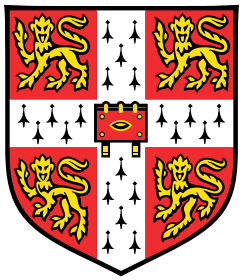
Efficient Gaussian Processes for data-driven decision making



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Abstract

This is where you write your abstract ...

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Chapter 1

Introduction

Bayesian inference has the potential to improve deep neural networks (DNNs) by providing 1) uncertainty estimates for robust prediction and downstream decision-making, and 2) an objective function (the marginal likelihood) for hyperparameter selection [MacKay, 1992a; 1992b; 2003]. The recent success of deep learning [Krizhevsky et al., 2012; Vaswani et al., 2017; Schrittwieser et al., 2020] has renewed interest in large-scale Bayesian Neural Networks (BNNs) as well, with effort mainly focused on obtaining useful uncertainty estimates [Blundell et al., 2015; Kingma et al., 2015; Gal and Ghahramani, 2016]. Despite already providing usable uncertainty estimates, there is significant evidence that current approximations to the uncertainty on neural network weights can still be significantly improved [Hron et al., 2018; Foong et al., 2020]. The accuracy of the uncertainty approximation is also linked to the quality of the marginal likelihood estimate [Blei et al., 2017]. Since hyperparameter learning using the marginal likelihood fails for most common approximations [e.g., Blundell et al., 2015], the accuracy of the uncertainty estimates is also questionable.

Damianou and Lawrence [2013] used Gaussian processes [Rasmussen and Williams, 2006] as layers to create a different Bayesian analogue to a DNN: the Deep Gaussian process (DGP). Gaussian processes (GPs) are a different representation of a single layer neural network, which is promising because it allows high-quality approximations to uncertainty [Titsias, 2009; David R. Burt et al., 2019]. DGPs are promising, since they seem to inherit these high-quality approximations, as indicated by the successful use of marginal likelihood approximations for hyperparameter learning [Damianou and Lawrence, 2013; Dutordoir et al., 2020b].

Despite their advantages, DGPs have not been adopted as widely as DNNs, which can mainly be attributed to their larger computational cost and the fact that their are challenging to optimise. In the past, these challenges were also present in DNNs, although decades of work has led to standard practices (e.g. ReLU activations [Glorot et al., 2011], Xavier weight initialisations [Glorot and Bengio, 2010], and batch normalisation [Ioffe and Szegedy, 2015]) that have largely eliminated them. So far, it has not been possible to directly apply these methods to DGPs due to the mathematical differences between the models.

1.1 Contributions and Layout of this Report

This report represents my learning and the research that I conducted during the first year of my PhD degree. Most notably, we developed a novel sparse approximation for (deep) Gaussian processes based on the decomposition of the kernel in Spherical harmonics. In chapter 2 we cover the necessary theoretical background.

Chapter 3 In this chapter we introduce a new class of inter-domain variational GPs where data is mapped onto the unit hypersphere in order to use spherical harmonic representations. The inference scheme is comparable to Variational Fourier Features, but it does not suffer from the curse of dimensionality, and leads to diagonal covariance matrices between inducing variables. This enables a speed-up in inference, because it bypasses the need to invert large covariance matrices. The experiments show that our model is able to fit a regression model for a dataset with 6 million entries two orders of magnitude faster compared to standard sparse GPs, while retaining state of the art accuracy.

The content of this chapter is largely based on:

Vincent Dutordoir, Nicolas Durrande, and James Hensman [2020a]. "Sparse Gaussian Processes with Spherical Harmonic Features". In: *Proceedings of the 37th International Conference on Machine Learning (ICML)*,

with the exception of the algorithm for computing the spherical harmonics in high dimensions.

Chapter 3 Following up on the previous chapter, we use the decomposition of zonal kernels to design an interdomain inducing variable that mimics the behaviour of activation functions is neural network layers.

The content of this chapter is largely based on:

Vincent Dutordoir, James Hensman, Mark van der Wilk, Carl Henrik Ek, Zoubin Ghahramani, and Nicolas Durrande [2021a]. "Deep Neural Networks as Point Estimate for Deep Gaussian Processes". In: *submission to NeurIPS*.

Chapter 4 In the last chapter of the report we will shed a light on what the future work will focus on: "Gaussian Decision Systems with Geometric Gaussian processes".

Chapter 2

Theoretical Framework

This chapter discusses Gaussian processes (GP) and deep Gaussian processes (DGPs), the composite model obtained by stacking multiple GP models on top of each other. We also review how to perform approximate Bayesian inference in these models, with a particular attention to Variational Inference. We also cover the theory of postive definite kernels and the Reproducing Kernel Hilbert Spaces (RKHS) they characterise.

2.1 Gaussian Processes

Gaussian processes (GPs) [Rasmussen and Williams, 2006] are non-parametric distributions over functions similar to Bayesian Neural Networks (BNNs). The core difference is that neural networks represent distributions over functions through distributions on weights, while a Gaussian process specifies a distribution on function values at a collection of input locations. This representation allows us to use an infinite number of basis functions, while still enables Bayesian inference [Neal, 1995].

Following from the Kolmogorov extension theorem, we can construct a real-valued stochastic process (i.e. function) on a non-empty set $\mathcal{X}$, $f : \mathcal{X} \to \mathbb{R}$, if there exists on all finite subsets $\{x_1, \dots x_N\} \subset \mathcal{X}$, a *consistent* collection of finite-dimensional marginal distributions over $f(\{x_1, \dots, x_n\})$. For a Gaussian process, in particular, the marginal distribution over every finite-dimensional subset is given by a multivariate normal distribution. This implies that, in order to fully specify a Gaussian process, it suffice to only define the mean and covariance (kernel) function because they are the sufficient statistics for every finite-dimensional marginal distribution. We can therefore denote the GP as

$$f \sim \mathcal{GP}(\mu, k), \tag{2.1}$$

where $\mu : \mathcal{X} \to \mathbb{R}$ is the mean function, which encodes the expected value of f at every x, $\mu(x) = \mathbb{E}_f[f(x)]$, and $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is the covariance (kernel) function that describes the

covariance between function values, $k(x, x') = \mathrm{Cov}(f(x), f(x'))$. The covariance function has to be a symmetric, positive-definite function. The Gaussianity, and the fact that we can manipulate function values at some finite points of interest without taking the behaviour at any other points into account (the marginalisation property) make GPs particularly convenient to manipulate and use as priors over functions in Bayesian models – as we will show next.

Throughout this report, we will consider f to be the complete function, and intuitively manipulate it as an infinitely long vector. Moreover, $f(\boldsymbol{x}) \in \mathbb{R}^N$ denotes the function evaluated at a finite set of points, whereas $f^{\setminus \boldsymbol{x}}$ denotes another infinitely long vector similar to f but excluding $f(\boldsymbol{x})$. From the marginalisation property it follows that integrating out over the infinitely many points that are not included in $\boldsymbol{x}$, we obtain a valid finite-dimensional density for $f(\boldsymbol{x})$

$$p(f(\boldsymbol{x})) = \int p(f)\, \mathrm{d}f^{\setminus \boldsymbol{x}}. \tag{2.2}$$

In the case of GPs, this finite-dimensional marginal is given by a multivariate Gaussian distribition, fully characterised by the mean μ and the covariance function k

$$p(f(\boldsymbol{x})) = \mathcal{N}(\boldsymbol{\mu}_{\mathbf{f}}, \mathbf{K}_{\mathbf{ff}}), \quad \text{where} \quad [\boldsymbol{\mu}_{\mathbf{f}}]_i = \mu(x_i) \text{ and } [\mathbf{K}_{\mathbf{ff}}]_{i,j} = k(x_i, x_j). \tag{2.3}$$

Conditioning the GP at this finite set of points leads to a conditional distribution for $f^{\setminus \boldsymbol{x}}$, which is given by another Gaussian process

$$p(f^{\setminus \boldsymbol{x}} \mid f(\boldsymbol{x}) = \mathbf{f}) = \mathcal{GP}(\mathbf{k}_{\mathbf{f}\cdot}^\top \mathbf{K}_{\mathbf{ff}}^{-1}(\mathbf{f} - \boldsymbol{\mu}_{\mathbf{f}}), \quad k(\cdot,\cdot) - \mathbf{k}_{\mathbf{f}\cdot}^\top \mathbf{K}_{\mathbf{ff}}^{-1} \mathbf{k}_{\mathbf{f}\cdot}), \tag{2.4}$$

where $[\mathbf{k}_{\mathbf{f}\cdot}]_i = k(x_i, \cdot)$. The conditional distribution over the whole function $p(f \mid f(\boldsymbol{x}) = \mathbf{f})$ has the exact same form as in eq. (2.4). This is mathematically slightly confusing because the random variable $f(\boldsymbol{x})$ is included both on the left and right-hand-side of the conditioning, but the equation is technically correct [Matthews et al., 2016].

2.1.1 The Beauty of Gaussian Process Regression: Exact Bayesian Inference

One of the key advantages of Gaussian processes for regression is that we can perform exact Bayesian inference. Assume a supervised learning setting where $x \in \mathcal{X}$ (typically, $\mathcal{X} = \mathbb{R}^d$) and $y \in \mathbb{R}$, and we are given a dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ of input and corresponding output pairs. For convenience, we sometimes group the inputs in $\boldsymbol{x} = \{x_i\}_{i=1}^N$ into a single design matrix and outputs $\boldsymbol{y} = \{y_i\}_{i=1}^N$ into a vector. We further assume that the data is generated by an unknown function $f : \mathcal{X} \to \mathbb{R}$, such that the outputs are perturbed versions of functions evaluations at the corresponding inputs: $y_i = f(x_i) + \epsilon_i$. In the case of regression we assume a Gaussian noise model $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$. We are interested in learning the function f that generated the data.

[General introduction to Bayesian modelling] The key idea in Bayesian modelling is to specify a prior distribution over the quantity of interest. The prior encodes what we know at that point in time about the quantity. In general term, this can be a lot or a little. We encode

this information in the form of a distribution. Then, as more data becomes available, we use the rules of probability, an in particlar Bayes' rule, to update our prior beliefs and compute a posterior distribution (see **bisschop**; MacKay [2003] for a thorough introduction).

Following the Bayesian approach, we specify a *prior* over the parameters of interests, which in the case of GPs is the function itself. The prior is important because it characterises the search space over possible solutions for f. Through the prior, we can encode strong assumptions, such as linearity, differentiability, periodicity, etc. or any combination thereof, which makes it possible to generalise well from very limited data. Compared to (Bayesian) parametric models, it is much more convenient and intuitive to specify priors directly in *function-space*, rather than on the weights of a parametric model [Rasmussen and Williams, 2006].

Following eq. (2.1) the prior over function evaluations at the datapoints is defined by the covariance function k. As we assume a à-priori zero mean function μ (without loss of generality) this can be written as:

$$p(f(\boldsymbol{x})) = \mathcal{N}(\mathbf{0}, \mathbf{K_{ff}}), \quad \text{where} \quad [\mathbf{K_{ff}}]_{i,j} = k(x_i, x_j). \tag{2.5}$$

Given the function f the likelihood factorises over datapoints and is given by a Gaussian:

$$p(\boldsymbol{y} \mid f) = \prod_{i=1}^{N} p(y_i \mid f) = \prod_{i=1}^{N} \mathcal{N}\Big(y_i \mid f(x_i), \sigma^2\Big) \tag{2.6}$$

We can obtain the posterior over the function using Bayes' rule and the marginalisation property

$$p(f \mid \boldsymbol{y}) = \frac{p(f)\, p(\boldsymbol{y} \mid f)}{p(\boldsymbol{y})} \tag{2.7}$$

$$= p(f^{\setminus \boldsymbol{x}} \mid f(\boldsymbol{x})) \frac{p(f(\boldsymbol{x})) \prod_{i=1}^{N} \mathcal{N}(y_i \mid f(x_i), \sigma^2)}{p(\boldsymbol{y})} \tag{2.8}$$

$$= \mathcal{GP}(\mathbf{k_{f\cdot}}^\top \mathbf{K_{ff}}^{-1} \mathbf{f}, \quad k(\cdot,\cdot) - \mathbf{k_{f\cdot}}^\top \mathbf{K_{ff}}^{-1} \mathbf{k_{f\cdot}}), \tag{2.9}$$

The marginal likelihood (model evidence)

$$p(\boldsymbol{y}) = \mathcal{N}\Big(\boldsymbol{y} \mid \mathbf{0}, \mathbf{K_{ff}} + \sigma^2 \mathbf{I}\Big) \tag{2.10}$$

1. Plot: Prior, Data, Posterior
2. occam's razor

Problems A common criticism for GPs is that any modification to this approach breaks the Gaussian assumption.

1. Non-Gaussian likelihoods
2. Large datasets

3. Transformations: log or square transform

Solutions

1. Laplace
2. Expectation Propagation
3. Sparse Variational Inference

2.2 Approximate Inference with Sparse Gaussian Processes

1. General introduction to Variational inference [Blei et al., 2017] variational inference (VI), where the problem of Bayesian inference is cast as an optimization problem—namely, to maximize a lower bound of the logarithm of the marginal likelihood.
2. Sparse approximations [Snelson and Ghahramani, 2005; Quiñonero-Candela and Rasmussen, 2005]

2.3 Interdomain Inducing Variables

The basis functions used in the approximate posterior mean TODO ref are determined by the covariance between the inducing variables and other function evaluations $[c_u(\cdot)]_m = \mathrm{Cov}(f(\cdot), u_m)$. Commonly, the inducing variables are taken to be function values $u_m = f(w_m)$, which leads to the kernel becoming the basis function $[c_u(\cdot)]_m = k(\boldsymbol{w}_m, \cdot)$. *Interdomain* inducing variables [Lázaro-Gredilla and Figueiras-Vidal, 2009] select different properties of the GP (e.g. integral transforms $u_m = \int f(\boldsymbol{x}) g_m(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}$), which modifies this covariance (see [van der Wilk et al., 2020; Leibfried et al., 2020] for an overview), and therefore gives control over the basis functions. Most current interdomain methods are designed to improve computational properties [Hensman et al., 2018; David R Burt et al., 2020; Dutordoir et al., 2020a]. Our aim is to control $c_u(\cdot)$ to be a typical NN actvation function like a ReLU or Softplus. This was also investigated by Sun et al. [2021], although they found less common saturating activation functions.

2.3.1 Example: heavyside inducing variable

$f \sim \mathcal{GP}$ defined on $\mathbb{S}^1$ (the unit circle), $f : [-\pi, \pi] \to \mathbb{R}, \theta \mapsto f(\theta)$.
kernel (Arc Cosine order 0):

$$k(\theta, \theta') = \kappa(\rho) = \pi - |\theta - \theta'| \tag{2.11}$$

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\Big|_{\theta=\theta_m} k(\theta, \theta') = \tag{2.12}$$

$$u_m = \mathcal{L}_m(f) \tag{2.13}$$

$$\mathcal{L}_m = \frac{\mathrm{d}}{\mathrm{d}\theta}\Big|_{\theta=\theta_m} + \int \mathrm{d}\theta \tag{2.14}$$

$$\begin{aligned} \mathrm{Cov}(u_m, f(\theta')) &= \mathbb{E}_f\left[\mathcal{L}_m(f)\, f(\theta')\right] && (2.15)\\ &= \mathcal{L}_m k(\theta', \cdot) && (2.16)\\ &= \frac{\mathrm{d}}{\mathrm{d}\theta}\Big|_{\theta=\theta_m} k(\theta', \theta) + \int_{-\pi}^{\pi} k(\theta', \theta)\mathrm{d}\theta && (2.17) \end{aligned}$$

2.4 Deep Gaussian Processes

Vincent Dutordoir, Hugh Salimbeni, Eric Hambro, John McLeod, Felix Leibfried, Artem Artemev, Mark van der Wilk, James Hensman, Marc P Deisenroth, and ST John [2021b]. "GPflux: A Library for Deep Gaussian Processes". In: *arXiv preprint arXiv:2003.01115*

2.5 Covariance Functions

1. Positive Definite and Symmetry
2. RKHS
3. Bochner's theorem
4. Mercer Decomposition
5. Examples of RKHS
6. RKHS through Spectral Decomposition
7. Representer Theorem
8. Show how sparse approximation links anchor points

Chapter 3

Spherical Harmonic Variational Gaussian Processes

3.1 ArcCosine kernel and Associated Reproducing Hilber Kernel Space

The first order Arc Cosine kernel mimics the computation of infinitely wide fully connected layers with ReLU activations. Cho and Saul [2009] showed that for $\sigma(t) = \max(0, t)$, the covariance between function values of $f(\boldsymbol{x}) = \sigma(\boldsymbol{w}^\top \boldsymbol{x})$ for $\boldsymbol{w} \sim \mathcal{N}\left(0, d^{-1/2}\mathbf{I}_d\right)$ and $\boldsymbol{w} \in \mathbb{R}^d$ is given by

$$k(\boldsymbol{x}, \boldsymbol{x}') = \mathbb{E}_{\boldsymbol{w}}\Big[\sigma(\boldsymbol{w}^\top \boldsymbol{x})\, \sigma(\boldsymbol{w}^\top \boldsymbol{x}')\Big] = \underbrace{||\boldsymbol{x}||||\boldsymbol{x}'||}_{\text{radial}}\ \underbrace{\frac{1}{\pi}(\sqrt{1-t^2} + t\,(\pi - \arccos t))}_{\text{angular (shape function) } s(t)}, \tag{3.1}$$

where $t = \frac{\boldsymbol{x}^\top \boldsymbol{x}'}{||\boldsymbol{x}||||\boldsymbol{x}'||}$. The factorisation of the kernel in a radial and angular factor leads to an RKHS consisting of functions of the form $f(\boldsymbol{x}) = ||\boldsymbol{x}||\, g(\frac{\boldsymbol{x}}{||\boldsymbol{x}||})$, where $g(\cdot)$ is defined on the unit hypersphere $\mathbb{S}^{d-1} = \{\boldsymbol{x} \in \mathbb{R}^d : ||\boldsymbol{x}||_2 = 1\}$ but fully determines the function on $\mathbb{R}^d$.

The shape function can be interpreted as a kernel itself, since it is the restriction of $k(\cdot, \cdot)$ to the unit hypersphere. Furthermore its expression only depends on the dot-product between the inputs so it is a zonal kernel (also known as a dot-product kernel [Bietti and Bach, 2020]). This means that the eigenfunctions of the angular part of $k(\cdot, \cdot)$ are the spherical harmonics $\phi_{n,j}$ (we index them with a level n and an index within each level $j \in \{1, \ldots, N_n^d\}$) [Wendland, 2005; Dutordoir et al., 2020a]. Their associated eigenvalues only depend on n:

$$\lambda_n = \frac{\omega_d}{C_n^{(\alpha)}(1)} \int_{-1}^{1} s(t)\, C_n^{(\alpha)}(t)\, (1-t^2)^{\frac{d-3}{2}}\, \mathrm{d}t, \tag{3.2}$$

where $C_n^{(\alpha)}(\cdot)$ is the Gegenbauer polynomial[1] of degree n, $\alpha = \frac{d-2}{2}$, ω_d is a constant that depends on the surface area of the hypersphere. Analytical expressions of λ_n are provided in **??**. The above implies that k admits the Mercer representation:

$$k(\boldsymbol{x}, \boldsymbol{x}') = ||\boldsymbol{x}||\,||\boldsymbol{x}'||\sum_{n=0}^{\infty}\sum_{j=1}^{N_n^d}\lambda_n\phi_{n,j}\left(\frac{\boldsymbol{x}}{||\boldsymbol{x}||}\right)\phi_{n,j}\left(\frac{\boldsymbol{x}'}{||\boldsymbol{x}'||}\right), \tag{3.3}$$

and that the inner product between any two functions g, $h \in \mathcal{H}$ is given by:

$$\langle g, h\rangle_{\mathcal{H}} = \sum_{n,j}\frac{g_{n,j}h_{n,j}}{\lambda_n} \tag{3.4}$$

where $g_{n,j}$ and $h_{n,j}$ are the Fourier coefficients of g and h, i.e. $g(\boldsymbol{x}) = \sum_{n,j} g_{n,j}||\boldsymbol{x}||\phi_{n,j}(\boldsymbol{x})$.

3.2 Spherical Harmonics

Spherical harmonics are a special set of functions defined on the hypersphere and play a central role in harmonic analysis and approximation theory [Wendland, 2005]. They originate from solving Laplace's equation, and form a complete set of orthogonal functions. Any sufficiently regular function defined on the sphere can be written as a sum of these spherical harmonics, similar to the Fourier series with sines and cosines. Spherical harmonics are defined in arbitrary dimensions [Efthimiou and Frye, 2014; Dai and Xu, 2013], but lack explicit formulations and practical implementations in dimensions larger than three.

In this section, we propose a novel algorithm to construct spherical harmonics in d dimensions. The algorithm is based on the existence of a fundamental system of points on the hypersphere, which we select in a greedy fashion through optimisation. This result in spherical harmonics that are a linear combination of zonal functions and form an orthnormal basis on $\mathbb{S}^{d-1}$. The algorithm lends itself well for implementation in Python and TensorFlow, which we provide at: https://github.com/vdutor/SphericalHarmonics. The code is accompagnied by a series of tests that show that the properties of spherical harmonics, as detailed below, hold. Before outlining the algorithm, we briefly define and cover the important properties of spherical harmonics in $\mathbb{R}^d$. We refer the interested reader to Dai and Xu [2013] and Efthimiou and Frye [2014] for a comprehensive overview.

We adopt the usual L_2 inner product for functions $f : \mathbb{S}^{d-1} \to \mathbb{R}$ and $g : \mathbb{S}^{d-1} \to \mathbb{R}$ restricted to the sphere

$$\langle f, g\rangle_{L_2(\mathbb{S}^{d-1})} = \frac{1}{\Omega_{d-1}}\int_{\mathbb{S}^{d-1}} f(x)\,g(x)\,\mathrm{d}\omega, \tag{3.5}$$

[1] See **??** for a primer on Gegenbauer polynomials and spherical harmonics.

where $\mathrm{d}\omega(x)$ is the surface area measure such that Ω_{d-1} denotes the surface area of $\mathbb{S}^{d-1}$

$$\Omega_{d-1} = \int_{\mathbb{S}^{d-1}} \mathrm{d}\omega(x) = \frac{2\pi^{d/2}}{\Gamma(d/2)}. \tag{3.6}$$

Throughout this section we use the following notation and definitions. For $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$ and $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}^d$, a monomial x^α is a product $x^\alpha = x_1^{\alpha_1} \ldots x_d^{\alpha_d}$, which has degree $|\alpha| = \alpha_1 + \ldots \alpha_d$. A real homogeneous polynomial $P(x)$ of degree n is a linear combination of monomials of degree n with real coefficients, that is $P(x) = \sum_{|\alpha|=n} c_\alpha x^\alpha$, with $c_\alpha \in \mathbb{R}$. We denote $\mathcal{P}_n^d$ as the space of real homogeneous polynomials of degree n, and can show that, counting the cardinality of the set $\{\alpha \in \mathbb{N}^d : |\alpha| = n\}$, that $\dim(\mathcal{P}_n^d) = \binom{n+d-1}{n}$. A function $f : \mathbb{R}^d \to \mathbb{R}$ is said to be *harmonic* if $\Delta f = 0$, where $\Delta = \partial_{x_1}^2 + \ldots + \partial_{x_d}^2$ and ∂_{x_i} the partial derivate w.r.t. the i-th variable.

Definition 1. *The spherical harmonics of degree n of d variables, denoted by $\mathcal{H}_n^d$, is the linear space of harmonic and homogeneous in degree n polynomials on $\mathbb{S}^{d-1}$, that is*

$$\mathcal{H}_n^d = \{p \in \mathcal{P}_n^d : \Delta p = 0 \text{ and } p : \mathbb{S}^{d-1} \to \mathbb{R}\}. \tag{3.7}$$

The dimensionality of $\mathcal{H}_n^d$ is given by

$$dim(\mathcal{H}_n^d) = \frac{2n+d-2}{n}\binom{n+d-3}{d-1} := N_n^d. \tag{3.8}$$

The space $\mathcal{H}_n^d$ has an orthonormal basis consisting of N_n^d functions, denoted by $\{\phi_{n,j}\}_{j=1}^{N_n^d}$. The basis satisfy the following properties

$$\mathcal{H}_n^d = \mathrm{span}\Big(\phi_{n,1}, \ldots, \phi_{n,N_n^d}\Big), \quad \text{and} \quad \langle \phi_{n,j}, \phi_{n',j'} \rangle_{L_2(\mathbb{S}^{d-1})} = \delta_{nn'}\delta_{jj'}. \tag{3.9}$$

From the completeness and orthonormality of the spherical harmonic basis $\{\phi_{n,j}\}_{n=0,j=1}^{\infty,N_n^d}$, it can be shown that they also form a basis of square-integrable functions [Efthimiou and Frye, 2014]. This means that we can decompose a function $f : \mathbb{S}^{d-1} \to \mathbb{R}$ as

$$f = \sum_{n=0}^{\infty} \sum_{j=1}^{N_n^d} \widehat{f}_{n,j}\phi_{n,j}, \quad \text{with} \quad \widehat{f}_{n,j} = \langle f, \phi_{n,j} \rangle_{L_2(\mathbb{S}^{d-1})}, \tag{3.10}$$

which can be seen as the spherical analogue of the Fourier decomposition of periodic functions onto a basis of sines and cosines.

Subsequently, we will coin the set $\{\phi_{n,j}\}$ as the spherical harmonics. They are indexed by n and j, where $n = 0, 1, 2, \ldots$ denotes the degree (or level) and $j = 1, \cdots, N_n^d$ denotes the orientation of the spherical harmonic. We are interested in finding $\{\phi_{n,j}\}$ in arbitrary dimension. For $d = 2$, is solving Laplace's equation ($\Delta p = 0$) directly relatively straightforward. Doing

so reveals that $N_0^2 = 1$ with $\phi_{0,1} = 1$ and $N_n^2 = 2$ for all $n > 0$ with $\phi_{n,1}(\theta) = \sqrt{2}\cos(n\theta)$ and $\phi_{n,2}(\theta) = \sqrt{2}\sin(n\theta)$. This shows that on the unit circle $\mathbb{S}^1$, the spherical harmonics correspond to the Fourier basis. For $d = 3$, we can also directly solve Laplace's diffential equation to find $N_n^d = 2n + 1$ and a closed form solution for $\{\phi_{n,j}\}$. However, for $d > 3$, explicit formulations for the spherical harmonics become very rare. To the best of our knowledge, the only explicit formulation we could find is in Dai and Xu [2013, Theorem 5.1], which consists of a product over polynomials. This makes the implementation cumbersome and numerically unstable, and only practically useful up to 10 dimensions [Dutordoir et al., 2020a]. However, making use of the following two theorems, in **??** we can derive another formulation for the basis of spherical harmonics as a sum of polynomials, rather than a product. The connection between spherical harmonics and orthogonal polynomials becomes clear in the next theorem.

Theorem 1 (Addition)**.** *Let $\{\phi_{n,j}\}_{j=1}^{N_n^d}$ be an orthonormal basis for the spherical harmonics of degree n and $x, x' \in \mathbb{S}^{d-1}$. Then the Gegenbauer polynomial $C_n^{(\alpha)} : [-1, 1] \to \mathbb{R}$ of degree n can be written as*

$$\sum_{j=1}^{N_n^d} \phi_{n,j}(x)\phi_{n,j}(x') = \frac{n+\alpha}{\alpha} C_n^{(\alpha)}(x^\top x') \quad \textit{with} \quad \alpha = \frac{d-2}{2}. \tag{3.11}$$

As a result of the relation between the Gegenbauer polynomial and the spherical harmonics, are the Gegenbauer polynomial sometimes referred to as ultraspherical polynomials. For $d = 2$, Theorem 1 recovers the addition formula of the cosine function, as indeed $\cos(\theta)\cos(\theta') + \sin(\theta)\sin(\theta') = \cos(\theta - \theta')$ and $C_n^{(0)}(t) = \cos(n \arccos(t))$. The Gegenbauer polynomials with $\alpha = 0$ are better known as the Chebyshev polynomials. Another connection between spherical harmonics and Gegenbauer polynomials is given by the Funk-Hecke theorem and applies to zonal functions. A zonal function on $\mathbb{S}^{d-1}$ is a function that is rotationally invariant w.r.t. to a point on the sphere, $\eta \in \mathbb{S}^{d-1}$. This means that the function only depends on the inner product $\eta^\top x$, or equivalently, on the geodestic distance between η and x.

Theorem 2 (Funk-Hecke)**.** *Let f be an integrable function such that $\int_{-1}^{1} \|f(t)\|(1-t^2)^{(d-3)/2}\mathrm{d}t$ is finite and $d \geq 2$. Then for every $\phi_{n,j}$ and $\eta \in \mathbb{S}^{d-1}$*

$$\frac{1}{\Omega_{d-1}} \int_{\mathbb{S}^{d-1}} f(\eta^\top x)\, \phi_{n,j}(x)\, \mathrm{d}\omega(x) = \lambda_n\, \phi_{n,j}(\eta), \tag{3.12}$$

where λ_n is a constant defined by

$$\lambda_n = \frac{\omega_d}{C_n^{(\alpha)}(1)} \int_{-1}^{1} f(t)\, C_n^{(\alpha)}(t)\, (1-t^2)^{\frac{d-3}{2}}\mathrm{d}t, \tag{3.13}$$

with $\alpha = \frac{d-2}{2}$ and $\omega_d = \frac{\Omega_{d-2}}{\Omega_{d-1}}$.

3.2.1 Zonal Spherical Harmonics

From the Funk-Hecke and the Addition theorem, it is clear that there is a strong connection between spherical harmonics and Gegenbauer polynomials. The next theorem develops this connection further as it states that a basis for spherical harmonics can be written as zonal Gegenbauer polynomials.

Theorem 3. *If* $\{\eta_1, \dots, \eta_{N_n^d}\} \in \mathbb{S}^{d-1}$ *is a fundamental system of points on the sphere, then* $\{C_n^{(\alpha)}(\eta_i \cdot)\}_{i=1}^{N_n^d}$ *is a basis for* $\mathcal{H}_n^d$*. A collection of points* $\{\eta_1, \dots, \eta_M\} \in \mathbb{S}^{d-1}$ *is called a fundamental system of degree* n *consisting of* M *points on the sphere if*

$$det \begin{bmatrix} C_n^{(\alpha)}(1) & \dots & C_n^{(\alpha)}(\eta_1^\top \eta_M) \\ \vdots & & \vdots \\ C_n^{(\alpha)}(\eta_M^\top \eta_1) & \dots & C_n^{(\alpha)}(1) \end{bmatrix} > 0. \tag{3.14}$$

Finding a basis for $\mathcal{H}_n^d$ is thus equivalent to finding a set of N_n^d points that satisfy eq. (3.14). Crucially, Dai and Xu [2013, Lemma 3] show that there always exists a fundamental system of degree n and N_n^d points.

Following the theoreom, if we wish to construct $\{\phi_{n,j}\}_{n,j}$, an *orthnormal* basis for the spherical harmonics, we firstly need a fundamental system of points. Secondly, while $\{C_n^{(\alpha)}(\eta_i \cdot)\}_{i=1}^{N_n^d}$ forms a basis for $\mathcal{H}_n^d$, the basis is not orthonormal. We will thus have to apply a Gram-Schmidt process for orthonormalising the basis. We detail both steps in the next paragraphs.

Construction of a fundamental system of points We propose to build a fundamental system of points in a greedy fashion by iteratively adding a point on the sphere that maximises the determinant as given in eq. (3.14). Therefore, let $\boldsymbol{\eta} = \{\eta_1, \dots, \eta_M\}$ contain the M points that are already in the fundamental system and define the following block-matrix of size $(M+1) \times (M+1)$ as

$$\mathbf{M}(\boldsymbol{\eta}, \eta_*) = \left[\begin{array}{c|c} C_n^{\alpha}(\boldsymbol{\eta}\boldsymbol{\eta}^\top) \in \mathbb{R}^{M \times M} & C_n^{(\alpha)}(\boldsymbol{\eta}\eta_*^\top) \in \mathbb{R}^{M \times 1} \\ \hline C_n^{(\alpha)}(\boldsymbol{\eta}\eta_*^\top)^\top \in \mathbb{R}^{1 \times M} & C_n^{(\alpha)}(1) \in \mathbb{R} \end{array}\right], \tag{3.15}$$

where $C_n^{(\alpha)}(\boldsymbol{\eta}\boldsymbol{\eta}^\top)$ corresponds to elementwise evaluating the Gegenbauer polynomial $C_n^{(\alpha)} : [-1, 1] \to \mathbb{R}$ for each element of $\boldsymbol{\eta}\boldsymbol{\eta}^\top \in \mathbb{R}^{M \times M}$. A new point η is added to the fundamental system if it maximises the determinant

$$\eta = \underset{\eta_* \in \mathbb{S}^{d-1}}{\operatorname{argmax}} \ \det(\mathbf{M}(\boldsymbol{\eta}, \eta_*)), \tag{3.16}$$

in order to satisfy the condition in eq. (3.14). Computing the determinant can be done efficiently using Schur' complement. Furthermore, as $\boldsymbol{\eta}$ and $C_n^{(\alpha)}(1.0)$ are constants the optimisation

problem boils down to

$$\eta = \underset{\eta_* \in \mathbb{R}^d}{\operatorname{argmin}} \; C_n^{(\alpha)}\left(\frac{\eta_*}{||\eta_*||}\boldsymbol{\eta}^\top\right)\left[C_n^{(\alpha)}(\boldsymbol{\eta}\boldsymbol{\eta}^\top)\right]^{-1} C_n^{(\alpha)}\left(\boldsymbol{\eta}\frac{\eta_*^\top}{||\eta_*||}\right). \tag{3.17}$$

The complete algorithm is given in algorithm 1.

Algorithm 1: Construction of fundamental system

Input: Degree n and dimension d

Result: Fundamental system $\boldsymbol{\eta} = \{\eta_0, \dots \eta_{N_n^d}\}$

$\eta_1 = (0, 0, \dots, 1)$ `// d-dimensional vector pointing north`

$\boldsymbol{\eta} = \{\eta_1\}$, $\alpha = \frac{d-2}{2}$, $i = 2$

while $i \leq N_n^d$ **do**

  $\eta = \text{argmax}_{\eta_* \in \mathbb{R}^d} \; \det(\mathbf{M}(\boldsymbol{\eta}, \frac{\eta_*}{||\eta_*||}))$ `// Using a local optimisation method (e.g., BFGS) and eq. (3.17)`

  Add η to $\boldsymbol{\eta}$

  i = i + 1

end

Orthonormalisation Proof $\langle C_n^{(\alpha)}(\eta_i^\top \cdot), C_n^{(\alpha)}(\eta_j^\top \cdot)\rangle_{L_2(\mathbb{S}^{d-1})} = C_n^{(\alpha)}(\eta_i^\top \eta_j)$ as a result of the Funk-Hecke theorem.

Theorem 4. *Let $\boldsymbol{\eta} = \{\eta_1, \dots, \eta_{N_n^d}\}$ be a fundamental system of degree n consisting of N_n^d points, and $\mathbf{L}$ the inverse cholesky factor of $C_n^{(\alpha)}(\boldsymbol{\eta}\boldsymbol{\eta}^\top)$. Then for $j = 1, \dots, N_n^d$ and*

$$\phi_{n,j}(x) = \sum_{i=1}^{N_n^d} \mathbf{L}_{j,i}\, C_n^{(\alpha)}(\eta_i^\top x) \tag{3.18}$$

is $\{\phi_{n,j}\}$ an orthnormal basis for the spherical harmonics $\mathcal{H}_n^d$.

Chapter 4

Deep Neural Networks as Point Estimates for Deep Gaussian Processes

MacKay [1992a; 1992b] noted very early that the Bayesian treatment of neural networks had large potential. To start, it can help to quantify estimates of the error bars on the network outputs, but it can also provide an objective that can be used for the comparison of alternative network architectures. The reality, however, was that Bayesian inference in neural networks was –and still is– challenging, and in practice one has to resort to either crude approximations (e.g., Laplace approximation [MacKay, 1998]) or lengthy computations (e.g., Markov Chain Monte Carlo [Neal, 1992]).

Building on the foundational work of MacKay, and driven by the amazing successes of large deterministic deep neural networks (DNNs), the literature has seen an upspring in the development of more scalable methods to perform approximate Bayesian inference in DNNs [Blundell et al., 2015; Kingma et al., 2015; Gal and Ghahramani, 2016]. However, it remains challenging to encode prior assumptions on functions through distributions on weights and the large number of parameters to be estimated makes it computationally prohibitive. Furthermore, the strong approximations used both during modelling and inference make it unclear to what extent these models approximate the true posterior distribution [Hron et al., 2018; Foong et al., 2020]. They also do not deliver on an important promise of Bayesian methods: an approximate marginal likelihood objective that can be used for automatic model selection and hyperparameter learning. A different approach may thus be necessary to unlock the Bayesian benefits in deep learning.

Neal [1995] showed that for infinitely wide single-layer BNNs the distribution over the non-linear functions are given by Gaussian processes. Williams [1998] and Cho and Saul [2009] extended this theory and derived the kernel corresponding to an infinite-width BNN

with Sigmoidal and ReLU activation function, respectively. The beauty of this connection is that performing Bayesian inference in the corresponding GP model can be done exactly and analytically – all in a single elegant framework [Rasmussen and Williams, 2006]. Since, various approximations to the exact GP framework have been developed to allow for non-Gaussian likelihoods [Kuss and Rasmussen, 2005; Hensman et al., 2013], large datasets [Hensman et al., 2015; Wang et al., 2019], and even neural network like structures such as convolutions [van der Wilk et al., 2017]. Crucially, the approximations to the marginal likelihood still enable the main Bayesian benefits: model uncertainty and learning model hyperparameters (e.g., [van der Wilk et al., 2018; Dutordoir et al., 2020b]).

More recently, Matthews et al. [2018] discovered the equivalence between *deep* (i.e. multi-layer) BNNs and GPs. This has led to the development of deep (fully connected and convolutional) neural network kernels for GPs (NN-GPs). Interestingly, the performance of the non-Bayesian neural nets significantly outperforms the corresponding GPs [Garriga-Alonso et al., 2018; Novak et al., 2019]. The discrepancy hints at the fact that these single-layer GPs, even when configured with very expressive DNN equivalent kernels, are missing a crucial component: the ability to learn feature representations from the data.

Deep Gaussian processes [Damianou and Lawrence, 2013, DGPs] are an interesting avenue to tackle these challenges. They are built by hierarchically stacking GPs on top of each other, which enables the learning of more powerful representations through compositional features. Moreover, their Bayesian approximations in function-space seem to be of higher quality than those of weight-space BNNs, e.g. as supported by the successful use of marginal likelihood estimates for hyperparameter learning [Damianou and Lawrence, 2013].

While promising, DGPs have struggled for relevance in applications due to the challenges and cost associated with Bayesian inference. Training DGPs is computationally expensive and requires very careful setting of the parameters. Furthermore, the hierarchical prior induced by naively stacking stationary kernels gives rise to pathological, "collapsed" samples Duvenaud et al. [2014]. Considerable progress for scalable inference in DGPs was made by Hensman and Lawrence [2014] and Salimbeni and Deisenroth [2017], who derived stochastic variational lower bounds. The formulation of these bounds closely resembles the computations of training a feed-forward neural network with regularisation terms, and has greatly inspired this work.

Building on Salimbeni and Deisenroth [2017] and to further improve the scalability of DGPs, Cutajar et al. [2017] used a Random Fourier Feature [Rahimi and Recht, 2008, RFF] approximation of the kernel. While successful, this approach introduces an approximation in both the prior and the posterior of the model. More recently, Rudner et al. [2020] proposed Fourier features of the Matérn RKHS, following Hensman et al. [2018, Variational Fourier Features (VFF)], to build inter-domain DGPs. Like for single layer VFF models, this approach can lead to faster training and improved performance, but is only computationally feasible for data of dimension one or two. In parallel with our work, Sun et al. [2021] explored the idea of using single-layer neural networks to parameterise inducing points in shallow GPs. Similar

to this paper, their method makes use of the spherical harmonic decomposition of a kernel. However, their works differs in the fact that they focus on shallow GPs, on bounded inducing functions (e.g., erf), and directly use the Nyström approximation to approximate the model's uncertainty estimates rather than the ELBO to learn the variational parameters.

The analysis of (Bayesian) neural networks has led to several probabilistic models: NN-GPs, GPs and DGPs. In this work, however, rather than focusing on the *prior* induced by these equivalent models, the emphasis lies on the connection between the DGP *posterior* and the DNN. This has received much less attention in the literature, though we argue it is a more interesting regime to study. The connection between GP piors and neural nets is established only in the infinite limit of the number of hidden units. The sparse posterior DGP, on the contrary, is built out of a finite set of basis functions and can thus immediately be connected to finite-width neural networks — in this paper we connect both models in their modus operandi.

We formulate a DGP configuration for which the approximate posterior mean has the same mathematical structure as a deep neural network with fully connected layers and non-linear activation functions. We can use this unification to train the DGP like a neural network which allow us to leverage all the great research in this area for DGP inference. Furthermore, this connection between DGPs posteriors and DNNs highlights the great potential of DGPs as a model for learning powerful representations from data while being fully Bayesian.

Chapter 5

Future Research

5.1 Geometric Gaussian Decision Systems

Problem setting

1. Black Box Functions $f : \mathcal{X} \to \mathcal{Y}$
2. We want to estimate a computable property $\mathcal{O}_{\mathcal{A}}(f)$
3. $\mathcal{A}$ is an algorithm $\mathcal{O}_{\mathcal{A}}(f) = \mathcal{A}(f)$
4. Evaluating f is *very* expensive (we can only evaluate it a limited amount of times)

Examples

1. Bayesian Optimisation: $\mathcal{A}(f) = \operatorname{argmax}_{x \in \mathcal{X}} f(x)$, which implies $\mathcal{O}_{\mathcal{A}}(f) = x^*$.
2. Sensor Placement (Active Learning): $\mathcal{O}_{\mathcal{A}}(f) = \operatorname{argmax}_{X \subset \mathcal{X}, |X|=T} \mathrm{MI}(f, f(X))$.
3. Level sets: $\mathcal{O}_{\mathcal{A}}(f) = \{X \subset \mathcal{X} : f(x) > C, \forall x \in X\}$.
4. Shortest path: $\mathcal{O}_{\mathcal{A}}(f) =$ shortest path between two nodes in a graph.

Model We model f by a Gaussian process

$$f \sim \mathcal{GP} \tag{5.1}$$

1. Low dimensions
2. Prior knowledge
3. Limited and very expensive data

Basically settings where DNNs are never going to be competitive with GPs - low-dim, very data-efficient, high-cost - not even if someone figures out how to do DNN uncertainty right, due to GP regret guarantees (under reasonable assumptions) matching the best possible regret achievable by any model/decision system.

Collaborators

1. Alex Terenin (Imperial College London)
2. Willie Neiswanger (Stanford University)

5.2 Projects in Progress

1. "Pay Attention to Deep Gaussian Processes"
   Transformer Layer Gaussian Processes using an explicit feature representation of the attention operation.
   $$\exp(\boldsymbol{x}^\top \boldsymbol{y}) = \Phi^\top(\boldsymbol{x})\Phi(\boldsymbol{y})$$
2. A Unifying Theory for Interdomain Gaussian Processes.
3. VISH-PI: Probabilistic Integration with Variational Inducing Spherical Harmonics.

References

Alberto Bietti and Francis Bach (2020). "Deep Equals Shallow for ReLU Networks in Kernel Regimes". In: *arXiv preprint arXiv:2009.14397*.

David M Blei, Alp Kucukelbir, and Jon D McAuliffe (2017). "Variational Inference: A Review for Statisticians". In: *Journal of the American Statistical Association*.

Charles Blundell, Julien Cornebise, Koray Kavukcuoglu, and Daan Wierstra (2015). "Weight Uncertainty in Neural Network". In: *Proceedings of The 32nd International Conference on Machine Learning (ICML)*.

David R Burt, Carl Edward Rasmussen, and Mark van der Wilk (2020). "Variational orthogonal features". In: *arXiv preprint arXiv:2006.13170*.

David R. Burt, Carl E. Rasmussen, and Mark van der Wilk (2019). "Rates of Convergence for Sparse Variational Gaussian Process Regression". In: *Proceedings of the 36th International Conference on Machine Learning (ICML)*.

Youngmin Cho and Lawrence K. Saul (2009). "Kernel Methods for Deep Learning". In: *Advances in Neural Information Processing Systems 22 (NIPS)*.

Kurt Cutajar, Edwin V. Bonilla, Pietro Michiardi, and Maurizio Filippone (2017). "Random feature expansions for deep Gaussian processes". In: *Proceedings of the 34th International Conference on Machine Learning (ICML)*.

Feng Dai and Yuan Xu (2013). *Approximation Theory and Harmonic Analysis on Spheres and Balls*. Springer.

Andreas Damianou and Neil D. Lawrence (2013). "Deep Gaussian Processes". In: *Proceedings of the 16th International Conference on Artificial Intelligence and Statistics (AISTATS)*.

Vincent Dutordoir, Nicolas Durrande, and James Hensman (2020a). "Sparse Gaussian Processes with Spherical Harmonic Features". In: *Proceedings of the 37th International Conference on Machine Learning (ICML)*.

Vincent Dutordoir, James Hensman, Mark van der Wilk, Carl Henrik Ek, Zoubin Ghahramani, and Nicolas Durrande (2021a). "Deep Neural Networks as Point Estimate for Deep Gaussian Processes". In: *submission to NeurIPS*.

Vincent Dutordoir, Hugh Salimbeni, Eric Hambro, John McLeod, Felix Leibfried, Artem Artemev, Mark van der Wilk, James Hensman, Marc P Deisenroth, and ST John (2021b). "GPflux: A Library for Deep Gaussian Processes". In: *arXiv preprint arXiv:2003.01115*.

Vincent Dutordoir, Mark van der Wilk, Artem Artemev, and James Hensman (2020b). "Bayesian Image Classification with Deep Convolutional Gaussian Processes". In: *Proceedings of the 23th International Conference on Artificial Intelligence and Statistics (AISTATS)*.

David Duvenaud, Oren Rippel, Ryan Adams, and Zoubin Ghahramani (2014). "Avoiding pathologies in very deep networks". In: *Proceedings of the 17th International Conference on Artificial Intelligence and Statistics (AISTATS)*.

Costas Efthimiou and Christopher Frye (2014). *Spherical Harmonics in p Dimensions*. World Scientific Publishing.

Andrew Y. K. Foong, David R. Burt, Yingzhen Li, and Richard E. Turner (2020). "On the Expressiveness of Approximate Inference in Bayesian Neural Networks". In: *Advances in Neural Information Processing Systems 33 (NeurIPS)*.

Yarin Gal and Zoubin Ghahramani (2016). "Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning Zoubin Ghahramani". In: *Proceedings of The 33rd International Conference on Machine Learning (ICML)*.

Adrià Garriga-Alonso, Carl E. Rasmussen, and Laurence Aitchison (2018). "Deep Convolutional Networks as shallow Gaussian Processes". In: *Proceedings of the 7th International Conference on Learning Representations (ICLR)*.

Xavier Glorot and Yoshua Bengio (2010). "Understanding the difficulty of training deep feedforward neural networks". In: *Proceedings of the 13th International Conference on Artificial Intelligence and Statistics (AISTATS)*.

Xavier Glorot, Antoine Bordes, and Yoshua Bengio (2011). "Deep Sparse Rectifier Neural Networks". In: *Proceedings of the 14th International Conference on Artificial Intelligence and Statistics (AISTATS)*.

James Hensman, Nicolas Durrande, and Arno Solin (2018). "Variational Fourier Features for Gaussian Processes". In: *Journal of Machine Learning Research*.

James Hensman, Nicolo Fusi, and Neil D. Lawrence (2013). "Gaussian Processes for Big Data". In: *Proceedings of the 29th Conference on Uncertainty in Artificial Intelligence (UAI)*.

James Hensman and Neil D. Lawrence (2014). "Nested Variational Compression in Deep Gaussian Processes". In: *arXiv preprint arXiv:1412.1370*.

James Hensman, Alexander G. de G. Matthews, and Zoubin Ghahramani (2015). "Scalable Variational Gaussian Process Classification". In: *Proceedings of the 18th International Conference on Artificial Intelligence and Statistics (AISTATS)*.

Jiri Hron, Alexander G. de G. Matthews, and Zoubin Ghahramani (2018). "Variational Bayesian dropout: pitfalls and fixes". In: *Proceedings of the 35th International Conference on Machine Learning (ICML)*.

Sergey Ioffe and Christian Szegedy (2015). "Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift". In: *Proceedings of The 32nd International Conference on Machine Learning (ICML)*.

Durk Kingma, Tim Salimans, and Max Welling (2015). "Variational Dropout and the Local Reparameterization Trick". In: *Advances in Neural Information Processing Systems 28 (NIPS)*.

Alex Krizhevsky, Ilya Sutskever, and Geoffrey E. Hinton (2012). "ImageNet Classification with Deep Convolutional Neural Networks". In: *Advances in Neural Information Processing Systems 25 (NIPS)*.

Malte Kuss and Carl E. Rasmussen (2005). "Assessing Approximate Inference for Binary Gaussian Process Classification". In: *Journal of Machine Learning Research*.

Miguel Lázaro-Gredilla and Aníbal Figueiras-Vidal (2009). "Inter-domain Gaussian Processes for Sparse Inference using Inducing Features". In: *Advances in Neural Information Processing Systems 22 (NIPS)*.

Felix Leibfried, Vincent Dutordoir, S. T. John, and Nicolas Durrande (2020). "A Tutorial on Sparse Gaussian Processes and Variational Inference". In: *arXiv preprint arXiv:2012.13962*.

David J. C. MacKay (1992a). "A Practical Bayesian Framework for Backpropagation Network". In: *Neural Computation*.

David J. C. MacKay (1992b). "Bayesian Model Comparison and Backprop Nets". In: *Advances in Neural Information Processing Systems 4 (NIPS 1991)*.

David J. C. MacKay (1998). "Choice of Basis for Laplace Approximation". In: *Machine Learning*.

David J. C. MacKay (2003). *Information Theory, Inference and Learning Algorithms*. Cambridge University Press.

Alexander G. de G. Matthews, James Hensman, Turner E. Richard, and Zoubin Ghahramani (2016). "On Sparse Variational Methods and the Kullback-Leibler Divergence between Stochastic Processes". In: *Proceedings of the 19th International Conference on Artificial Intelligence and Statistics (AISTATS)*.

Alexander G. de G. Matthews, Mark Rowland, Jiri Hron, Richard E. Turner, and Zoubin Ghahramani (2018). "Gaussian process behaviour in wide deep neural networks". In: *Proceedings of the 6th International Conference on Learning Representations (ICLR)*.

Radford M. Neal (1992). "Bayesian Mixture Modeling". In: *Maximum Entropy and Bayesian Methods*.

Radford M. Neal (1995). *Bayesian Learning for Neural Networks*. Springer.

Roman Novak, Lechao Xiao, Jaehoon Lee, Yasaman Bahri, Greg Yang, Jiri Hron, Daniel A. Abolafia, Jeffrey Pennington, and Jascha Sohl-Dickstein (2019). "Bayesian deep convolutional networks with many channels are Gaussian processes". In: *Proceedings of the 7th International Conference on Learning Representations (ICLR)*.

Joaquin Quiñonero-Candela and Carl E. Rasmussen (2005). "A Unifying View of Sparse Approximate Gaussian Process Regression". In: *Journal of Machine Learning Research*.

Ali Rahimi and Benjamin Recht (2008). "Random Features for Large-Scale Kernel Machines". In: *Advances in Neural Information Processing Systems 20 (NIPS 2007)*.

Carl E. Rasmussen and Christopher K. I. Williams (2006). *Gaussian Processes for Machine Learning*. MIT Press.

Tim G. J. Rudner, Dino Sejdinovic, and Yarin Gal (2020). "Inter-domain Deep Gaussian Processes". In: *Proceedings of the 37th International Conference on Machine Learning (ICML)*.

Hugh Salimbeni and Marc P. Deisenroth (2017). "Doubly Stochastic Variational Inference for Deep Gaussian Processes". In: *Advances in Neural Information Processing Systems 30 (NIPS)*.

Julian Schrittwieser et al. (2020). "Mastering Atari, Go, Chess and Shogi by Planning with a Learned Model". In: *Nature*.

Edward Snelson and Zoubin Ghahramani (2005). "Sparse Gaussian Processes using Pseudo-inputs". In: *Advances in Neural Information Processing Systems 4 (NIPS 2005)*.

Shengyang Sun, Jiaxin Shi, and Roger B. Grosse (2021). "Neural Networks as Inter-Domain Inducing Points". In: *3rd Symposium on Advances in Approximate Bayesian Inference*.

Michalis K. Titsias (2009). "Variational Learning of Inducing Variables in Sparse Gaussian Processes". In: *Proceedings of the 12th International Conference on Artificial Intelligence and Statistics (AISTATS)*.

Mark van der Wilk, Matthias Bauer, S. T. John, and James Hensman (2018). "Learning Invariances using the Marginal Likelihood". In: *Advances in Neural Information Processing Systems 31 (NeurIPS)*.

Mark van der Wilk, Vincent Dutordoir, S. T. John, Artem Artemev, Vincent Adam, and James Hensman (2020). "A Framework for Interdomain and Multioutput Gaussian Processes". In: *arXiv preprint arXiv:2003.01115*.

Mark van der Wilk, Carl E. Rasmussen, and James Hensman (2017). "Convolutional Gaussian Processes". In: *Advances in Neural Information Processing Systems 30 (NIPS)*.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin (2017). "Attention is All you Need". In: *Advances in Neural Information Processing Systems 30 (NIPS)*.

Ke Wang, Geoff Pleiss, Jacob Gardner, Stephen Tyree, Kilian Q. Weinberger, and Andrew Gordon Wilson (2019). "Exact Gaussian Processes on a Million Data Points". In: *Advances in Neural Information Processing Systems 32 (NeurIPS)*.

Holger Wendland (2005). *Scattered Data Approximation*. Cambridge University Press.

Christopher K. I. Williams (1998). "Computing with Infinite Networks". In: *Advances in Neural Information Processing Systems 11 (NIPS 1997)*.