Gaussian Process Surrogate Models for Neural Networks

Abstract

Not being able to understand and predict the behavior of deep learning systems makes it hard to decide what architecture and algorithm to use for a given problem. In science and engineering, *modeling* is a methodology used to understand complex systems whose internal processes are opaque. Modeling replaces a complex system with a simpler surrogate that is more interpretable. Drawing inspiration from this, we construct a class of surrogate models for neural networks using Gaussian processes. Rather than deriving kernels for infinite neural networks, we learn kernels empirically from the naturalistic behavior of finite neural networks. We demonstrate our approach captures existing phenomena related to the spectral bias of neural networks, and then show that our surrogate models can be used to solve practical problems such as identifying which points most influence the behavior of specific neural networks and predicting which architectures and algorithms will generalize well for specific datasets.

1 INTRODUCTION

Deep learning systems are ubiquitous in machine learning but sometimes exhibit unpredictable and undesirable behavior when deployed in real-world applications [Geirhos et al., 2020, D'Amour et al., 2020]. This gap between idealized and real-world performance has driven calls for explainability, transparency, and interpretability of deep learning systems [Lipton, 2016, Doshi-Velez and Kim, 2017, Samek et al., 2017], especially as these systems are more widely applied [Bommasani et al., 2021].

Machine learning is not unique in seeking to understand a complex system whose inputs and outputs are observable but whose internal processes are opaque—this challenge occurs across the empirical sciences and engineering. An explanatory tool that is foundational across these disciplines is that of *modeling*, that is, representing a complex and opaque system with a simpler one that is more amenable to interpretation.[1] Modeling makes precise assumptions about how a system may operate while abstracting away details that are irrelevant for a given level of understanding or a given downstream use case. These properties are valuable for a framework for understanding deep learning as they are in other scientific and engineering disciplines.

As the popularity of deep learning has grown, a number of proposals have been made for modeling these systems. Numerous mathematical models of deep learning have been developed [Roberts et al., 2022], and some surprising phenomena, such as adversarial examples [Szegedy et al., 2014], have been captured with a mathematical analysis [Ilyas et al., 2019]. However, existing mathematical models are unable to capture the properties of machine learning systems as applied in practice [Nakkiran, 2021]. Beyond mathematical models, specific models have aimed to explain the predictions of machine learning systems on a per-example basis [Ribeiro et al., 2016, Koh and Liang, 2017, Zhou et al., 2022, Ilyas et al., 2022], but these approaches are, by construction, only partial explanations of the end-to-end system.

In this paper, we pursue an alternative modeling approach that draws on two domains for inspiration. In engineering design, *surrogate models* [Wang and Shan, 2006] emulate the input-output behavior of a complex physical system, allowing practitioners to simulate effects that are consequential for design or analysis without relying on costly or otherwise prohibitive queries from the system itself. In cognitive science, *cognitive models* [Sun, 2008, McClelland, 2009] describe how unobservable mental processes such as memory or attention produce the range of people's observed be-

[1] Though some architectural components of a deep learning system are commonly referred to as a *model*—as in "neural network model"—we use *modeling* to refer to the methodology of idealizing a complex system as a simpler one.

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haviors. Both domains abstract away internal details, such as real-world constraints on a physical system or neural circuitry in the brain, instead treating the target process or system as a *black box*. At the same time, both surrogate and cognitive models are constructed to replicate the end-to-end behavior of the target system and thus are complete where localized explanations are not.

We explore an analogous approach to investigate deep learning systems by constructing *Gaussian process surrogate models for neural networks*. Gaussian processes (GPs) are a natural choice, with appealing theoretical properties specific to the study of neural networks (NNs); namely, certain limiting cases of NN architectures are realizable as GPs [Neal, 1996, Li and Liang, 2018, Jacot et al., 2018, Allen-Zhu et al., 2019, Du et al., 2019]. However, in contrast to these theoretical approaches, we explore the scientific and practical utility of idealizing NNs with GPs using a *data-driven* approach to estimating the kernel functions of finite NNs. With this approach, we capture a number of known phenomena, including a bias towards low frequencies and pathological behavior at initialization, in a cohesive framework. Finally, we demonstrate the practical benefits of this framework by identifying points that strongly influence NN predictions and predicting the generalization behavior of models in a NN family.

2 BACKGROUND

In **surrogate modeling**, we approximate a complex black-box function with a simpler surrogate model that is more amenable to interpretation. Surrogate models have many applications: In optimization, they are often used to approximate queries from expensive-to-evaluate functions [Snoek et al., 2012, Shahriari et al., 2016]; in other applications, surrogate models have been used to gain insight into large physical systems [Camps-Valls et al., 2015].

Cognitive models have been used by cognitive scientists since the 1950s to gain insight into the human mind [Newell et al., 1958]. Bayesian models of cognition offer a way to describe the inductive biases of learning systems as a prior distribution [Griffiths et al., 2010]. As deep NNs have become more prevalent, researchers have used methodologies from cognitive science to interrogate opaque models [Ritter et al., 2017, Geirhos et al., 2019, Hawkins et al., 2020]. The success of these efforts suggests that other methods from cognitive science—namely, cognitive modeling—may be applicable to machine learning systems.

Gaussian processes [GPs; Rasmussen and Williams, 2006] are probabilistic models that specify a distribution over functions. A GP models any *finite* set of N observations as a multivariate Gaussian distribution on $\mathbb{R}^D$, where the nth point is interpreted as the function value, $f(\mathbf{x}_n)$, at the input point $\mathbf{x}_n$. GPs are fully characterized by a mean function $m(\mathbf{x})$, usually taken to be degenerate as $m(\mathbf{x}) = \mathbf{0}, \forall \mathbf{x}$, and a positive-definite kernel function $k(\mathbf{x},\ \mathbf{x}')$ that gives the covariance between $f(\mathbf{x})$ and $f(\mathbf{x}')$ as a function of $\mathbf{x}$ and $\mathbf{x}'$.

Formally, let $\mathbf{X}$ be a matrix of inputs and $\mathbf{y}$ be a vector of output responses. Due to the marginalization properties of the Gaussian distribution, the posterior predictive distribution of a GP for a new input $\mathbf{x}_*$, conditioned on dataset $\mathcal{D} = \{\mathbf{X}, \mathbf{y}\}$ and assuming centered Gaussian observation noise with variance σ^2, is Gaussian with closed-form expressions for the mean and variance:

$$\mathbb{E}[f(\mathbf{x}_*) \mid \mathcal{D}] = m(\mathbf{x}_*) + {\mathbf{k}_*}^T(\mathbf{K} + \sigma^2\mathbf{I})^{-1}(\mathbf{y} - m(\mathbf{x}_*)) \tag{1}$$

$$\mathbb{V}[f(\mathbf{x}_*) \mid \mathcal{D}] = k(\mathbf{x}_*, \mathbf{x}_*) - {\mathbf{k}_*}^T(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\mathbf{k}_* \tag{2}$$

where $\mathbf{K}$ is the $N \times N$ Gram matrix of pairwise covariances, $k(\mathbf{x}_i, \mathbf{x}_j)$, and $\mathbf{k}_* = [k(\mathbf{x}_1, \mathbf{x}_*), \ldots, k(\mathbf{x}_N, \mathbf{x}_*)]^T$.

The kernel function k specifies the prior on what kind of functions might be represented in observed data, for example, expressing expected smoothness or periodicity. Parametric kernels have hyperparameters θ that affect this prior and thus the posterior predictive. These kernel hyperparameters can be adapted to the properties of a dataset, thus defining a prior over functions that is appropriate for that context. GP kernel hyperparameters are typically learned via gradient-based optimization to maximize the GP marginal likelihood, $p(\mathbf{y} \mid \mathbf{X})$. Again due to properties of the GP, this marginal likelihood has the closed-form expression:

$$\begin{aligned}\log p(\mathbf{y} \mid \mathbf{X}) = &-\frac{1}{2}\mathbf{y}^T\left(\mathbf{K}_\theta + \sigma_n^2 I\right)^{-1}\mathbf{y} \\ &-\frac{1}{2}\log|\mathbf{K}_\theta + \sigma_n^2 I| - \frac{n}{2}\log 2\pi\,.\end{aligned} \tag{3}$$

We write the Gram matrix as $\mathbf{K}_\theta$ to indicate that it depends on kernel hyperparameters via a particular parameterization. In this work, we make use of two kernel parameterizations: the **Matérn kernel** [MK; Matérn, 1960] and the **spectral mixture kernel** [SMK; Wilson and Adams, 2013]. Specifically, following Snoek et al. [2012], we use the automatic relevance determination (ARD) $5/2$ MK, given by:

$$\begin{aligned}k(\mathbf{x}, \mathbf{x}') = \theta_0 &\left(1 + \sqrt{5r^2(\mathbf{x}, \mathbf{x}')} + \tfrac{5}{3}r^2(\mathbf{x}, \mathbf{x}')\right) \\ &\exp\left\{-5\sqrt{5r^2(\mathbf{x}, \mathbf{x}')}\right\}\end{aligned} \tag{4}$$

where $r^2(\mathbf{x}, \mathbf{x}') = \sum_{d=1}^{D}(x_d - x'_d)^2/\theta_d^2$ and each θ_d is a lengthscale parameter capturing smoothness along dimension d. The SMK is derived by modeling the spectral density associated with a kernel as a scale-location mixture of Gaussians [Wilson and Adams, 2013], giving:

$$k(\tau) = \sum_{q=1}^{Q} w_q \cos\left(2\pi^2\tau^T\mu_q\right)\prod_{p=1}^{P}\exp\left\{-2\pi^2\tau_p^2 v_q^{(p)}\right\}. \tag{5}$$

Here, $k(\tau)$ gives the covariance between function values $f(\mathbf{x})$ and $f(\mathbf{x}')$ whose corresponding input values $\mathbf{x}$ and $\mathbf{x}'$ are a distance τ apart. For a Q-component spectral mixture, $w = \{w_i\}_{i=1}^{Q}$ are scalar mixture weights, and $\mu_i, v_i \in \mathbb{R}^P$ are component-wise Gaussian means and variances, respectively. See Section A.4 of the supplement for details on how the hyperparameters of the MK and the SMK control the respective priors on functions.

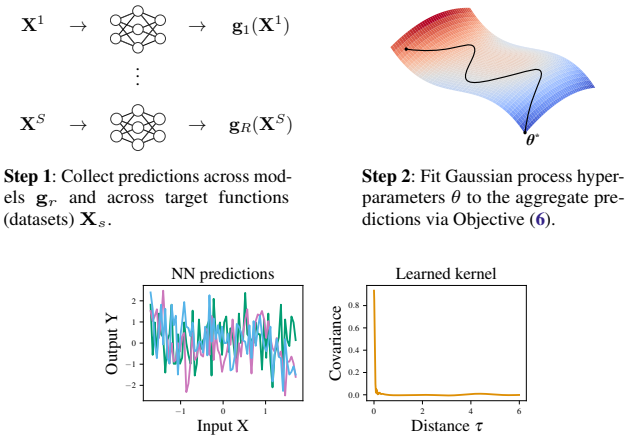
3 LEARNING A GP SURROGATE MODEL FROM NN PREDICTIONS

In this section, we detail the goals and approach of the surrogate modeling framework. In brief, our approach involves collecting neural network predictions across a set of neural network models and across a set of datasets, and estimating GP kernel hyperparameters from these predictions by maximizing the marginal likelihood across model-and-dataset pairs; see Fig. (1) for a schematic.

3.1 FORMAL FRAMEWORK

Our goal is to capture shared properties among a family of neural network models $\mathfrak{F}$ as applied to a family of datasets $\mathfrak{D}$ (with untrained neural networks being the special case where $\mathfrak{D}$ is empty). Here, a model family $\mathfrak{F}$ is a set of neural networks $\{\mathbf{g}_0, \ldots, \mathbf{g}_R\}$ that share in design choices (*e.g.,* architecture, training procedure, random initialization scheme) but differ in quantities that are randomized prior to or during training (*e.g.,* parameter initializations).Similarly, a dataset family $\mathfrak{D}$ is a set of datasets $\{\mathcal{D}_0, \ldots, \mathcal{D}_S\}$ that share some underlying structure as in multi-task and meta-learning settings [Caruana, 1997, Hospedales et al., 2020]. We consider supervised learning, in which each dataset consists of inputs and targets, $\mathcal{D} = (\mathbf{X}, \mathbf{y})$. Importantly, we fit surrogate model parameters θ to a *behavioral dataset* of the model family evaluated on the dataset family, and not the ground truth datasets themselves.

Data. We construct a component of the surrogate model training dataset as follows: We sample a model index r and a dataset index s. The corresponding dataset is split into a training set and an evaluation set, $\mathcal{D}_s = \mathcal{D}_s^{\text{train}} \cup \mathcal{D}_s^{\text{eval}}$. The corresponding model $\mathbf{g}_r$ is fit the training set $\mathcal{D}_s^{\text{train}} = (\mathbf{X}_s^{\text{train}}, \mathbf{y}_s^{\text{train}})$ according to the training procedure specified by the choice of model family $\mathfrak{F}$, producing $\mathbf{g}_r^{\text{fit}}$. We then collect the predictions of the trained model on the evaluation set, $\mathbf{g}_r^{\text{fit}}(\mathbf{X}_s^{\text{eval}})$, to produce the component $(\mathbf{X}_s^{\text{eval}}, \mathbf{g}_r^{\text{fit}}(\mathbf{X}_s^{\text{eval}}))$ consisting of the *ground truth inputs* paired with the *neural network behavioral targets* from the evaluation set. We aggregate the ground truth inputs and the neural network behavioral targets across pairs to produce the *surrogate model training dataset*, $\big((\mathbf{X}_{s_1}^{\text{eval}}, \mathbf{g}_{r_1}^{\text{fit}}(\mathbf{X}_{s_1}^{\text{eval}})), \ldots, (\mathbf{X}_{s_T}^{\text{eval}}, \mathbf{g}_{r_T}^{\text{fit}}(\mathbf{X}_{s_T}^{\text{eval}}))\big)$.



Step 1: Collect predictions across models $\mathbf{g}_r$ and across target functions (datasets) $\mathbf{X}_s$.

Step 2: Fit Gaussian process hyperparameters θ to the aggregate predictions via Objective (6).

Step 3: Analyze the kernel learned from the aggregate predictions. Here, the learned surrogate kernel reveals the quickly varying behavior of particular neural networks.

Figure 1: Outline of the surrogate modeling approach. We learn a Gaussian process surrogate model for a neural network family applied to a task family by learning kernel hyperparameters from aggregated neural network predictions across datasets. We interpret the learned kernel to derive insights into the properties of the neural network family; for example, biases towards particular frequencies (see Section (4.1)), or expected generalization behavior on a new dataset (see Section (4.3)).

Surrogate model. We fit the GP using type-II maximum likelihood. Let $P_\theta(\mathbf{g}^{\text{fit}}(\mathbf{X}^{\text{eval}}) \mid \mathbf{X}^{\text{eval}})$ be the GP marginal likelihood of the dataset component $\big(\mathbf{X}^{\text{eval}}, \mathbf{g}^{\text{fit}}(\mathbf{X}^{\text{eval}})\big)$ under a GP with kernel hyperparameters θ, as given in Eq. (3). We fit the surrogate model jointly across model-and-task pairs in the surrogate model training dataset by maximizing the joint marginal likelihood with respect to θ:

$$\max_{\theta} \prod_{(r,s)} P_\theta(\mathbf{g}_r^{\text{fit}}(\mathbf{X}_s^{\text{eval}}) | \mathbf{X}_s^{\text{eval}}) \,. \tag{6}$$

By optimizing Objective (6), we encourage the kernel hyperparameters θ to capture the implicit prior distribution over functions induced by the models in the family $\mathfrak{F}$ as applied to the datasets in the family $\mathfrak{D}$. Algorithm (1) gives the complete surrogate model training and evaluation process.

Motivating the framework. By estimating a prior over functions for a neural network family directly from neural network behavior, we aim to capture shared properties that determine the model family's behavior on data, *i.e.,* **the model family's *inductive biases***. The inductive biases of neural networks (*e.g.,* invariances and equivariances, Markovian assumptions, compositionality) play an important role in their performance by determining their extrapolation behavior [Mitchell, 1980].

GPs, in particular, offer several advantages as surrogate models of NNs. Firstly, GPs **are flexible models that are also often interpretable** in the sense that the learned hyperparameters can provide insights into properties of the datasets on which they are trained [Wilson and Adams, 2013]. Secondly, the use of GP surrogate models is also motivated by

Algorithm 1: Training and evaluation of a GP surrogate.

hyperparameters : model family $\mathfrak{F}$,
dataset family $\mathfrak{D}$,
model-dataset count T,
GP parameterization θ

`// Step 1 in Fig. (1)`

for $t \in 1 \ldots T$ **do**

  Sample a model, $\mathbf{g}_{r_t} \sim \text{Unif}(\mathfrak{F})$

  Sample a dataset, $\mathcal{D}_{s_t} \sim \text{Unif}(\mathfrak{D})$

  Train the model, $\mathbf{g}^{\text{fit}}_{r_t} \leftarrow \text{train}(\mathbf{g}_{r_t}, \mathcal{D}^{\text{train}}_{s_t})$

  Evaluate $\mathbf{g}^{\text{fit}}_{r_t}(\mathcal{D}^{\text{eval}}_{s_t})$

end

`// Step 2 in Fig. (1)`

Optimize Objective (6) for θ^*

`// Step 3 in Fig. (1)`

Analyze θ^* via P_{θ^*}

the **theoretical connections between GPs and NNs.** Neal [1996] showed that a prior over the parameters of certain single-layer multi-layer perceptrons (MLPs) converges to a GP as the MLP's width approaches infinity, and recent works [Lee et al., 2017, Matthews et al., 2018, Novak et al., 2019, Garriga-Alonso et al., 2019, Yang, 2019] have extended this correspondence to deep MLPs and more modern NN architectures. The connections between GPs and NNs can provide insight because they transform the priors implicit in NNs designs into explicit priors expressed through a GP. However, our strategy differs from this prior theoretical work that derives analytic kernels for limiting cases of NNs—we instead take an empirical approach by learning GP kernels from the predictions of arbitrary classes of finite NNs.

Lastly, GPs have **analytic** marginal likelihoods and leave-one-out predictive distributions, a property that we will exploit in Sections (4.2) and (4.3) to amortize the computation of two quantities useful for practitioners.

3.2 DEMONSTRATION: COMPARING LEARNED GP PRIORS WITH NN PRIORS

We briefly demonstrate the framework of Section (3.1) by verifying that GP surrogates learned from various NN families exhibit meaningful variation in behavior.

NN hyperparameters. We consider ensembles of 50 randomly initialized (about zero with weight variance $\sigma_w^2 = 1.5$ and bias variance $\sigma_b^2 = 0.05$) fully connected NNs with rectified linear unit (ReLU) or sine (sin) activations and 16 or 32 hidden layers of 128 hidden units each.

GP surrogate. For each ensemble, we learn the hyperparameters of a randomly initialized SMK with $Q = 10$ mixture components by optimizing Objective (6) for 350 iterations with batch gradient descent and the adaptive momentum (Adam) optimizer [Kingma and Ba, 2015] with learning rate $\eta = 0.1$. We choose the kernel hyperparameters with highest objective value across three random initializations.

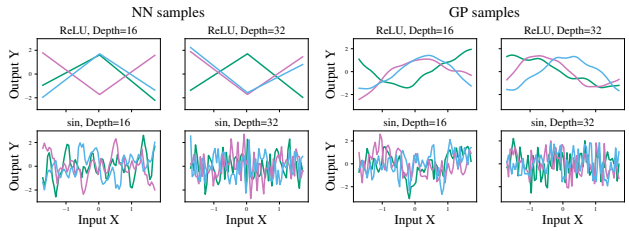


Figure 2: Demonstration: Comparing learned GP priors with NN priors. Samples from GP prior (**right**) with kernel hyperparameters inferred from the predictions of NN families (**left**). GPs are flexible enough to capture properties of each NN family; for example, the samples from the learned GP prior reflect the quickly varying behavior of the 32-layer sinusoidal NNs and the increasing-decreasing behavior of rectifier NNs.

Results. We plot NN predictions and samples from the learned GP priors in Fig. (2). The learned GP captures the periodicity of the sinusoidal neural networks (sinusoidal NNs), and partially captures the increasing-decreasing behavior of rectifier neural networks (rectifier NNs) about a cusp; though, due to the SMK parameterization, it cannot capture the discontinuity at the cusp. The GP also captures differences in depths for the sinusoidal NNs: The GP prior samples for the 32-layer networks are quickly varying, indicating shorter learned lengthscales. Taken together, the results of this demonstration show that GP surrogates can capture certain NN behavior. In Section A.1 of the supplement, we apply the same framework to study pathologies that emerge with increasing depth in randomly initialized NNs.

4 EXPERIMENTS

We provide a series of demonstrations of the value of the approach of Section (3). Each experiment aims to investigate the properties of one or more neural network families, specified by **neural network (NN) hyperparameters**, as evaluated on one or more dataset families, parameterized as **target functions**, by analyzing the corresponding **Gaussian process (GP) surrogate model**. In Section (4.1), we capture a previously established NN phenomenon, in Section (4.2), we identify influential points for NNs, and in Section (4.3), we predict NN generalization behavior.

4.1 REPRODUCTION: SPECTRAL BIAS

Rahaman et al. [2019] demonstrated that deep rectifier NNs exhibit *spectral bias*, the preference to learn lower frequencies in the target function before higher frequencies. To demonstrate this, the authors studied the Fourier spectrum of rectifier NNs fit to a sum of sinusoidal functions of varying frequencies. In this section, we take an alternative approach:

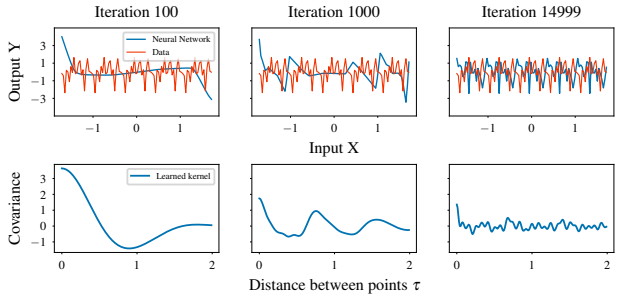


Figure 3: Capturing spectral bias in neural networks. (**Top**) Neural network predictions as training progresses on the sum-of-sines target function described in Section (4.1). (**Bottom**) Spectral mixture kernel fit to neural network predictions as training progresses. The kernel reveals a spectral bias for this neural network family, with the range of spectral frequencies expressed in the kernel increasing with the number of iterations of training.

We learn kernels from NN predictions at various stages of training and demonstrate that the evolution of these learned kernels captures the spectral bias.

NN hyperparameters. As in Rahaman et al. [2019], we train an NN with 6 hidden layers of 256 units and ReLU activations using full-batch gradient descent with Adam and a learning rate of $\eta = 3 \times 10^{-4}$.

Target function. The target functions are sums of sine functions with frequencies in $(5, 10, \ldots, 45, 50)$ and phases drawn from $U(0, 2\pi)$, evaluated at 200 points evenly spaced between $[0, 1]$, as in Rahaman et al. [2019].

GP surrogate. We learn the parameters of a spectral mixture kernel (SMK) with $Q = 10$ mixture components by optimizing Objective (6) with Adam for 350 iterations with a learning rate of $\eta = 0.1$. Since the marginal likelihood of the SMK is multi-modal in its frequency parameters, we repeat this optimization for three different random initializations of the kernel parameters and choose the hyperparameters with the largest marginal likelihood value (the value of Objective (6)). We randomly initialize the length-scales v_i by sampling from a truncated normal distribution whose variance depends on the maximum distance between input points. We set the signal variances w to the variance of the target function values divided by the number of mixture components. The frequency hyperparameters of the SMK are sometimes initialized by sampling from a uniform distribution whose upper limit is the Nyquist frequency [Wilson and Adams, 2013]; since this target function's largest frequency is smaller than the Nyquist frequency, we instead set a smaller frequency as the upper limit.

Results. Fig. (3) displays the NN predictions and the kernel of the corresponding GP surrogate at different iterations of NN training. The kernel function, which is given in Eq. (5), reflects how the similarity between function values varies with the distance between their input points.[2] The structure of the learned kernel reflects the properties of the NN family: Initially, the learned kernel only captures low frequencies in the NN's predictions—seen in the long period of the kernel—consistent with the spectral bias of Rahaman et al. [2019]. However, with more training, the periodicity of the surrogate kernel reflects both low and high frequencies.

4.2 AMORTIZED INFLUENCE ESTIMATION

The primary computational bottleneck of fitting a GP is the $O(N^3)$ cost of Gram matrix inversion. However, once this matrix is inverted, certain computations that seem costly can actually be performed cheaply. For example, the leave-one-out predictive (LOO) distributions can be computed analytically given the inverted Gram matrix and the training data [Rasmussen and Williams, 2006].These distributions characterize how GP predictions change after removing a training point. In this section, we leverage this nice property of GPs to perform influence function analysis in the spirit of [Koh and Liang, 2017]. In particular, we use the LOO predictive distributions of a surrogate GP to detect influential points for NNs with Fourier feature layers [Tancik et al., 2020], which enable NNs to learn higher frequencies. Similar architectures have achieved state-of-art performance in a number of important tasks in computer vision and computer graphics [Mildenhall et al., 2020]. We show that the surrogate LOO predictions are consistent with NN LOO predictions obtained from costly retraining.

NN hyperparameters. As in Tancik et al. [2020], we train an NN with 4 hidden layers of 1024 units, ReLU activations. The inputs to the NNs are passed through a single Fourier feature layer with parameter p that controls the spectral bias of the NN. We set $p = 1$ and choose Fourier feature mappings with frequencies ranging from 1 to 4. We train the network using full-batch gradient descent with stochastic gradient descent (SGD) and a learning rate of $\eta = 10^{-3}$ for 2000 iterations.

Target functions. We consider a target function inspired by one used in the leave-one-out GP literature [Ginsbourger and Scharer, 2021]. The functional form is given by $f(x) = \sin(30(x - 0.95)^4)\cos(2(x - 0.95)) + (x - 0.95)/2$. This target function is non-stationary with higher frequency behavior in the left half of its input domain and lower frequency behavior in the right.

GP surrogate. We fit a SMK with $Q = 10$ mixture components to trained neural network predictions at 300 input points evenly spaced between (0, 3). We initialize frequency hyperparameters by sampling uniformly from 0 to 20.

[2] Since the SMK is a stationary covariance function, we graph against the distance between input points rather than the absolute value of the input points themselves.

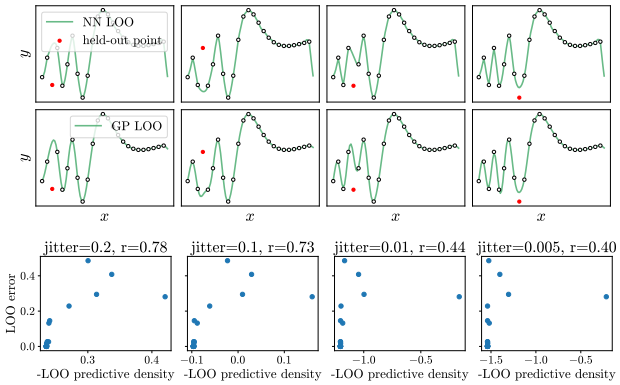


Figure 4: NN and GP surrogate leave-one-out predictions compared. (**Top**) Neural network predictions obtained from re-training on target function with influential (red) training points removed. (**Middle**) GP surrogate predictions on same datasets with kernel learned from trained NN predictions. Columns correspond to different held-out training points. (**Bottom**) Correlation between LOO error and (negative) GP LOO predictive probability of held-out points; a lower negative LOO predictive probability means a less influential point. The GP and NN LOO predictions are qualitatively consistent and the LOO error correlates positively with the negative LOO predictive probability.

We briefly overview leave-one-out cross-validation (LOO-CV) in the context of GPs. The GP LOO predictive probability when leaving out training example i is

$$\log p(y_i|X_{-i}, \mathbf{y}_{-i}) = -\frac{1}{2}\log\sigma_i^2 - \frac{(y_i-\mu_i)^2}{2\sigma_i^2} - \frac{1}{2}\log 2\pi \tag{7}$$

The notation $\mathbf{y}_{-i}$ indicates all training targets *besides* the ith target. The LOO-CV predictive mean μ_i and variance σ_i^2 can be computed directly from the inverted Gram matrix:

$$\mu_i = y_i - \frac{[K^{-1}y]_i}{[K^{-1}]_{ii}}, \quad \text{and} \quad \sigma_i^2 = \frac{1}{[K^{-1}]_{ii}} \tag{8}$$

Importantly, to compute these predictive means and variances, we can reuse the inverse of the Gram matrix computed to perform GP inference (Eqs. (1) and (3)). In our analysis, we will quantify the influence of a point (x_i, y_i) using the predictive log probability $\log p(y_i|X_{-i}, \mathbf{y}_{-i})$. We can interpret points with lower log probability as more "surprising" or "influential" under the assumptions of a kernel.

Results In the first two rows of Figure 4, we compare the surrogate GP LOO and NN LOO predictions for some of the most influential points. Indeed, the GP LOO predictions at the influential points are consistent with the NN LOO prediction. In the last row of Figure 4, we show that the (negative) LOO log probability at an input point is positively correlated with the actual LOO error at the training input, where the LOO error is computed as the difference between the NN LOO predictions and the predictions of the NN trained on the full dataset. We validate this result across different levels of jitter added to the Gram matrix.

4.3 PREDICTING THE GENERALIZATION GAP

In these sections, we predict generalization using kernels learned from trained NNs. To do this, we characterize trained NN properties on the *validation set* and compare these properties to the training data. We focus on the validation set because it is more informative of extrapolation. If the NN extrapolates well, its predictions on the validation set should be "similar" in some sense to the dataset. On the other hand, significant discrepancies could indicate poor extrapolation. This intuition motivates us to compare a kernel from the training data with a surrogate kernel fit to NN predictions on a validation set. We find that a lower similarity between these kernels correlates with a larger *generalization gap* (*i.e.,* poorer extrapolation), defined as the difference between test error and training error [*e.g.,* Jiang et al., 2020].

4.3.1 Initial demonstration

NN hyperparameters. We train ensembles of randomly initialized NNs with sigmoid-weighted linear unit (SiLU) [Elfwing et al., 2018], Gaussian error linear unit (GELU) [Hendrycks and Gimpel, 2016], ReLU [Fukushima, 1975, Nair and Hinton, 2010], or hyperbolic tangent ($\tanh$) activations, and two layers of 128 hidden units. We use the LeCun normal initialization with a scale of 1.5 [LeCun et al., 2012]. We train 25 NNs with full-batch gradient descent using Adam with a learning rate of $\eta = 0.003$. We want to assess if our approach can distinguish between NNs with similar training behavior but varying generalization performance, so we train NNs either for a maximum number of iterations, a hyperparameter, or until training error reaches zero.

Target functions. We consider a set of naturalistic regression tasks from the UC Irvine Machine Learning Repository (UCI) dataset [Dua and Graff, 2017], spanning a range of dataset sizes and input dimensions. We split each of the datasets into a 72/8/20 train/validation/test split. Both the data input and output are standardized by mean-centering and dividing by the standard deviation dimension-wise so that the target values and each dimension of the data input have near zero mean and unit variance. We subsample 2,000 datapoints for datasets with more than 2,000 datapoints, as in Simpson et al. [2021] and Liu et al. [2020].

GP surrogate. We learn a *data kernel* directly from the training dataset. We also learn a *surrogate kernel* from NN predictions on the validation set. In both cases, we use the Matérn kernel (MK) since the SMK can struggle for higher-dimensional inputs. We learn a separate lengthscale for each input dimension (*i.e.,* feature) of the data. We denote the lengthscales for a kernel as its *lengthscale profile*. We call the data kernel's lengthscales the *data lengthscales* and the surrogate kernel's lengthscales the *surrogate lengthscales*. To quantify the mismatch between NN validation predic-

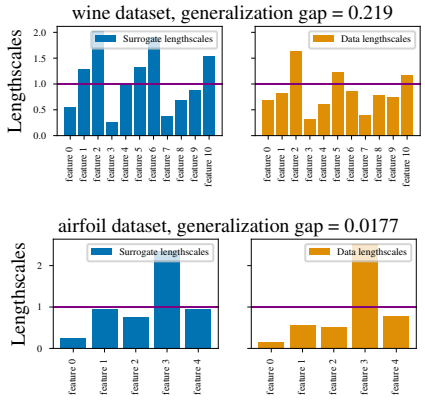


Figure 5: Qualitative connection between lengthscale profile discrepancy and generalization gap. Each subfigure compares normalized lengthscales learned from neural network predictions on validation set (*i.e.,* surrogate lengthscales) after training and normalized lengthscales learned from training data (*i.e.,* data lengthscales). A lengthscale greater than 1 indicates an "unimportant" feature. The title indicates the UCI dataset and generalization gap defined in Fig. (6). Data and surrogate lengthscales for some features are different (*e.g.,* features 1, 4, 6), reflected in a high generalization gap (**top**). Data and surrogate lengthscales for the same features are generally similar, reflected in a low generalization gap (**bottom**). This suggests a connection between the generalization gap and discrepancy between surrogate and data lengthscales.

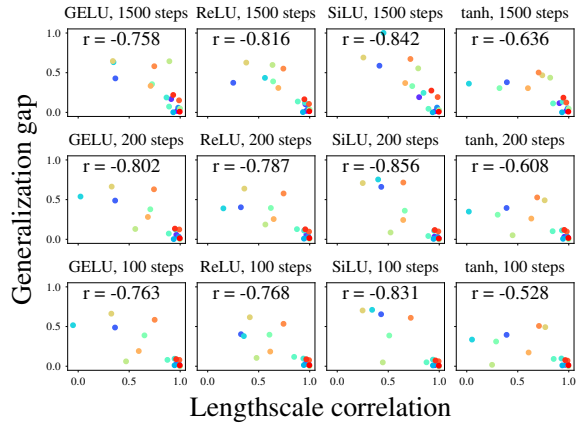


Figure 6: Inverse relationship between generalization error and lengthscale correlation on UCI datasets. Each point represents the lengthscale correlation (between surrogate and data lengthscales) and the generalization gap for a neural network ensemble to which the surrogate model is fit, on a single UCI dataset. Each panel corresponds to a particular neural family; see Section (4.3) for details about hyperparameters of these families, including architectures. Colors correspond to a particular UCI dataset. Across datasets and architectures, a larger lengthscale correlation (*i.e.,* higher similarity between the data and surrogate representations) corresponds to a lower generalization gap (*i.e.,* better extrapolation).

tions and the training data, we consider the *correlation in lengthscale profiles across features*. This is the correlation between the data and surrogate lengthscales.

Results. Fig. (5) gives intuition for our more general result in Fig. (6). For two UCI datasets, we compare the data lengthscales and the surrogate lengthscales for a two-layer GELU NN. The vertical axis corresponds to (normalized) learned lengthscales for each input dimension.[3] When the generalization gap is small, the data kernel and surrogate kernel are similar; the same features have similar lengthscales (Fig. (5), bottom). When the generalization gap is large, the data kernel and surrogate kernel have discrepancies. For example, the surrogate lengthscales for features 1 and 6 are larger than 1, but the data lengthscales for feature 1 and 6 are smaller than 1 (Fig. (5), top).

In Fig. (6), we summarize our results across different architectures, datasets, and maximum training iterations. We display the generalization gap against the correlation in lengthscale profiles across features. The similarity in lengthscale profiles negatively correlates with generalization gap across a range of architectures and max iterations. The Pearson correlation coefficients range from -0.856 to -0.528. In Section A.3 of the supplement, we additionally demonstrate that these results are insensitive to outlier datasets by performing a dataset-sensitivity analysis.

[3]For this visualization, we divide the learned lengthscale for each dimension by the difference between the maximum feature value and minimum feature value for each dimension. We can thus interpret a lengthscale that is much greater than 1 as suggesting that the NN predictions do not vary much along that dimension.

4.3.2 Larger-scale demonstration

In this section we extend the analysis in the previous section to a larger hyperparameter sweep of models, more closely emulating the kind of analysis a practitioner would use in selecting a model for a dataset.

NN hyperparameters. We train ensembles of randomly initialized NNs with four activations (SiLU, GELU, ReLU, or tanh), two depths (2, 4), two widths (32, 64), and two learning rates with Adam (0.03, 0.003), generating 32 hyperparameter combinations. We use the LeCun normal initialization with a scale of 1.5.We train 50 NNs for 500 iterations with full-batch gradient descent using Adam.

Target functions. We consider a subset of UCI datasets that satisfy two criteria: the number of unique feature values for each dimension is greater than 2 and the range in lengthscale correlations between neural network and datasets is greater than 0.025; the first condition ensures that we can learn sensible lengthscales for the dataset, while the second ensures that there is meaningful variation in NN behavior within a dataset.

As in Section (4.3.1), we split each of the datasets into a 72/8/20 train/validation/test split, subsample 2,000 datapoints if necessary, and standardize data inputs and outputs.

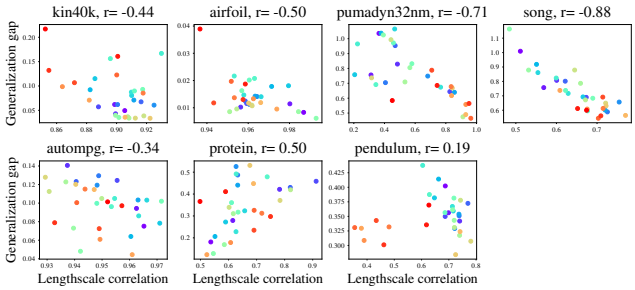


Figure 7: Inverse relationship between generalization error and lengthscale correlation on UCI datasets across hyperparameter sweep of neural networks. Each point represents the lengthscale correlation (between surrogate and data lengthscales) and the generalization gap for a neural network ensemble to which the surrogate model is fit. Each panel corresponds to a particular UCI dataset; see Section (4.3.2) for details about hyperparameters and architectures. In 5/7 datasets, a larger lengthscale correlation (*i.e.,* higher similarity between the data and surrogate representations) corresponds to a lower generalization gap (*i.e.,* better extrapolation).

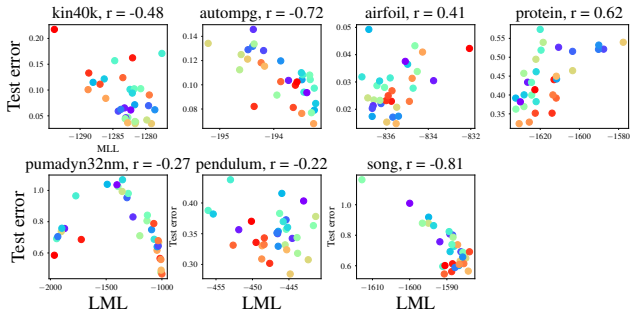


Figure 8: Inverse relationship between test error and marginal likelihood on UCI datasets Each point represents the marginal likelihood of the training data (using the surrogate kernel for a neural network family) and the test error for a neural network ensemble to which the surrogate model is fit. Each panel corresponds to a particular UCI dataset; see Section (4.3.2) for details about hyperparameters of these families, including architectures. Each color corresponds to a particular neural network ensemble. In 5/7 datasets, a larger marginal likelihood correlates with lower test error.

GP surrogate. In addition to the correlation in lengthscale profiles across features from Section (4.3.1), we consider the marginal likelihood of the training dataset under the surrogate kernel for each family of neural networks.

Results. Figure (7) plots the generalization gap against the correlation in lengthscale profiles across features. In contrast to Fig. (6), each panel corresponds to a particular dataset and each data point corresponds to a particular neural network family with a set of hyperparameters described above. The majority of datasets exhibit negative correlation between correlation the in lengthscale profiles and generalization gap. There are two exceptions: pendulum and protein. For the pendulum dataset, the positive correlation is driven by neural networks with tanh activations (the dots in different shades of red). We think the Matern kernel may struggle to model the tanh networks. This is consistent with Fig. (6) where the correlations were consistently lower for the tanh networks. For the protein dataset, the positive correlations might be related to challenges in fitting GPs to this dataset; recent work showed that exact GP regression on a training dataset (without any subsampling) from the protein dataset attains high test RMSE [Wang et al., 2019].

In Fig. (8), we plot the test error against the marginal likelihood of the training data under the various surrogate kernels for each neural network ensemble. That is, each point corresponds to the marginal likelihood of the training data using the surrogate kernel learned from each neural network family. We find the marginal likelihood correlates with test error on several of the datasets (each dataset is indicated by the subplot title). Consistent with previous work [Lotfi et al., 2022], we find that this result is sensitive to the jitter (which we set to 0.5). In Section A.2 of the supplement, we sanity check this analysis on synthetic datasets.

5 DISCUSSION

In this work, we illustrated the potential of empirically characterizing neural networks with Gaussian process surrogates. We captured the spectral bias of deep rectifier networks by examining how the surrogate kernel evolves during training (Section (4.1)). We further demonstrated that Gaussian process surrogates can be used to identify influential datapoints (Section (4.2)) and predict neural network generalization (Section (4.3)). Taken together, these results suggest that Gaussian process surrogates may be a valuable empirical tool for investigating deep learning, and future work could aim to use this framework to complement existing approaches to interpretability [*e.g.,* Ribeiro et al., 2016] and examining extrapolation behavior [*e.g.,* Xu et al., 2021].

We note some limitations of our current study. First, though the framework is, in principle, applicable to broader settings, we restricted this first exploration to regression tasks and feed-forward neural network architectures. A broader study of more architectures and tasks would be challenging due to the need to scale Gaussian processes but potentially rewarding, as characterizing properties of neural networks as used in practice is a significant open problem with far-reaching implications [Sejnowski, 2020]. We could leverage classic techniques such as inducing points [*e.g.,* Titsias, 2009].

Second, we learn point estimates of kernel hyperparameters [type II maximum likelihood; Gelman et al., 2013]. Although this is standard, we could infer the posterior over hyperparameters using Markov chain Monte Carlo (MCMC) or variational inference [Lalchand and Rasmussen, 2020, Murray and Adams, 2010] to perform a fully Bayesian analysis. We could also explore a richer set of kernels, such as compositional kernels [Duvenaud et al., 2013]. These directions are exciting avenues for future work.

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