Imperial College London

# Uncertainty in Deep Models
## using Gaussian Processes

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- This talk is loosely based on the paper **Bayesian Image Classification with Deep Convolutional Gaussian Processes**, Vincent Dutordoir, Mark van der Wilk, Artem Artemev, James Hensman; AISTATS 2020.

# Overview

# Uncertainty: a matter of life or death


TESLA MODEL S MODEL 3 MODEL X MODEL Y ROADSTER

Blog Videos

A Tragic Loss

The Tesla Team • 30 June 2016

We learned yesterday evening that NHTSA is opening a preliminary evaluation into the performance of Autopilot during a recent fatal crash that occurred in a Model S. This is the first known fatality in just over 130 million miles where Autopilot was activated. Among all vehicles in the US, there is a fatality every 94 million miles. Worldwide, there is a fatality approximately every 60 million miles. It is important to emphasize that the NHTSA action is simply a preliminary evaluation to determine whether the system worked according to expectations.

Following our standard practice, Tesla informed NHTSA about the incident immediately after it occurred. What we know is that the vehicle was on a divided highway with Autopilot engaged when a tractor trailer drove across the highway perpendicular to the Model S. Neither Autopilot nor the driver noticed the white side of the tractor trailer against a brightly lit sky, so the brake was not applied. The high ride height of the trailer combined with its positioning across the road and the extremely rare circumstances of



Deep learning applied in the wild, but what would you do

- in a previously unseen situation, or ambiguous stimulus?
- if you were 10% sure there was an obstruction?

# Automatic machine learning

Current learning procedure:

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3. Train multiple models with different hyperparameters (layers, topology, ...)
4. Cross-validate and deploy model with best performance

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Can we

- **automatically** pick hyperparameters and data augmentation?
- **update** model based on new observations?

Goals:

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1. Good uncertainty

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2. Automatic model selection

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# Related problems

in the Bayesian framework

# Overview

Goals

Bayesian Deep Learning

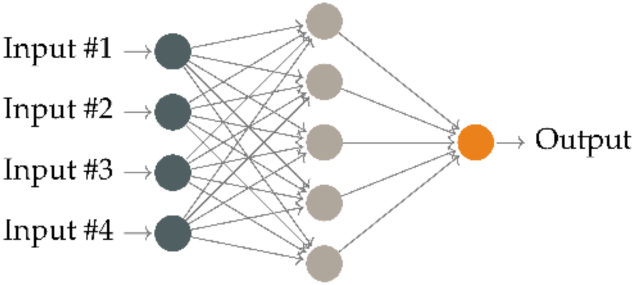
Gaussian Processes

Deep Gaussian Processes

Application & results

Conclusions

# Neural networks are basis function models

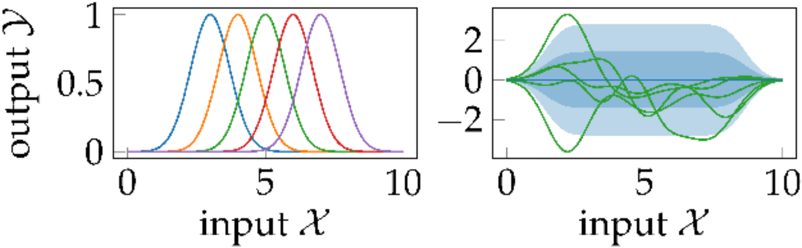



$$f(\mathbf{x}) = \sum_{b=1}^{B} w_b \phi_b(\mathbf{x}) = \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x})$$

$$\phi_b(\mathbf{x}) = \sigma\left(\sum_{d=1}^{D} \tilde{w}_d x_d\right) = \sigma(\tilde{\mathbf{w}}^\top \mathbf{x})$$

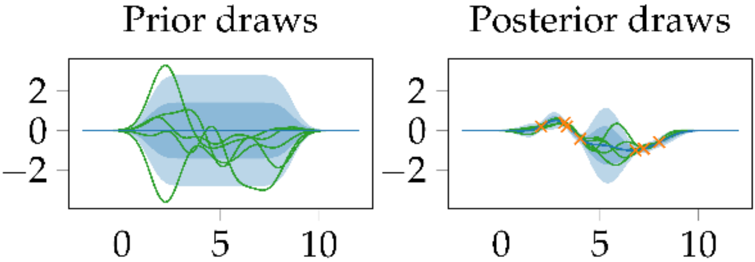
# Bayesian Neural Networks are a prior over functions

Placing priors on **w** gives us a distribution over functions:




$$f(\mathbf{x}) = \sum_{b=1}^{B} w_b \phi_b(\mathbf{x}) = \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x}), \qquad \mathbf{w} \sim \mathcal{N}\left(\mathbf{w}; 0, \sigma_w^2 I\right).$$

# Bayesian advantages




Using the prior, we can obtain the **posterior** to quantify **uncertainty**:

$$p(\mathbf{w}|\mathbf{y},\theta) = \frac{\prod_n p(y_n|\mathbf{w},\theta)p(\mathbf{w}|\theta)}{p(\mathbf{y}|\theta)}$$

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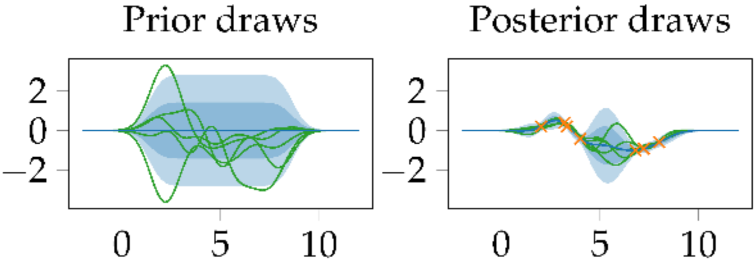


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Using the **marginal likelihood** we can find hyperparameters (properties of the prior):

$$p(\theta\,|\,\mathbf{y}) = \frac{\prod_n p(\mathbf{y}\,|\,\theta)p(\theta)}{p(\mathbf{y})}$$

# Variational Inference

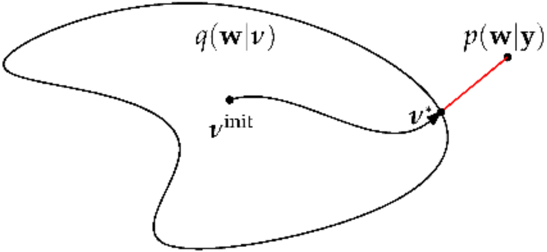


Figure adopted from Blei et al.'s NIPS-2016 tutorial

- Find approximation of a probability distribution (e.g., posterior) by optimization:
  1. Define a (parametrized) family of approximating distributions $q_\nu$
  2. Define KL[approx||posterior] to be measure of similarity
  3. Optimise measure w.r.t. variational parameters $\nu$
- Inference ⏩ Optimization

# Variational Inference in Bayesian Neural Networks

Variational inference is most commonly used for approximate inference in BNNs:

$$q(\mathbf{w}) = \underset{q(\mathbf{w})\in\mathcal{Q}}{\operatorname{argmin}} \mathrm{KL}[q(\mathbf{w})||p(\mathbf{w}\,|\,\mathbf{y},\theta)]$$

$$\log p(\mathbf{y}\,|\,\theta) - \mathrm{KL}[q(\mathbf{w})||p(\mathbf{w}\,|\,\mathbf{y},\theta)] = \mathrm{ELBO} = \mathcal{L}$$

ELBO becomes:

$$\mathcal{L} = \mathbb{E}_{q(\mathbf{w})}[\log p(\mathbf{y}\,|\,\mathbf{w},\theta)] - \mathrm{KL}[q(\mathbf{w})||p(\mathbf{w})]$$

$$\text{with e.g. } q(\mathbf{w}) = \prod_{p=1}^{P} \mathcal{N}\left(w_i; \mu_i, \sigma_i^2\right)$$

E.g. Blundell et al. *Weight Uncertainty in Neural Networks* [2015]

# Is variational inference working?

From Blundell et al. *Weight Uncertainty in Neural Networks* [2015]:

> cross-validation where possible. Empirically we found optimising the parameters of a prior $P(\mathbf{w})$ (by taking derivatives of (1)) to not be useful, and yield worse results.

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- ELBOs not tight enough for model comparison
- Observation: Bounds are so loose that they prefer a noise model over fitting the data (i.e. variance of $\mathbb{V}_{p(\mathbf{w}\,|\,\theta_{\text{opt}})} = 0$)

$$\mathcal{L} + \text{KL}[q(\mathbf{w})||p(\mathbf{w}\,|\,\mathbf{y})] = \log p(\mathbf{y}\,|\,\theta)$$

$$\mathcal{L}(\mathbf{v}_{\text{opt}}, \theta_{\text{opt}}) \gg \mathcal{L}(\mathbf{v}_{\text{good}}, \theta_{\text{good}})$$

$$\implies \text{KL}[q(\mathbf{w})||p(\mathbf{w}\,|\,\mathbf{y}, \theta)] = \text{large!}$$

# Problems

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Bayesian deep learning using Variational Inference

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We could be doing a lot better!

# Overview

# Gaussian Processes

A Gaussian process is a **distribution over functions** with Gaussian marginals. Its properties are defined by the **kernel function** $k(\mathbf{x}, \mathbf{x}')$:

$$p(f(\mathbf{x}_1), f(\mathbf{x}_2), f(\mathbf{x}_3), \dots) = p(f(X)) = \mathcal{N}(f(X); 0, \boldsymbol{K})$$
$$[\boldsymbol{K}]_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$$

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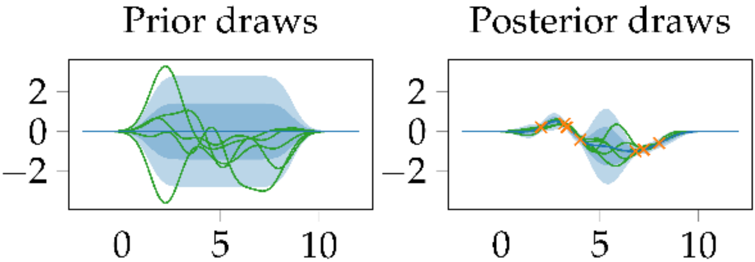
- Behaves as a basis function model
- Can have infinite basis functions
- Posteriors can be represented accurately

# Finite basis functions

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- How many basis functions?

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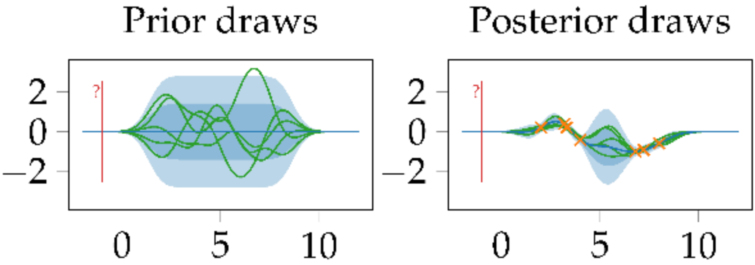


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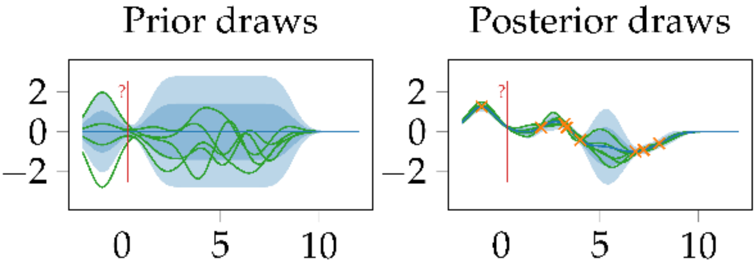


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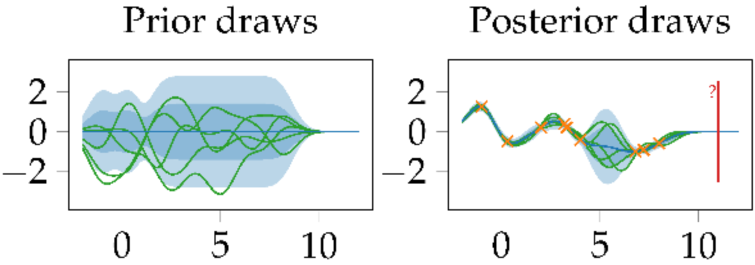


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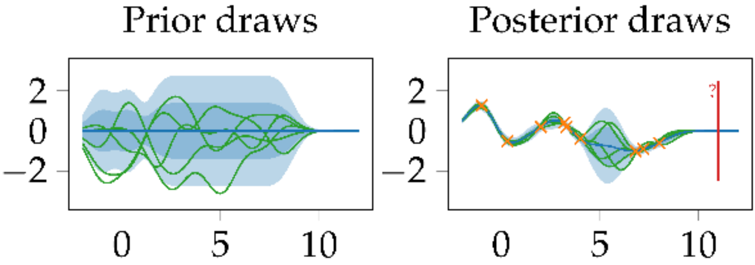


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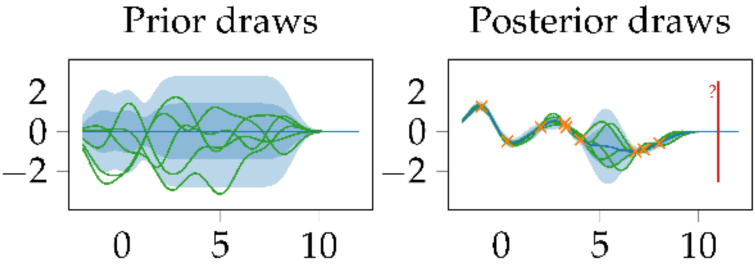
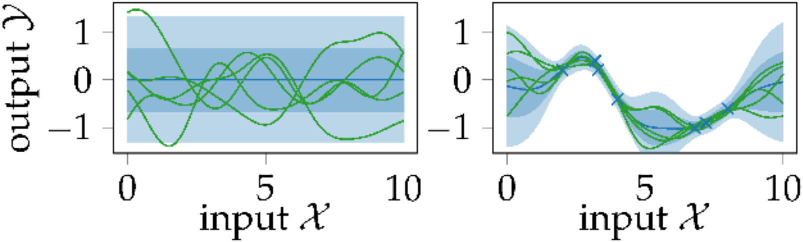



- Should we be so certain far from the data?
- How many basis functions?

Solution: Use an infinite number of basis functions?

# Infinite basis functions




- Should we be so certain far from the data? → **No, and we don't have to be!**
- How may basis functions? → **infinite!**

# Inference in Gaussian Processes

Predictions are made using the posterior:

$$p(f(X^*) \mid \mathbf{y}, \theta) = \int p(f(X^*) \mid f(X), \theta) \frac{\prod_n p(y_n \mid f(\mathbf{x}_n)) p(f(X) \mid \theta)}{p(\mathbf{y} \mid \theta)} \mathrm{d} f(X)$$

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- Prior is computationally costly. Covariance matrix inverse and determinant scale as $O(N^3)$.
- Need approximate inference for non-Gaussian likelihoods.

# Variational Inference for Gaussian Processes

In VI for GPs, we minimise the KL divergence between the approximate posterior over functions $q(f(\cdot))$ and the true posterior over functions $p(f(\cdot) \mid \mathbf{y}, \theta)$:

$$\mathrm{KL}[q(f(\cdot))||p(f(\cdot) \mid \mathbf{y}, \theta)]$$

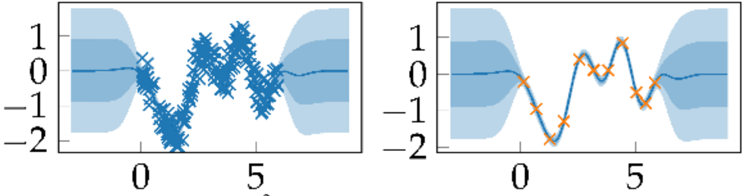
This is well-defined, [Matthews et al. 2016], and leads to a tractable ELBO [Hensman et al. 2013]:

$$\mathcal{L} = \sum_{n=1}^{N} \mathbb{E}_{q(f(\mathbf{x}_n))}[\log p(y_n \mid f(\mathbf{x}_n)] - \mathrm{KL}[q(f(\cdot))||p(f(\cdot))]$$

(We abuse notation of densities over functions to mean the appropriate Gaussian process measures, or a distribution over an arbitrary set of function values.)

# Set of approximate posteriors

Gaussian process prior, but with constrained behaviour at $M$ points




$$q(f(\mathbf{x}_n)) = \int p(f(\mathbf{x}_n) \mid f(Z)) q(f(Z)) \mathrm{d}f(Z)$$

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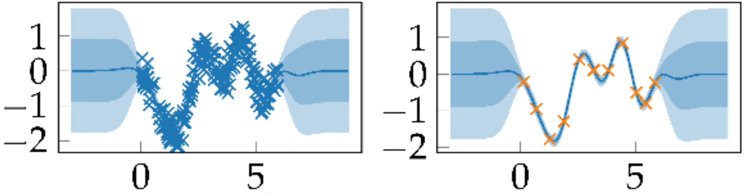


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- Computationally efficient [Titsias 2009]
- Can be minibatched [Hensman et al. 2013]
- Works with arbitrary likelihoods [Hensman et al. 2016]
- Can be arbitrarily accurate [Burt et al. 2019]

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# Gaussian Processes as a Layer

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[Damianou & Lawrence 2013]

# Deep Gaussian Processes

Define model through

- function composition (like deep NNs),
- Gaussian process priors on each layer.

$$f(\mathbf{x}) = f_L(f_{L-1}(f_{L-2}(\dots f_1(\mathbf{x})\dots))) = (f_L \circ f_{L-1} \circ \dots f_1)(\mathbf{x})$$
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How do we find the posterior?

$$p(f_1(\cdot), f_2(\cdot), \dots \mid \mathbf{y}) = \frac{\prod_{n=1}^{N} p(y_n \mid f(\mathbf{x}_n), \mathbf{x}_n) \prod_{\ell=1}^{L} p(f_\ell(\cdot) \mid \theta)}{p(\mathbf{y} \mid \theta)} \quad (1)$$

# Variational Inference for Gaussian Processes

We again minimise the KL divergence between the distributions over functions, only we have more now.

$$\mathrm{KL}[q(f_1, \ldots, f_L) \| p(f_1, \ldots, f_L \,|\, \mathbf{y})]$$

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The ELBO has a similar structure, and can be optimised using Monte Carlo estimates of the expectations:

$$\mathcal{L} = \sum_{n=1}^{N} \mathbb{E}_{q(f_1,\ldots,f_L)}[\log p(y_n \mid (f_L \circ \cdots \circ f_1)(\mathbf{x}_n))] - \sum_{\ell=1}^{L} \mathrm{KL}[q(f_\ell(Z)) \| p(f_\ell(Z))]$$

Monte Carlo estimate only needs to evaluate $f_\ell(\cdot)$ at the output of $f_{\ell-1}(\cdot)$, starting with $f_1(\mathbf{x})$ [Salimbeni & Deisenroth 2017].

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- stack Gaussian process layers with convolutional structure [v.d. Wilk 2017],
- introduce modelling capacity compared to Blomqvist et al. [2018],
- apply the straightforward variational inference procedure from Salimbeni & Deisenroth [2017].

We obtain

- an ELBO that we maximise for **selecting hyperparameters**,
- **competitive performance** on MNIST,
- **better uncertainty estimates** compared to NNs.

# Deep Convolutional Gaussian Processes: Uncertainty


Applying theory simply works!

1. ELBO tight enough for hyperparameter optimisation
2. Evidence supporting KL[approx||posterior] is small

# Deep Convolutional Gaussian Processes: Results

Table 2: DCGP [Blomqvist et al., 2019] (reproduced with our code) and Deep TICK-GP (our method) on MNIST and CIFAR-10.

| | | MNIST | | CIFAR-10 | |
|---|---|---|---|---|---|
| depth | metric | Conv | TICK | Conv | TICK |
| 1 | top-1 error (%) | 1.87 | **1.19** | 41.06 | **37.10** |
| | NLL full | 0.06 | **0.04** | 1.17 | **1.08** |
| | neg. ELBO ($\times 10^3$) | 8.29 | **5.83** | 65.72 | **63.51** |
| 2 | top-1 error (%) | 0.96 | **0.67** | 28.60 | **25.59** |
| | NLL full | 0.04 | **0.02** | 0.84 | **0.75** |
| | neg. ELBO ($\times 10^3$) | 5.37 | **4.25** | 52.81 | **48.31** |
| 3 | top-1 error (%) | 0.93 | **0.64** | 25.33 | **23.83** |
| | NLL full | 0.03 | **0.02** | 0.74 | **0.69** |
| | neg. ELBO ($\times 10^3$) | 5.045 | **4.19** | 49.38 | **47.53** |

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- DGPs are behind in performance, but steadily improving.
- DGPs are slow, but getting faster.
- BDL starts from current methods that perform well, and try to make inference work.
- DGPs start from inference that works, and try to make it perform well.

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Thank you!

# References

Key references. See paper for more.


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