\mathrm{KL}(q_\phi(\mathbf{u}) | p_\theta(\mathbf{u})) = -\mathbb{E}_q \left[\log \frac{p_\theta(\mathbf{u})}{q_\phi(\mathbf{u})} \right] = -\mathbb{E}_q \left[T_{\Omega^\star}(\mathbf{u}) \right]$$

[Mescheder et. al., 2017]

Challenges: KL-evaluation

Poor prior fit, important in complex models [Knoblauch et al. 2019]



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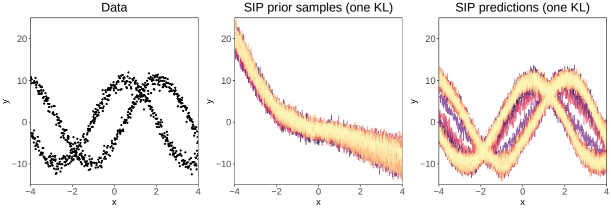

Solution: Exchange KL by the symmetrized KL-divergence

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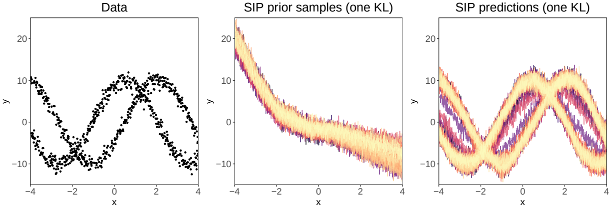

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KL as regularization in the ELBO $\Rightarrow$ changes often improve results

- Easy to compute dependencies w.r.t. θ
- Good empirical results + little added computational cost

[Wenzel et. al., 2020]

Final setup

Final objective function (with α-divergences + symmetrized KL):

$$\boxed{\mathcal{L}_{\alpha}^{\star}(\phi, \theta) = \frac{1}{\alpha} \sum_{i=1}^{N} \log \mathbb{E}_{q_{\phi,\theta}}[p(y_i|f_i)^{\alpha}] - \frac{1}{2} \left[\mathrm{KL}(q_{\phi}||p_{\theta}) + \mathrm{KL}(p_{\theta}||q_{\phi})\right]}$$

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GP approximation ($\sim$VIP)

$$\mathbb{E}[f(\mathbf{x})] = m^{\star}_{MLE}(\mathbf{x}) + \mathbf{K}_{\mathbf{f},\mathbf{u}}(\mathbf{K}_{\mathbf{u},\mathbf{u}} + \mathbf{I}\sigma^2)^{-1}(\mathbf{u} - m^{\star}_{\mathrm{MLE}}(\mathbf{X}))\,,$$
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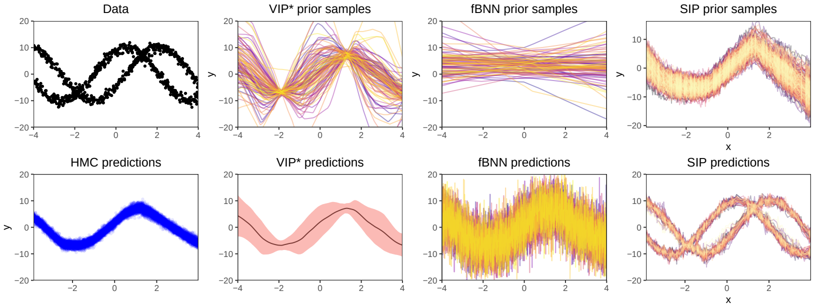
Predictions approximated by Monte Carlo (mixture of Gaussians):

$$p(f(\mathbf{x}_*)|\mathbf{y}, \mathbf{X}) \approx \frac{1}{S} \sum_{s=1}^{S} p_\theta(f(\mathbf{x}_*)|\mathbf{u}_s)\,, \qquad \mathbf{u} \sim q_\phi(\mathbf{u})$$

Synthetic data experiments



VIP regularization term is not used

Same BNN prior for all methods

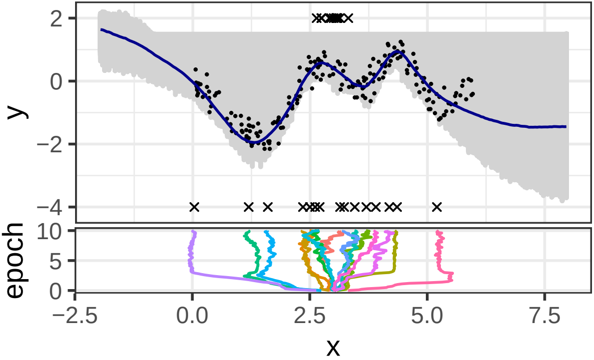
SIP is the only one with **fitted prior samples** and **bimodal predictive distribution**

SIP corrects the model bias that induces the wrong posterior!

- Combination of flexibility of the framework + α-divergences

Evolution of the inducing points

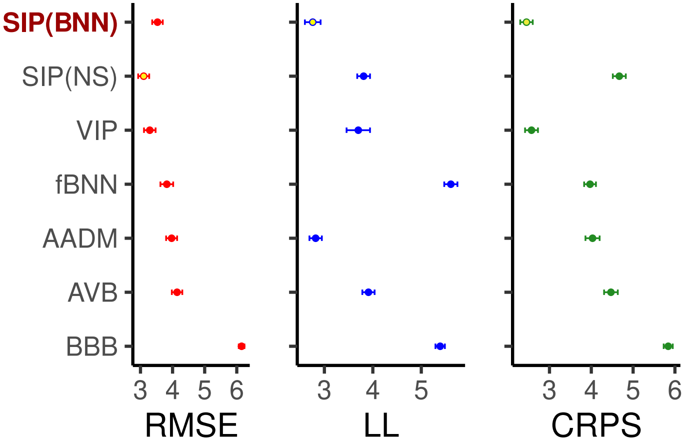
Inducing points spread and cover the whole training data range



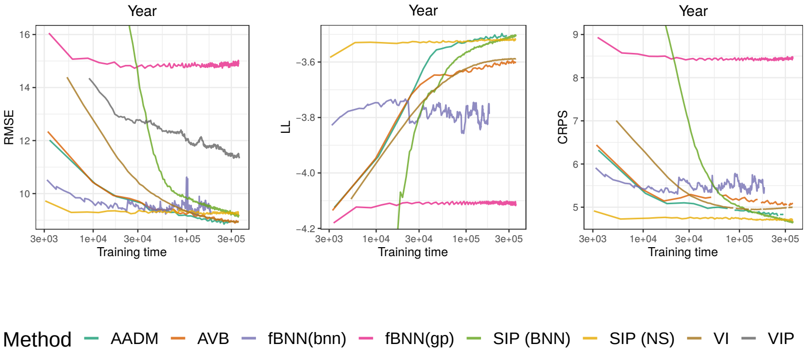
Posterior parameters are not trained for this example:
slight underfitting + *adversarial initialization*

Regression results

Ranking analysis (lower is better, 8 UCI datasets, 20 splits each, 2σ)



Convergence experiments



$\mathbf{SIP_{NS}}$ is clearly faster, $\mathbf{SIP_{BNN}}$ performs the best overall

Conclusions

1. Approximate inference in parameter space presents intrinsic difficulties

2. Approximate inference in function space is advantageous but hard

   ! Allowing the model to train all of its parameters

   ! Provide flexible predictive distributions

3. **SIP** has new important properties
   - ✓ Can learn the prior parameters
   - ✓ Flexible posterior approximation via mixture of Gaussians
   - ✓ Scalable with large amounts of data
   - ✓ SIP can use other flexible priors based on implicit processes
   - ✓ Capable of correcting wrong model bias from the formulation

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Thanks for your attention!

`https://github.com/simonrsantana/sparse-implicit-processes`

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