Gaussian processes and Bayesian NNs in function space

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Computing $p(\text{Data})$ is intractable! $\Rightarrow$ different **approximate solutions**, such as **BNNs** (*VI, EP, AVB, etc.*) or **GPs**

Non-paremetric approaches *s.a.* **GPs** could help ease our job (real-world problems are complicated!)

$\rightarrow$ *Intrinsic advantages and issues!*

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Stablished methods ⇒ lack some properties, while exceed at others

Could we combine some of them to improve overall?

Brief mention of kernel methods

- Widespread models based on learning **kernel functions**
- **Instance based methods** $\Rightarrow$ Learn parameters for each training data point (*must remember these*)
- **Predictions** $\Rightarrow$ Similarity function $k(\cdot, \cdot)$ between train and test points (**kernel**)
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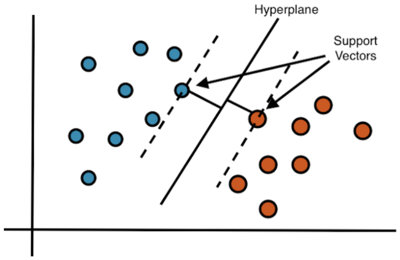
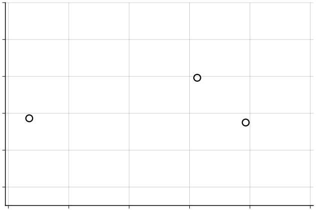
$$k(x,x') = \phi(x)^T\phi(x')$$

- Many different kernels to choose from
- Flexible approach $\Rightarrow$ many different usages (SVMs, GPs, PCA...)



Approximate inference and GPs



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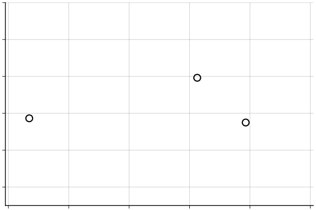

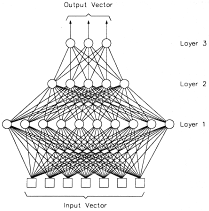

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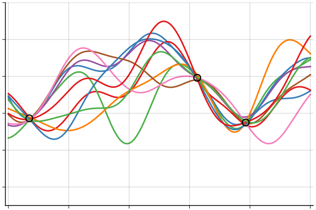

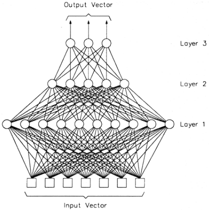

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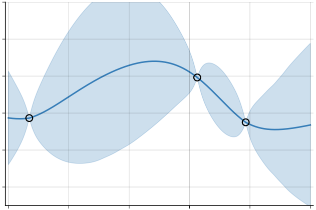

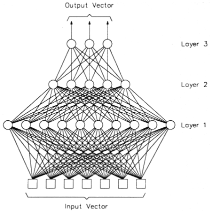

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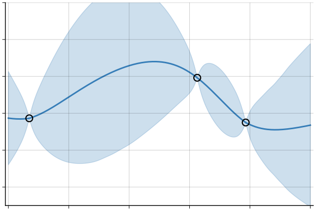

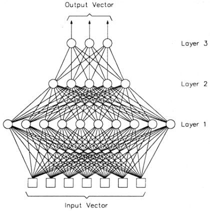

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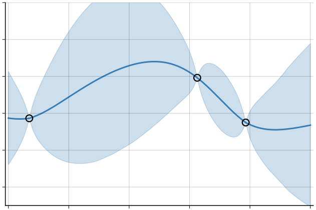

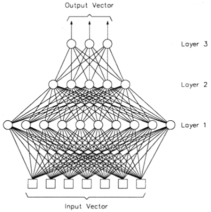

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Challenges: Non-parametric models would simplify our job (problems can be complex!) and computing $p(\text{Data})$ is intractable!

Hint: One (*vanilla*) solution is simply setting $p(\mathbf{W}) \sim \mathcal{N}(\mathbf{W}|0, \sigma^2\mathbf{I})$

Gaussian Processes

GPs: Distribution over functions $f(\cdot)$ so that for any finite $\{\mathbf{x}_i\}_{i=1}^N$, $(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_N))^\mathsf{T}$ follows an N-dimensional Gaussian distribution.

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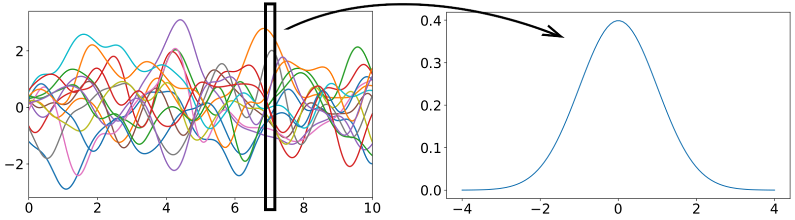

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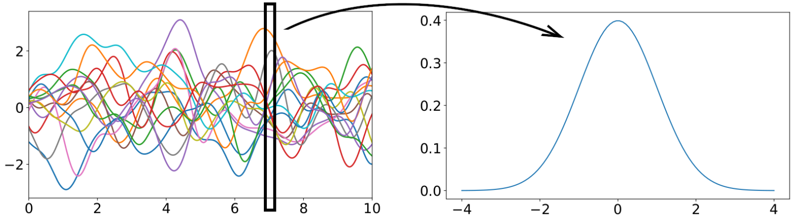

Regression with GPs

$$\hat{y}_i = y_i + \epsilon_i, \qquad \text{with} \qquad p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}), \quad \epsilon_i \sim \mathcal{N}(0, \beta^{-1})$$

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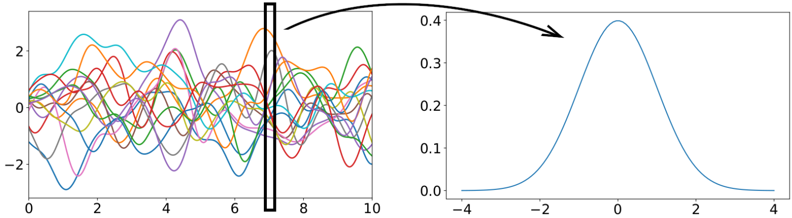

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Due to Gaussian form, there are **closed-form solutions** for many useful questions about finite data!

Gaussian Processes

- The **joint distribution** for $\mathbf{y}^\star$ at test points $\{\mathbf{x}_m^\star\}_{m=1}^M$ and $\mathbf{y}$:

$$p(\mathbf{y}^\star, \mathbf{y}) = \mathcal{N}\left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \boldsymbol{\kappa}_\theta & \mathbf{k}_\theta^\mathsf{T} \\ \mathbf{k}_\theta & \mathbf{K}_\theta \end{bmatrix}\right)$$

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- These **matrices** are computed from the covariance $C(\cdot, \cdot; \theta)$:

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$$\mathbf{y}^\star \sim \mathcal{N}(\mathbf{m}, \boldsymbol{\Sigma})$$

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- The log of the **marginal likelihood**, $p(\mathbf{y}|\theta)$, is:

$$\log p(\mathbf{y}) = -\frac{N}{2} \log 2\pi - \frac{1}{2} \log |\mathbf{K}_\theta| - \frac{1}{2} \mathbf{y}^\mathsf{T} \mathbf{K}_\theta^{-1} \mathbf{y}$$

An Example of a Covariance Function

Squared Exponential: $$C(\mathbf{x}, \mathbf{x}') = \sigma^2 \exp\left\{\frac{1}{2}\sum_{j=1}^{d}\left(\frac{x_j - x_j'}{l_j}\right)^2\right\}$$

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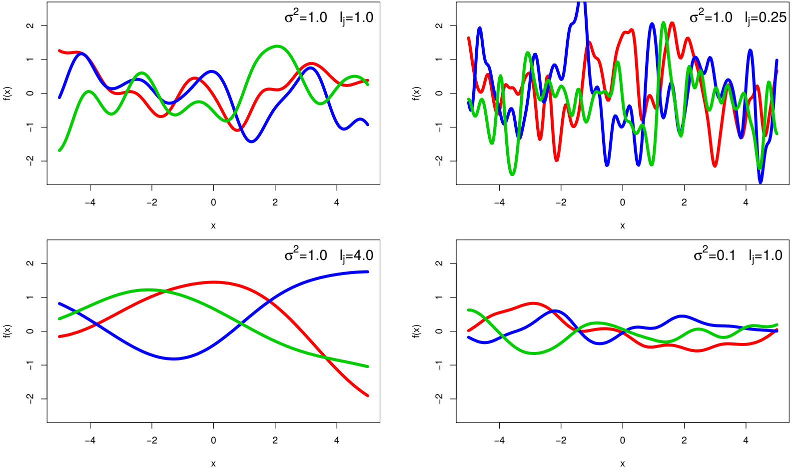
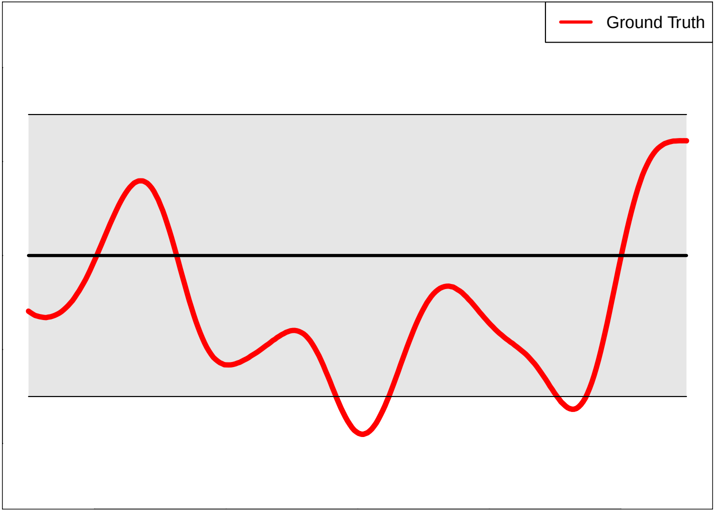


From the Prior to the Posterior

GP regression provides a **closed-form** posterior distribution for $f(\cdot)$.



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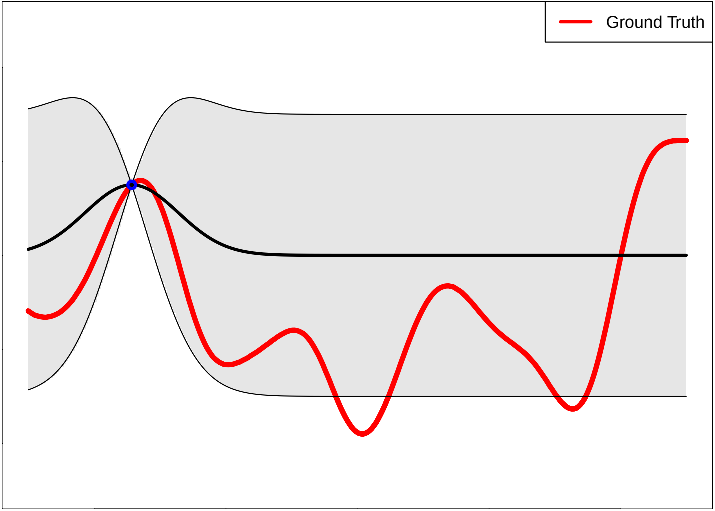

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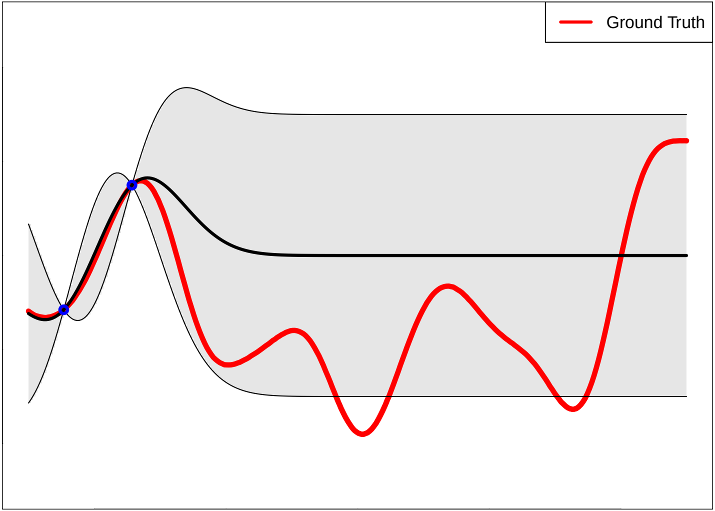

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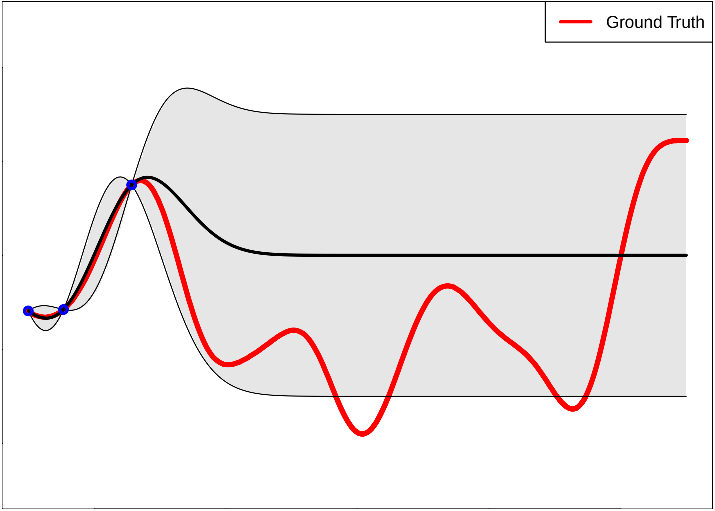

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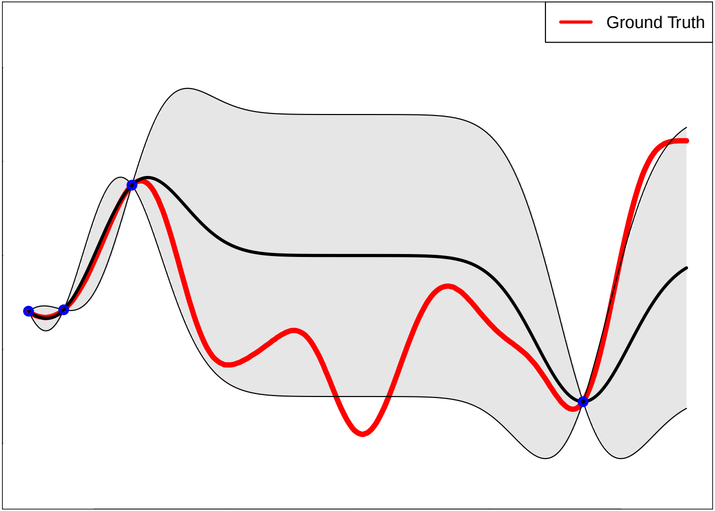

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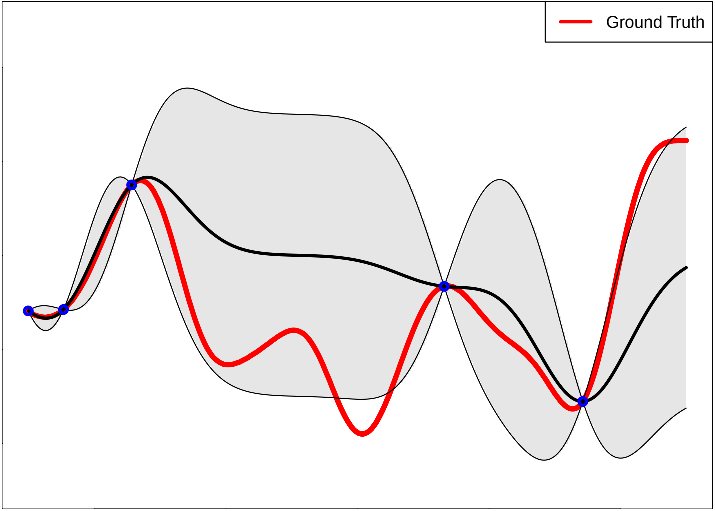

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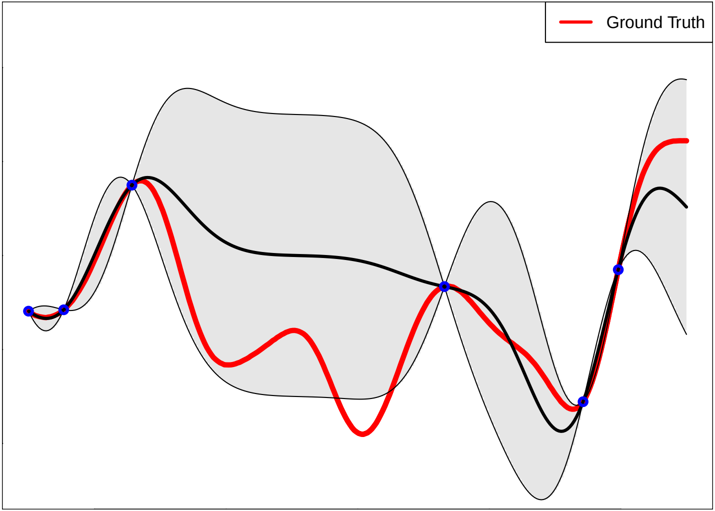

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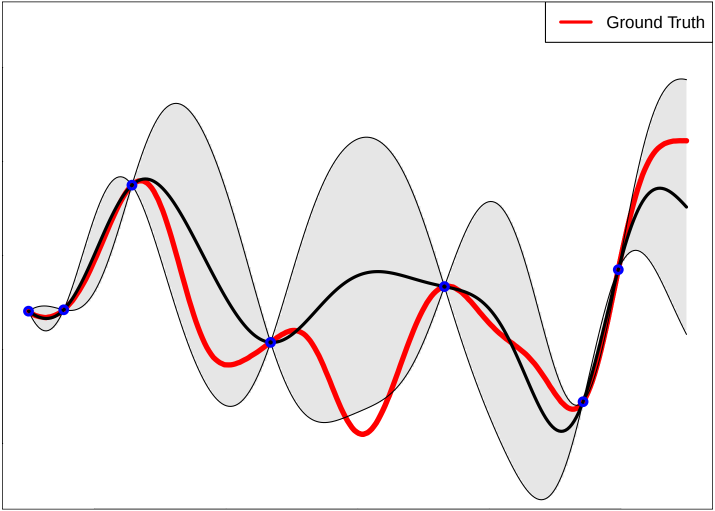

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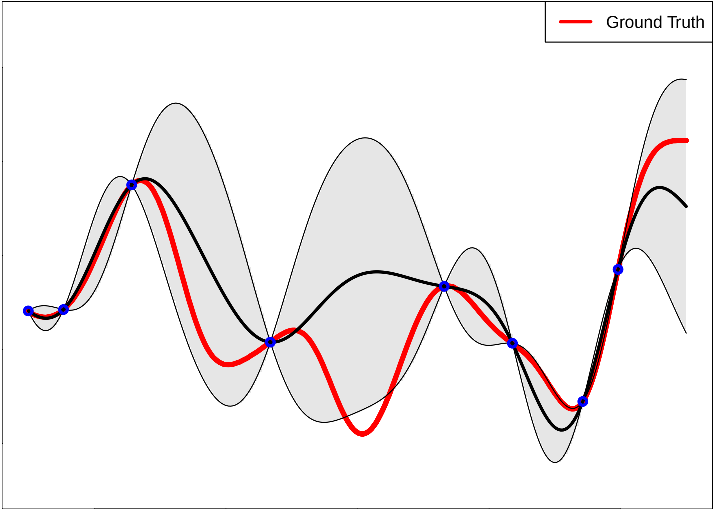

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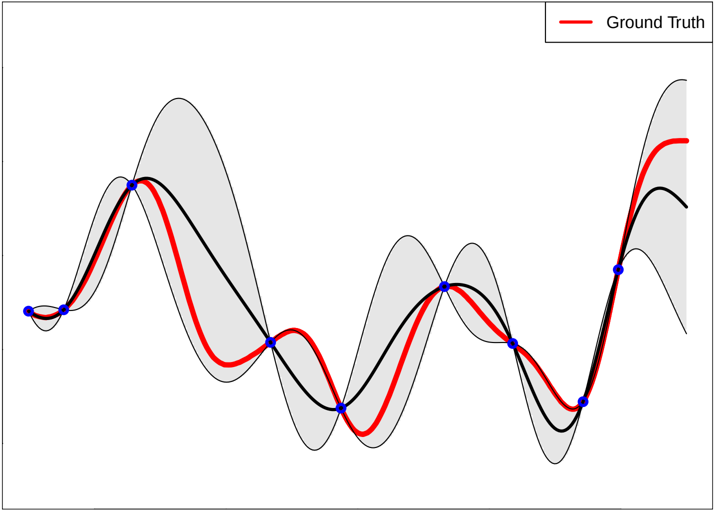

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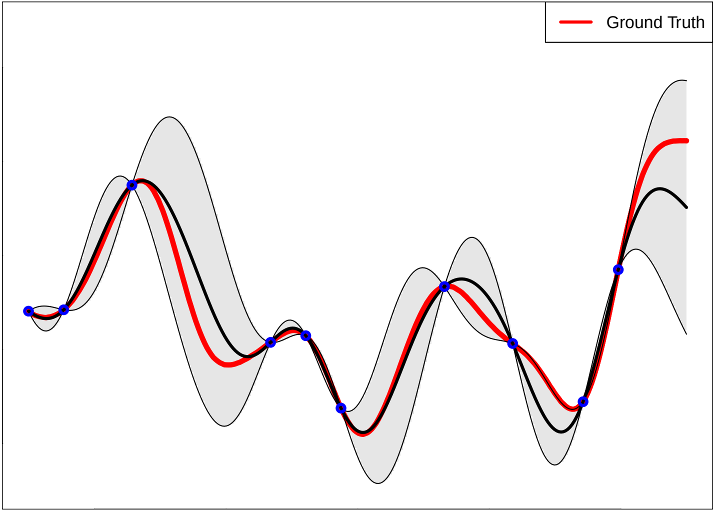

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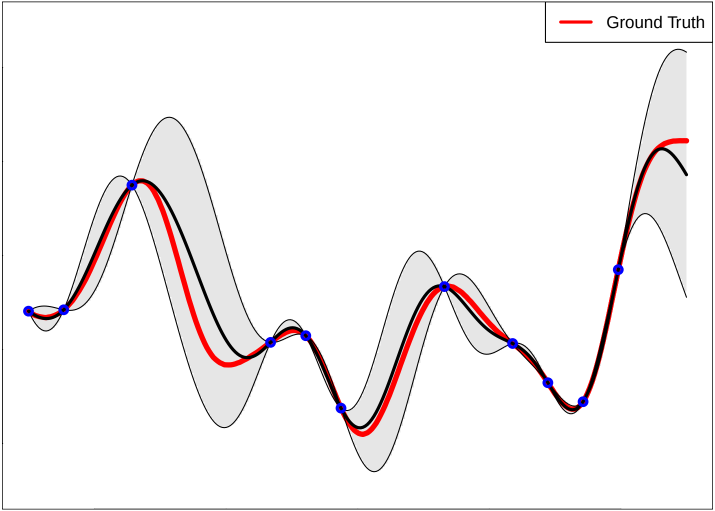

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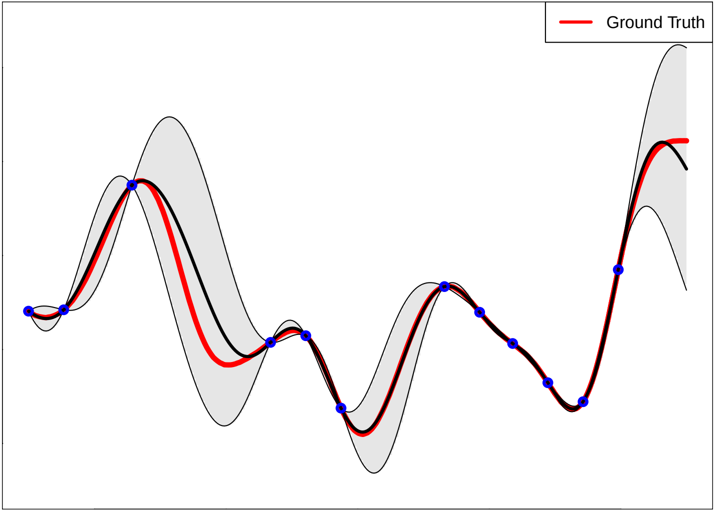

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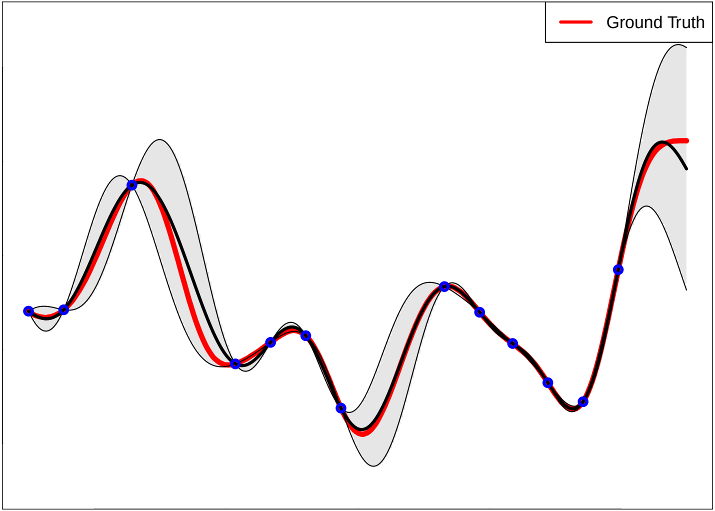

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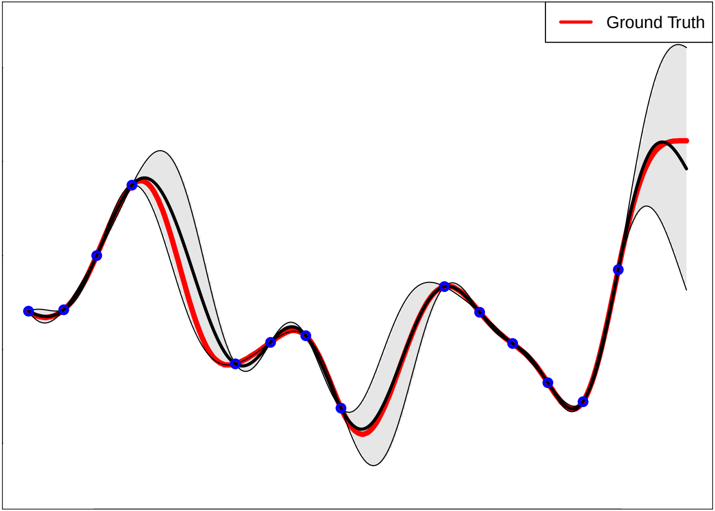

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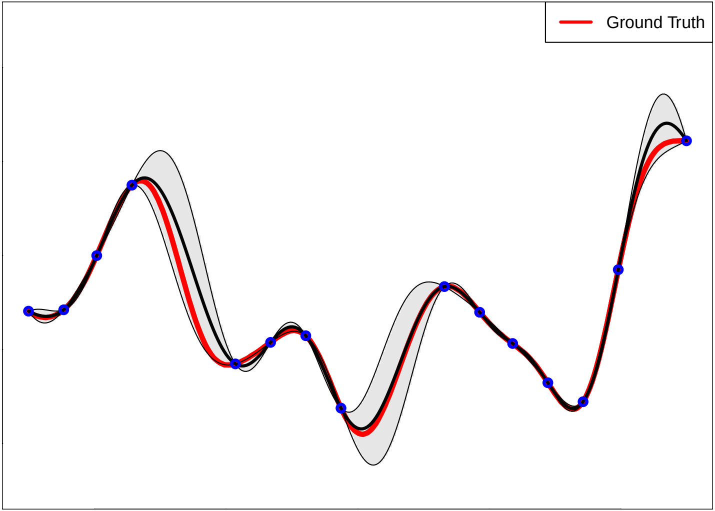

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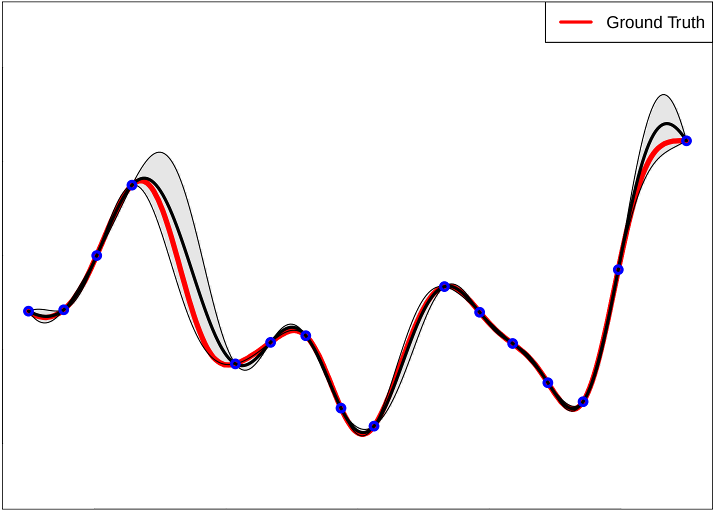

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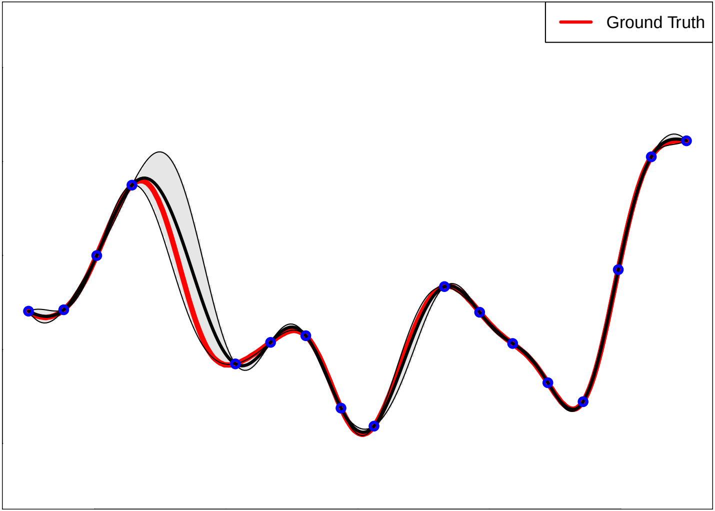

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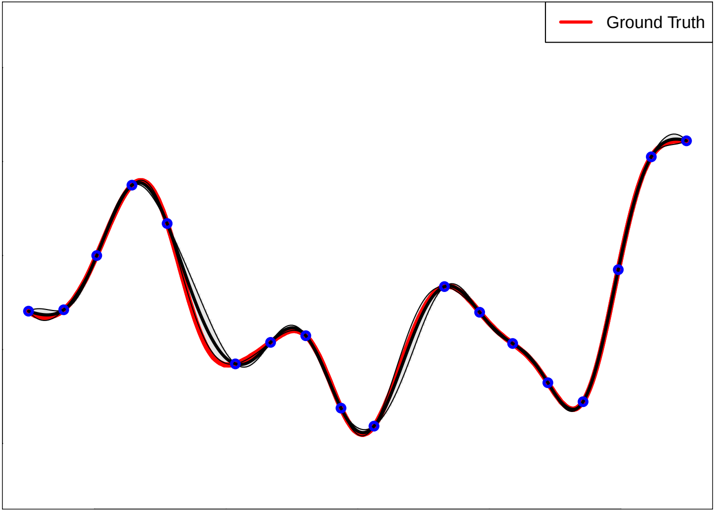

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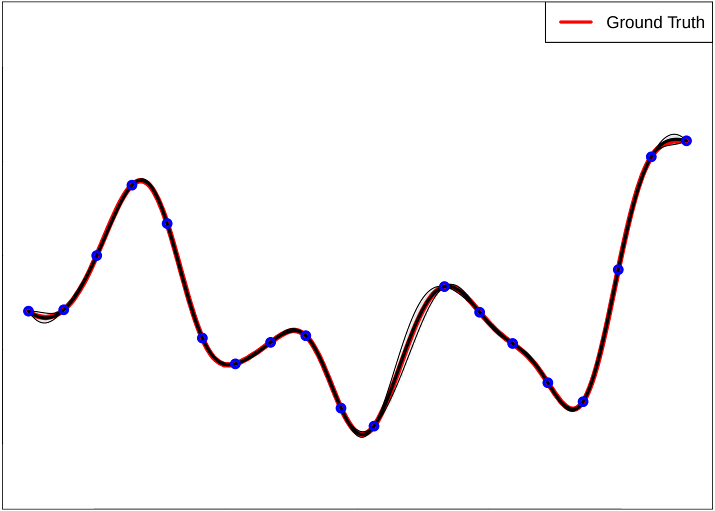

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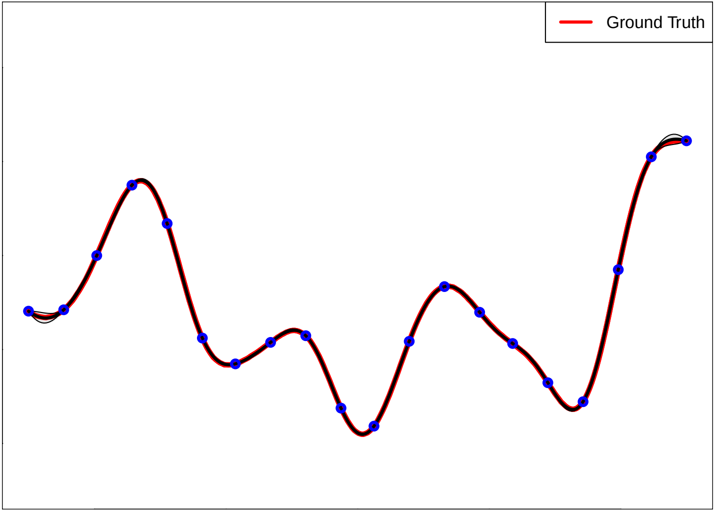

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Can we get the benefits of the two approaches?

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How do we approximate these quantities?

Variational Inference - a quick reminder

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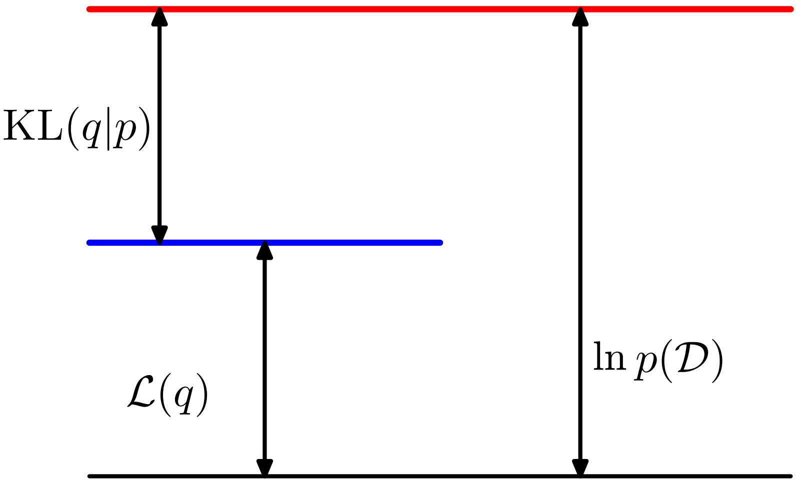
$p(\mathbf{W}, \mathcal{D})$, the product of the prior and the likelihood factors, **simplifies with the logarithm** and $\mathcal{L}(q)$ is **feasible to evaluate**.

Decomposition of the Marginal Likelihood



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Stochastic optimization techniques enable VI on deep neural networks and massive datasets!

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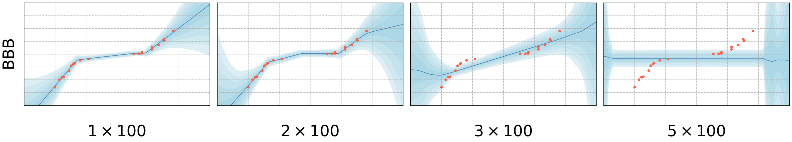

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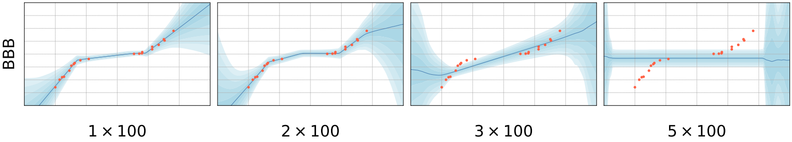

Undesirable behavior as more units or layers are added!

(Sun et al., 2019)

Why use the function space?

Benefits:

1. Avoids symmetric modes in the posterior of parameter space!
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Approximate inference is challenging since it involves working with random functions rather than with finite sets of variables!

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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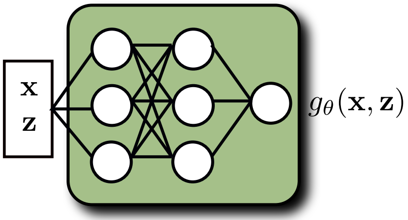
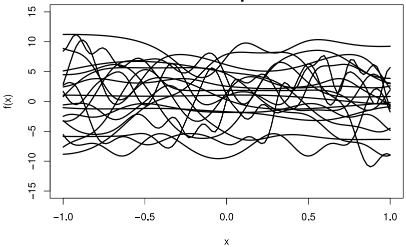
Neural sampler



Prior samples



Learning under Implicit Process Priors

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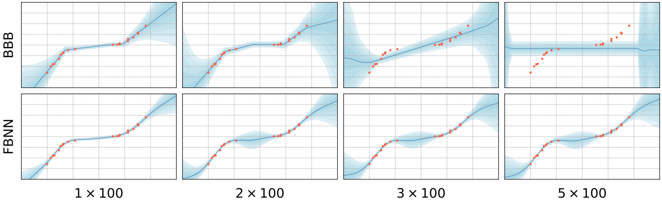

Inference with IPs and inducing points

Implicit process $f(\mathbf{x}) = h_\phi(\mathbf{x}, \epsilon)$ as approximate implicit posterior distribution of the process specified in the prior (as in *FBNNs*)

Approximate Inference via functional variational inference (*f-ELBO*):

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Challenges:

1. Avoid increasing the number of latent variables with N (as GPs)
   - $M \ll N$ **inducing points** ($\overline{\mathbf{X}}$, $\mathbf{u}$)
2. Compute the conditional posterior (intractable)
   - **MonteCarlo GP approximation** for the posterior approximation $p(\mathbf{f}|\mathbf{u})$ (as in *VIPs*)

Training the system

Our posterior approximation becomes

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

The variational inference objective is:

$$\begin{aligned}\mathcal{L}(q) &= \mathbb{E}_q \left[\log \frac{p(\mathbf{y}|\mathbf{f}) \cancel{p_\theta(\mathbf{f}|\mathbf{u})} p_\theta(\mathbf{u})}{\cancel{p_\theta(\mathbf{f}|\mathbf{u})} q_\phi(\mathbf{u})} \right] \\ &= \sum_{i=1}^{N} \mathbb{E}_{q_{\phi,\theta}} [\log p(y_i|f_i)] - \mathrm{KL}(q_\phi(\mathbf{u}) | p_\theta(\mathbf{u}))\end{aligned}$$

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$$= \sum_{i=1}^{N} \mathbb{E}_{q_{\phi,\theta}} [\log p(y_i|f_i)] - \mathrm{KL}(q_\phi(\mathbf{u})|p_\theta(\mathbf{u}))$$

KL-divergence is **intractable** (**implicit** q and p) $\Rightarrow$ **classifier** to estimate the log-ratio inside the KL-divergence:

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

$T_{\Omega^\star}(\mathbf{u}) \Rightarrow$ Optimized DNN discriminating samples of $q_\phi(\mathbf{u})$ and $p_\theta(\mathbf{u})$

Conditional Distribution and Predictions

It is critical to compute $p_\theta(\mathbf{f}|\mathbf{u})$ in the model.

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Approximated using a GP (as in VIP)

$$\mathbb{E}[f(\mathbf{x})] = m^\star_{MLE}(\mathbf{x}) + \mathbf{K}_{\mathbf{f},\mathbf{u}}(\mathbf{K}_{\mathbf{u},\mathbf{u}} + \mathbf{I}\sigma^2)^{-1}(\mathbf{u} - m^\star_{\mathrm{MLE}}(\mathbf{X}))\,,$$
$$\mathrm{Var}(f(\mathbf{x})) = \mathbf{K}_{\mathbf{f},\mathbf{f}} - \mathbf{K}_{\mathbf{f},\mathbf{f}}(\mathbf{K}_{\mathbf{u},\mathbf{u}} + \mathbf{I}\sigma^2)^{-1}\mathbf{K}_{\mathbf{u},\mathbf{f}}$$

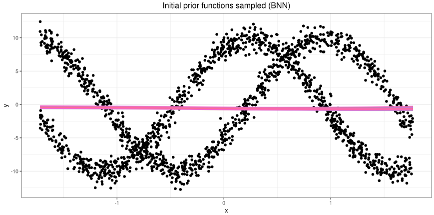
Covariances $\Rightarrow$ Monte Carlo methods by sampling from the prior

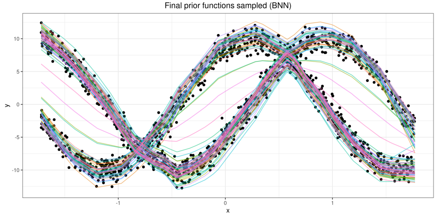
Predictions can also be approximated by Monte Carlo:

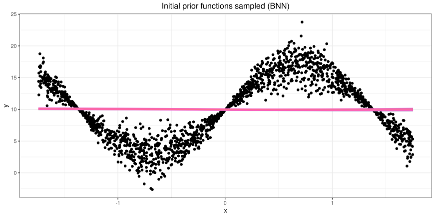
$$p(f(\mathbf{x}_*)|\mathbf{y},\mathbf{X}) \approx \frac{1}{S}\sum_{s=1}^{S} p_\theta(f(\mathbf{x}_*)|\mathbf{u}_s)\,, \qquad \mathbf{u} \sim q_\phi(\mathbf{u})\,.$$

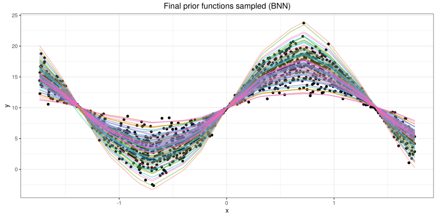
Flexibility of the prior functions

Synthetic data with different features to test the functions the prior is able to learn



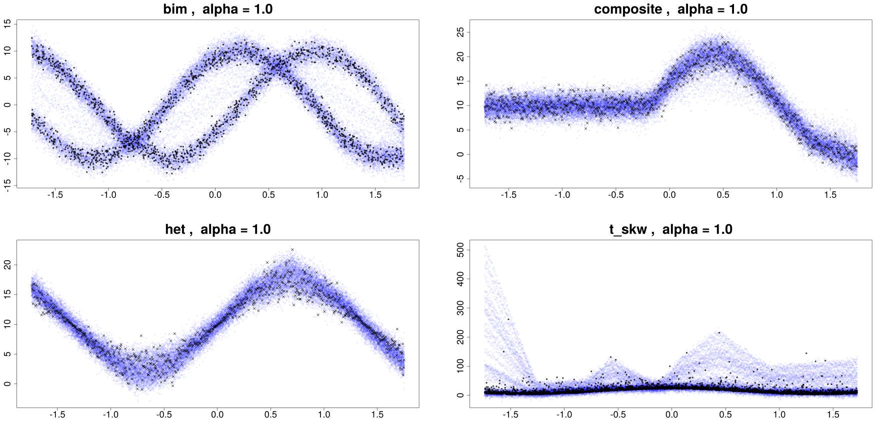






Predictive distribution and results

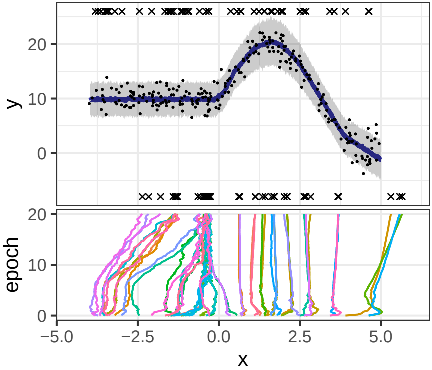
Flexible final predictions in different synthetic datasets



Evolution of the inducing points

Inducing points tend to gather in the regions where data changes most
The data here follows a constant function first, and suddenly change into a sine function

- The matching point between both behaviors tend to have more concentration of IPs ($M = 50$)



Conclusions

1. Gaussian Processes and Bayesian neural networks provide partial solutions for estimating uncertainty in the predictions.
   - GPs: simple and work fine for small data, but have flexibility and scalability problems
   - Sparse GPs: scalable, but predictions remain only Gaussian
   - BNNs: intractable inference and issues in the optimization procedure
2. Approximate inference in function space may be advantageous over weight space
3. Implicit processes are a difficult but very useful tool to deal with all these issues
   - Availability to **learn the hyperparameters** θ (*IP* prior) ✓
   - Flexibility in the posterior approximation (*IP* model - NS) with mixture of Gaussians predictions $\Rightarrow$ General predictive dist. ✓
   - **Scalability** in memory ($\mathcal{O}(M^3)$) and convergence time ✓

Thank you for your attention!

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