Characterizing Deep Gaussian Processes via Nonlinear Recurrence Systems

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Abstract
Recent advances in Deep Gaussian Processes (DGPs) show the potential to have more expressive representation than that of traditional Gaussian Processes (GPs). However, there exists a pathology of deep Gaussian processes that their learning capacities reduce significantly when the number of layers increases. In this paper, we present a new analysis in DGPs by studying its corresponding nonlinear dynamic systems to explain the issue. Existing work reports the pathology for the squared exponential kernel function. We extend our investigation to four types of common stationary kernel functions. The recurrence relations between layers are analytically derived, providing a tighter bound and the rate of convergence of the dynamic systems. We demonstrate our finding with a number of experimental results.

1 Introduction
Deep Gaussian Process [DGP] (Damianou and Lawrence 2013) is a new promising class of models which are constructed by a hierarchical composition of Gaussian processes. The strength of this model lies in its capacity to have richer representation power from the hierarchical construction and its robustness to overfitting from the probabilistic modeling. Therefore, there have been extensive studies (Hensman and Lawrence 2014; Dai et al. 2016; Bui et al. 2016; Cutajar et al. 2017; Salimbeni and Deisenroth 2017; Havasi, Hernández-Lobato, and Murillo-Fuentes 2018; Salimbeni et al. 2019; Lu et al. 2020; Ustyuzhaninov et al. 2020) contributing to this research area.

There exists a pathology, stating that the increase in the number of layers degrades the learning power of [DGP] (Duvenaud et al. 2014). That is, the functions produced by [DGP] priors become flat and cannot fit data. It is important to develop theoretical understanding of this behavior, and therefore to have proper tactics in designing model architectures and parameter regularization to prevent the issue. Existing work (Duvenaud et al. 2014) investigates the Jacobian matrix of a given model which can be analytically interpreted as the product of those in each layer. Based on the connection between the manifold of a function and the spectrum of its Jacobian, the authors show the degree of freedom is reduced significantly at deep layers. Another work (Dunlop et al. 2018) studies the ergodicity of the Markov chain to explain the pathology.

To explain such phenomena, we study a quantity which measures the distance of any two layer outputs. We present a new approach that makes use of the statistical properties of the quantity passing from one layer to another layer. Therefore, our approach accurately captures the relations of the distance quantity between layers. By considering kernel hyperparameters, our method recursively computes the relations of two consecutive layers. Interestingly, the recurrence relations provide a tighter bound than that of (Dunlop et al. 2018) and reveal the rate of convergence to fixed points. Under this unified approach, we further extend our analysis to five popular kernels which are not analyzed yet before. For example, the spectral mixture kernels do not suffer the pathology. We further provide a case study in [DGP] showing the connection between our recurrence relations and learning [DGPs].

Our contributions in this paper are: (1) we provide a new perspective of the pathology in [DGP] under the lens of chaos theory; (2) we show that the recurrence relation between layers gives us the rate of convergence to a fixed point; (3) we give a unified approach to form the recurrence relation for several kernel functions including the squared exponential kernel function, the cosine kernel function, the periodic kernel function, the rational quadratic kernel function and the spectral mixture kernel; (4) we justify our findings with numerical experiments. We use the recurrence relations in debugging [DGPs] and explore a new regularization on kernel hyperparameters to learn zero-mean [DGPs].

2 Background
Notation Throughout this paper, we use the boldface as vector or vector-value function. The superscript i.e. \( f^{(d)}(x) \) is the \( d \)-th dimension of vector-valued function \( f(x) \).

2.1 Deep Gaussian Processes
We study [DGPs] in composition formulation where GP layers are stacked hierarchically. An \( N \)-layer [DGP] is defined as

\[
    f_N \circ f_{N-1} \circ \cdots \circ f_1(x),
\]

where, at layer \( n \), for dimension \( d \), \( f^{(d)}_n | f_{n-1} \sim GP(0, k_n(\cdot, \cdot)) \) independently. Note that the GP priors have the mean functions set to zero. The non-zero-mean case is discussed later (Section 4.4). We shorthand \( f_n \circ f_{n-1} \circ \cdots \circ f_1(x) \)
Recurrence relation: \(E[Z_n] = h(E[Z_{n-1}]; \theta)\)

Figure 1: Studying the squared distance, \(Z_n\), between outputs of two consecutive layers. The asymptotic property (middle plot) of the recurrence relation of this quantity between two consecutive layers decides the existence of pathology for a very deep model. Here, \(\theta\) indicates kernel hyperparameters. The middle plot is the bifurcation plot providing the state of DGP at very deep layer. The pathology is identified by the zero-value region where \(E[Z_n] \to 0\). Note that this bifurcation plot is for illustration purpose only.

\[
\cdots \circ f_1(x) \overset{\text{as}}{=} f_n(x) \quad \text{and write} \quad k_n(f_{n-1}(x), f_{n-1}(x')) \quad \text{as} \quad k_n(x, x'). \quad \text{Let} \ m \ \text{be the number of output of} \ f_n. \quad \text{All layers have the same hyperparameters.}
\]

**Theorem 2.1** (Dunlop et al. 2018). Assume that \(k(x, x')\) is given by the squared exponential kernel function with variance \(\sigma^2\) and lengthscale \(\ell^2\) and that the input \(x\) is bounded. Then if \(\sigma^2 < \ell^2 / m\),

\[
P(\|f_n(x) - f_n(x')\|_2 \to 0 \quad \text{for all} \ x, x' \in D) = 1
\]

where \(P\) denotes the law of process \(\{f_n\}\).

This theorem tells us the criterion that the event of vanishing in output magnitude happens infinitely often with probability 1.

### 2.2 Analyzing dynamic systems with chaos theory

Recurrence maps representing dynamic transitions between DGP layers are nonlinear. Studying the dynamic states and convergence properties for nonlinear recurrences is not as well-established as those of linear recurrences. As an example, given a simple nonlinear model like the logistic map: \(u_n = ru_{n-1}(1 - u_{n-1})\), its dynamic behaviors can be complicated (May 1976).

Recurrent plots or bifurcation plots have been used to analyze the behavior of chaotic systems. The plots are produced by simulating and recording the dynamic states up to very large time points. This tool allows us to monitor the qualitative changes in a system, illustrating fixed points asymptotically, or possible visited values. Other techniques, e.g. transient chaos (Poole et al. 2016), recurrence relations (Schoenholz et al. 2017) have been used to study deep neural networks.

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Figure 2: Bifurcation plot of the logistic function \(u_n = ru_{n-1}(1 - u_{n-1})\).

3 Moment-generating function of distance quantity

Throughout this paper, we are interested in quantifying the expectation of the squared Euclidean distance between any two outputs of a layer and thereby study the dynamics of this quantity from a layer to the next layer. Figure 3 shows that we can make use of the found recurrence relations to study the pathology of DGP.

For any input pair \(x\) and \(x'\), we define such quantity at layer \(n\) as \(Z_n = ||f_n(x) - f_n(x')||^2 = \sum_{d=1}^m (f_n^{(d)}(x) - f_n^{(d)}(x'))^2\). When the previous layer \(f_{n-1}\) is given, the difference between any \(f_n^{(d)}(x)\) and \(f_n^{(d)}(x')\) is Gaussian,

\[
(f_n^{(d)}(x) - f_n^{(d)}(x')) | f_{n-1} \sim \mathcal{N}(0, s_n).
\]

Here \(s_n = k_n(x,x) + k_n(x',x') - 2k_n(x,x')\) which is obtained from subtracting two dependent Gaussians. We can normalize the difference between \(f_n^{(d)}(x)\) and \(f_n^{(d)}(x')\) by a factor \(\sqrt{s_n}\) to obtain the form of standard normal distribu-
The second equality is followed by 
\[
\frac{1}{\sqrt{s_n}} \text{E}_{n-1} \sim \mathcal{N}(0, 1).
\]
Since all dimensions \(d\) in a layer are independent, we can say that \(\frac{Z_n}{s_n} = f_{n-1} \sim \chi^2_m\) is distributed according to the Chi-squared distribution with \(m\) degrees of freedom.

One useful property of the Chi-squared distribution is that the moment-generating function of \(\frac{Z_n}{s_n} | f_{n-1}\) can be written in an analytical form, with \(t \leq 1/2\),
\[
M_{\frac{Z_n}{s_n} | f_{n-1}}(t) = \mathbb{E} \left[ \exp \left( t \frac{Z_n}{s_n} | f_{n-1} \right) \right] = (1 - 2t)^{-m/2}.
\]

We shall see that the expectation of the distance quantity \(Z_n\) is computed via a kernel function which, in most cases, involves exponentiations. Given that the input of this kernel is governed by a distribution, i.e., \(\chi^2\), the moment-generating function becomes convenient to obtain our desired expectations.

Figure 3 depicts our approach to extract a function \(h(.)\) which models the recurrence relation between \(\mathbb{E}[Z_n]\) and \(\mathbb{E}[Z_{n-1}]\). This is also the main theme of this paper.

4 Finding recurrence relations

This section presents the formalization of the recurrence relation of \(\mathbb{E}[Z_n]\) for each kernel function. We start off with the squared exponential kernel function.

4.1 Squared exponential kernel function

The squared exponential kernel (SE) is defined in the form of
\[
\text{SE}(\mathbf{x}, \mathbf{x'}) = \sigma^2 \exp \left( -\frac{\| \mathbf{x} - \mathbf{x'} \|^2}{2\ell^2} \right).
\]

**Theorem 4.1 (DGP with SE).** *Given a triplet \((m, \sigma^2, \ell^2)\), \(m \geq 1\) such that the following sequence converges to 0:
\[
u_n = 2m \sigma^2 \left( 1 - (1 + \nu_{n-1}/m^2)^{-m/2} \right),
\]
Then, \(\mathbb{P}(\|f_n(\mathbf{x}) - f_n(\mathbf{x'})\|_2^n \to 0 \text{ for all } \mathbf{x}, \mathbf{x'} \in D) = 1."
\]

**Proof.** Note that we do not directly have access to \(\mathbb{E}[Z_n]\) but \(\mathbb{E}[Z_n | f_{n-1}]\) because of the Markov structure of the DGP construction. Getting \(\mathbb{E}[Z_n]\) is done via \(\mathbb{E}[Z_n | f_{n-1}]\) where we use the law of total expectation \(\mathbb{E}[Z_n] = \mathbb{E}[f_{n-1} | \mathbb{E}[Z_n | f_{n-1}]]\).

Now, we study the term \(\mathbb{E}[Z_n | f_{n-1}]\):
\[
\mathbb{E}[Z_n | f_{n-1}] = \mathbb{E}[\sum_{d=1}^m (f_n^{(d)}(\mathbf{x}) - f_n^{(d)}(\mathbf{x'}))^2 | f_{n-1}] = 2m \sigma^2 - 2m k_n(\mathbf{x}, \mathbf{x'}).\]

The second equality is followed by \(\mathbb{E}[(f_n^{(d)}(\mathbf{x}))^2] = \mathbb{E}[(f_n^{(d)}(\mathbf{x'}))^2] = \sigma^2\) and \(\mathbb{E}[f_n^{(d)}(\mathbf{x}) f_n^{(d)}(\mathbf{x'})] = k_n(\mathbf{x}, \mathbf{x'}).\)

![Figure 4](image)

**Figure 4:** (a) Bifurcation plot of the recurrence relation of SE kernel for \(m = 1\). (b) Contour plot of \(u_n\) at layer \(n = 300\) and \(m = 1\). The misalignment between the red line \((\sigma^2/\ell^2 = 1)\) and the zero-level contour is due to numerical errors. (c): Increase \(m > \sigma^2/\ell^2\) to avoid pathology.

Recall that we write \(k_n(\mathbf{x}, \mathbf{x'}) = k_n(f_{n-1}(\mathbf{x}), f_{n-1}(\mathbf{x'})).\) By the definition of SE kernel, we have
\[
\mathbb{E}[Z_n | f_{n-1}] = 2m \sigma^2 \left( 1 - \exp \left( -\frac{Z_{n-1}}{2\ell^2} \right) \right).
\]

Applying the law of total expectation, we have
\[
\mathbb{E}[Z_n] = 2m \sigma^2 \left( 1 - \mathbb{E} \left[ \exp \left( -\frac{Z_{n-1} | f_{n-2}}{2\ell^2} \right) \right] \right).\]

Again, we can only compute \(\mathbb{E}[\exp(-Z_{n-1} | f_{n-2})] = \mathbb{E}[f_{n-2} | \mathbb{E}[\exp(-Z_{n-1} | f_{n-2})]]\). The expectation will be computed by the formula of the moment-generating function with respect to \(\frac{Z_{n-1} | f_{n-2}}{\sqrt{s_{n-1}}} \) where \(t = -\frac{s_{n-1} | f_{n-2}}{2\ell^2}\) in Equation (1). Choosing this value also satisfies the condition \(t \leq 1/2\). Now, we have
\[
\mathbb{E}[Z_n] = 2m \sigma^2 \left( 1 - \mathbb{E} \left[ \left( \frac{1 + s_{n-1} | f_{n-2}}{\ell^2} \right)^{-m/2} \right] \right) \leq 2m \sigma^2 \left( 1 - \left( 1 + \mathbb{E}[s_{n-1} | f_{n-2}] \right)^{-m/2} \right).\]

Here, Jensen’s inequality is used as \((1 + x)^{-a}\) is convex for any \(x > 0\). By Equation 4, we have
\[
\mathbb{E}[Z_{n-1} | f_{n-2}] = 2\sigma^2 - 2k_{n-1}(\mathbf{x}, \mathbf{x'}) = s_{n-1}.
\]
Replacing \(s_{n-1}\) in Equation (5) and applying the law of total expectation for the case of \(Z_{n-1}\), we obtain recurrence relation between layer \(n - 1\) and layer \(n\) is
\[
\mathbb{E}[Z_n] \leq 2m \sigma^2 \left( 1 - \left( 1 + \mathbb{E}[Z_{n-1} | f_{n-2}] \right)^{-m/2} \right).
\]

Using the Markov inequality, for any \(\epsilon\), we can bound \(\mathbb{P}(Z_n \geq \epsilon) \leq \frac{\mathbb{E}[Z_n]}{\epsilon} = \frac{\epsilon}{2m \sigma^2}.
\]

At this point, \(u_n\) defined in Equation 5 is considered as the upper bound of \(\mathbb{E}[Z_n]\). We condition that \(\{u_{n}\}\) converges to 0, then \(\mathbb{E}[Z_n]\) converges to 0 as well. By the first Borel-Cantelli lemma, we have \(\mathbb{P}(\lim \sup_{n \to \infty} Z_n \geq \epsilon) = 0\), which leads to the conclusion in the same manners as Dunlop et al. 2018.

**Analyzing the recurrence** Figure 4 illustrates the bifurcation plot of Equation 3 with \(m = 1\). The non-zero contour
region in Figure 4b tells us that $\sigma^2/\ell^2$ should be smaller than 1 to escape the pathology. When $m > 1$, Figure 4c shows that if $m > \sigma^2/\ell^2$, $u_n$ does not approach to 0, implying the condition to prevent the pathology. This result is consistent with Theorem 2.1 in (Dunlop et al. 2018).

**Discussion** Note that the relation between $\mathbb{E}[Z_n]$ and $\mathbb{E}[Z_{n-1}]$ presents a tighter bound than existing work (Dunlop et al. 2018). If we construct the recurrence relation based on (Dunlop et al. 2018), $\mathbb{E}[Z_n]$ is bounded by

$$
\mathbb{E}[Z_n] \leq \frac{m \sigma^2}{\ell^2} \mathbb{E}[Z_{n-1}] - m \sigma^2 \mathbb{E}[Z_{n-1}] - \frac{m^2 \sigma^2}{\ell^2}.$$

One can show that $(1 + x)^a \geq 1 - ax$, $a < 0, x > 0$, implying

$$2m \sigma^2 (1 - (1 + \mathbb{E}[Z_{n-1}]/(m^2))^{-m/2}) \leq m \sigma^2 \mathbb{E}[Z_{n-1}] - \frac{m^2 \sigma^2}{\ell^2}.$$

In fact, a numerical experiment shows that our bound of $\mathbb{E}[Z_n]$ is found to be close to the true $\mathbb{E}[Z_n]$ (Section 6.1). That is, we can see the trajectory of $\mathbb{E}[Z_n]$ for every layer of a given model of which the depth is not necessary to be infinitely many.

One can reinterpret the recurrence relation for each dimension $d$ as

$$\mathbb{E}[Z_n^{(d)}] \leq 2 \sigma^2 \left(1 - \left(1 + \mathbb{E}[Z_{n-1}^{(d)}]/\ell^2\right)^{-m/2}\right),$$

where $\mathbb{E}[Z_n^{(d)}] = \mathbb{E}[Z_n]/\mathbb{E}[Z_{n-1}]$ with $Z_n^{(d)} = (f_n^{(d)}(x) - f_n^{(d)}(x'))^2$.

**A guideline to obtain a recurrence relation** Given a specific kernel function, one may follow these steps to acquire the corresponding recurrence relation: (1) considering the form of kernel input where it may be distributed according to either the Chi-squared distribution or its variants (presented in the next sections); (2) checking whether there is a way to represent the kernel function under representations such that statistical properties of kernel inputs are known; (3) caring about the convexity of the function after choosing a proper setting (as we bound the expectation with Jensen’s inequality in the proof of Theorem 4.1).

### 4.2 Cosine kernel function

The cosine kernel (COS) function takes inputs as the distance between two points instead of the squared distance like in the case of SE kernel. We will mainly work with $\sqrt{Z_n}$ in this subsection. The cosine kernel function $k(x, x') = \cos(\langle x, x' \rangle)$ is defined as

$$\cos(\langle x, x' \rangle) = \sigma^2 \cos(\pi \|x - x'\|_2/p).$$

Starting with Equation 4b and using the definition of Cos kernel, we have

$$\mathbb{E}[Z_n|f_{n-1}] = 2m \sigma^2 - 2m \sigma^2 \cos(\pi \sqrt{Z_{n-1}/p})
= 2m \sigma^2 - m \sigma^2 \exp(i \pi \sqrt{Z_{n-1}/p})
- m \sigma^2 \exp(-i \pi \sqrt{Z_{n-1}/p}).$$

Here, Euler’s formula is used to represent $\cos(\cdot)$ and $i$ is the imaginary unit ($i^2 = -1$). To obtain $\mathbb{E}[Z_n]$, we use the law of total expectation and compute the two following expectations: $\mathbb{E}[\exp(i \pi \sqrt{Z_{n-1}/p})f_{n-1}]$ and $\mathbb{E}[\exp(-i \pi \sqrt{Z_{n-1}/p})f_{n-2}]$. From $Z_n = \mathbb{E}[Z_{n-1} | f_{n-1}]$, we have $\sqrt{Z_n} f_{n-1} \sim \chi^2$, where $\sqrt{Z_n} f_{n-1}$ is distributed according to the Chi distribution. This observation follows the first step in the guideline. The characteristic function of the Chi distribution for random variable $\sqrt{Z_n} f_{n-1}$ is

$$\varphi_{\sqrt{Z_n}/\sqrt{s_n}}(t) = \mathbb{E}\left[\exp(it \sqrt{Z_n}/s_n)\right]
= \frac{m}{2} \frac{1}{2} \frac{1}{2} + \sqrt{n}2^{(m+1)/2} \Gamma(m/2) \frac{1}{1 - F_1(\frac{m}{2}, \frac{1}{2}, \frac{3}{2})}.$$

where $F_1(a, b, z)$ is Kummer’s confluent hypergeometric function (see Definition in Appendix A.2). This is considered as the second step in the guideline. Back to our process of finding the recurrence function, we consider the case $Z_{n-1}/s_n \sim \chi_m$. By choosing $t = \pm \frac{\sqrt{Z_{n-1}/s_n}}{p}$ for its characteristic function, we can obtain

$$\mathbb{E}[Z_n] = 2m \sigma^2 \left[1 - 1 - F_1(\frac{3}{2}, \frac{1}{2}, \frac{\pi^2}{2p^2}) \mathbb{E}[Z_{n-1}|f_{n-2}]\right].$$

This is because the imaginary parts of $\varphi(t = \pm \sqrt{Z_{n-1}/s_n}/p)$ and $\varphi(-\frac{\sqrt{Z_{n-1}/s_n}}{p})$ are canceled out.

As the third step in the guideline, we perform a sanity check about the convexity of $1F_1$. Only with $m = 1$, $1F_1(\frac{3}{2}, \frac{1}{2}, \frac{1}{2}) = \exp(-\frac{1}{4})$ is convex. Our result in this case is restricted to $m = 1$. Now, we can state that the recurrence relation is

$$u_n = 2 \sigma^2 \left[1 - \exp(-\frac{\pi^2}{4p^2})\right].$$

### 4.3 Spectral mixture kernel function

In this paper, we consider the spectral mixture (SM) kernel (Wilson and Adams 2013) in one-dimensional case with one mixture:

$$SM(r) = \exp(-\frac{\pi^2}{4r^2} \cos(2\pi \mu r)),$$

where $r = \|x - x'\|_2$ and $\sigma^2, \mu > 0$. We can rewrite this kernel function as $\frac{1}{2} w^2(\exp(-\frac{\pi^2}{4r^2} \cos(2\pi \mu r)) + \exp(-\frac{\pi^2}{4r^2} \cos(2\pi \mu r))$. Here we simplify the kernel by change in variables as $w^2 = \exp(-\frac{\mu}{2\sigma^2})$, $\nu^2 = 2\sigma^2 \sigma^2$, and $u = \frac{\mu}{2\sigma^2}$. With a similar approach, we compute the expectation of $\mathbb{E}[\exp(-\frac{\pi^2}{4r^2} \cos(2\pi \mu r))].$ We can identify that $(\sqrt{Z_{n-1} + iu})^2/f_{n-2} \sim \chi^2(\lambda)$ is distributed according to a non-central Chi-squared distribution of which the moment-generating function is

$$M_{\chi^2}(t; \lambda) = (1 - 2t)^{-1/2} \exp(\lambda t/(1 - 2t)),$$

where the noncentrality parameter $\lambda = -u^2/s_{n-1}$. By choosing an appropriate $t = -u^2/s_{n-1}$, we obtain the recurrence as

$$\mathbb{E}[Z_n] \leq 2(1 - w^2 M_{\chi^2}(t; -u^2/s_{n-1}) \mathbb{E}[Z_{n-1}]; \lambda = -u^2/s_{n-1}]).$$

Note that the convexity requirement is satisfied. This recurrence relation of SM kernel has one additional exponent term when comparing to that of SE. We provide a precise formula and an extension to the high-dimensional case in Appendix C.
5.1 Identify the pathology

Table 1 provides the recurrence relations of two more kernel functions: the periodic (PER) kernel function and the rational quadratic (RQ) kernel function. The detailed derivation is in Appendix B and D.

5.2 Rate of convergence

Recall that $h(\cdot)$ is the function modeling the recurrence relation between $E[Z_n]$ and $E[Z_{n-1}]$. According to Banach fixed-point theorem (Kamis 2001), the rate of convergence is decided by the Lipchitz constant of $h(\cdot)$, $L = \sup h'(\cdot)$. The more curved the functions are, the faster the convergence will be. Note that $x$ is not input data but plays the role of $E[Z_n]$.

To the best of our knowledge, this is the first analytical explanation for the nonexistence of pathology in nonzero-mean DGPs. In practice, there is existing work choosing mean functions (Salimbeni and Deisenroth 2017). (Dunlop et al. 2018) briefly makes a connection between nonzero-mean DGPs and stochastic differential equations. However, there is no clear answer given for this case, yet. We use our approach to analyze two cases including mean DGPs and stochastic differential equations. However, the convergence rate of $E[Z_n]$ is never equal to zero since both $\sigma^2$ and $\mu$ are positive.

4.4 Extension to non-pathological cases

We use our approach to analyze two cases including nonzero-mean DGPs and input-connected DGPs where there is no pathology occurring.

**Nonzero-mean DGPs** Let $f_n(d)(x) \sim \mathcal{GP}(\mu_n(x), k_n(x,x'))$ with the mean function $\mu_n(x)$, the difference between two outputs, $(f_n(d)(x) - f_n(d)(x')) \sim \mathcal{N}(\nu_n, s_n)$ with $\nu_n = \mu_n(x) - \mu_n(x')$. This leads to $f_n(x) \sim \chi^2_{\nu_n}$, the noncentral Chi-squared distribution with the non-central parameter $\lambda = m\sigma_n^2$.

Since we already provide an analysis involving the non-central Chi-squared distribution with spectral mixture kernels, no pathology of nonzero-mean DGPs can be shown by our analysis (Section 4.3). That is, there is no pathology as $\lambda > 0$. When $\lambda = 0$, this case falls back to zero-mean or constant-mean. Mean functions greatly impact the recurrence relation because $\lambda$ is inside an exponential function.

To the best of our knowledge, this is the first analytical explanation for the nonexistence of pathology in nonzero-mean DGPs. In practice, there is existing work choosing mean functions (Salimbeni and Deisenroth 2017). (Dunlop et al. 2018) briefly makes a connection between nonzero-mean DGPs and stochastic differential equations. However, there is no clear answer given for this case, yet.

**Input-connected DGPs** Previously, (Neal 1995; Duvenaud et al. 2014) suggest to make each layer connect to input. The corresponding dynamic system is

$$u_n = 2m\sigma^2(1 - (1 + u_{n-1}/m\sigma^2)^{-m/2}) + c,$$

with $c$ is computed from the kernel function taking input data $x$. By seeing its bifurcation plot in Figure 5 we can confirm the solution from (Neal 1995; Duvenaud et al. 2014). That is, $u_n$ converges to the value which is greater than zero, and avoids the pathology. However, the convergence rate of $E[Z_n]$ stays the same.

5 Analysis of recurrence relations

This section explains the condition of hyperparameters that causes the pathology for each kernel function. Then we discuss the rate of convergence for the recurrence functions.

**Cos kernel** Similar to SE, the condition to escape the pathology is $\pi^2\sigma^2/p^2 > 1$.

**PER kernel** If we increase $\ell$, then we should decrease the periodic length $p$ to prevent the pathology.

**RQ kernel** The behavior of this kernel resembles that of SE. We also observe that the change in the hyperparameter $\alpha$ does not affect the condition to avoid the pathology (Appendix E, Figure 15).

**SM kernel** Interestingly, this kernel does not suffer the pathology. If $(\sigma^2, \mu)$ goes to $(0, 0)$, $E[Z_n]$ approaches to 0. However, $E[Z_n]$ is never equal to 0 since both $\sigma^2$ and $\mu$ are positive.
Table 1: Kernel functions (middle column) and corresponding recurrence relations (right column)

| Kernel Function   | Recurrence Relation |
|-------------------|---------------------|
| Rational quadratic (RQ) | \( \sigma^2 \left( 1 + \frac{\|x - x\|^2}{2\alpha \ell^2} \right)^{-\alpha} \) |
| Periodic (PER)    | \( \sigma^2 \exp \left( -\frac{2 \sin^2(\pi m \|x - x\| / \ell)}{\ell^2} \right) \) |

6.1 Correctness of recurrence relations

We set up a DGP model with 10 layers with SE kernel. The inputs are \( x_0 = 0 \) and \( x_1 = 1 \). We will track the value \( Z_n = \| f_n(x_0) - f_n(x_1) \|_2^2 \) for \( n = 1 \ldots 10 \). Given a kernel \( k(x, x') \), we can exactly compute the expectations \( \mathbb{E}[Z_n] \).

From the model, we collect 2000 samples for each layer \( n \) to obtain the empirical expectation of \( \mathbb{E}[Z_n] \). Then, we would like to compare the true and empirical estimates. Figure 8 plots the comparisons for SE kernel and SM kernel. This numerical experiment supports the claim that our estimation \( \mathbb{E}[Z_n] \) is tight and even close to the true estimation. On the other hand, \( \mathbb{E}[Z_n] \) computed based on (Dunlop et al. 2018) Equation (6) grows exponentially, and cannot fit in Figure 8. The additional plots with different settings of hyperparameter and \( m \) can be found in Appendix F (Figure 17 and 18).

6.2 Justifying the conditions of pathology

From \( N_{\text{data}} \) inputs, we generate the outputs of DGP and measure the root mean squared distance (RMSD) among the outputs \( \text{RMSD}(n) = \sqrt{\frac{1}{N_{\text{data}}(N_{\text{data}}-1)} \sum_{i \neq j} \| f_n(x_i) - f_n(x_j) \|_2^2} \). We record this quantity as we increase \( n \). We replicate the procedure 30 times to aggregate the statistics of RMSD(n). Here, we only consider the case \( m = 1 \).

**SE kernel** We set up models in one dimension with inputs of each model in range \((-5, 5)\) with \( N_{\text{data}} = 100 \). The kernel hyperparameter \( \sigma^2 \) is set to 1 while \( 1/\ell^2 \) runs from 0.1 to 5. Figure 9 shows the trace of RMSD computed up to layer 100. When \( \sigma^2/\ell^2 > 1 \), the models start escaping the pathology.

**Cos kernel** With a similar setup to that of SE, Figure 9 shows that when \( \pi^2 \sigma^2/\ell^2 > 1 \), the models do not suffer the pathology.

**PER kernel** Since the PER kernel has three hyperparameters, \( \sigma^2, \ell^2, \alpha \), we fix \( \sigma^2 \) and vary \( \ell^2 \) and \( \alpha \). In this case, we collected the RMSDs at layer 100. We then compare the contour plot of these RMSDs with the values of the lower bound of \( \mathbb{E}[Z_n] \) computed when \( n \) is large. We can find a similarity between Figure 10 and Figure 6. The lower left of both plots has low values, identified as the region that causes the pathology.

**RQ kernel** Analogous to PER, only the RMSDs at layer 100 are gathered. We chose two different values of \( \alpha = \{0.5, 3\} \), and varying values of \( \sigma^2 \) and \( \ell^2 \). Figure 10 shows two contour plots of RMSDs for the two settings of \( \alpha \). Both of the two plots share the same area of which the contour level is close to 0.

**SM kernel** This kernel shows no sight of pathology (Figure 10b). We can find the similarity between this plot with the contour plot of \( \mathbb{E}[Z_n] \) in Figure 6.

6.3 Using recurrence relations in DGPs

Here, we use the recurrence relation as a tool to analyze DGP regression models. We learned the models where the number of layers, \( N \), ranges from 2 to 6 and the number...
of units per layer, \( m \), is from 2 to 9. We trained our models on Boston housing data set (Dheeru and Karra Taniskidou 2017) and diabetes data set (Efron et al. 2004). For each data set, we train our models with 90% of the data set and hold out the remaining for testing. The inference algorithm is based on (Salimbeni and Deisenroth 2017). We considered two settings: (1) standard zero-mean DGPs with SE kernel; (2) the SE kernel hyperparameters are constrained to avoid pathological regions with \( \ell^2 \in (0, c_0 m \sigma^2] \), constraint coefficient \( 0 < c_0 < 1 \).

Figure 11 plots the root mean squared errors (RMSEs) and quantity \( \mathbb{E}[Z_n] / \sigma^2 \) which describes changes between layers. For the case of standard zero-mean DGPs we can observe that models can not learn effectively at deeper layers and there are drops in terms of \( \mathbb{E}[Z_n] / \sigma^2 \) at the last layer. In the case of constraining hyperparameters, we see fewer drops and the results are improved when comparing to non-constrained cases. It seems that the drop pattern of \( \mathbb{E}[Z_n] / \sigma^2 \) correlates to model performances. We provide detailed figures and an additional result on the diabetes data set with a similar observation in Appendix F.

### 6.4 High-dimensional data set with zero-mean DGPs

We test on MNIST data set (LeCun and Cortes 2010) with the two models like previous experiments. The number of units per layer, \( m \), is chosen as \( m = 30 \). We consider the number of layers, \( N = 2, 3, 4 \).

The standard zero-mean DGP without any regularization fails to learn from data with accuracy \( \approx 10\% \). This means that the output of this model is just a flat function, making this 10-class classifier have such an accuracy. On the other hand, the constrained zero-mean DGP can alleviate the model performance with accuracy at best 91.21%. Figure 12 provides the results with different settings of \( c_0 \).

To have a better understanding of the above models, we visualize the loss landscape (Li et al. 2018) of the two cases in Figure 12. The standard zero-mean DGP easily falls into unsafe pathological hyperparameters during optimization and cannot escape the unsafe state (see Figure 12a). In contrary, the loss landscape of constrained DGPs (Figure 12b) shows an improved loss surface. However, we note that it still has a flat region where the optimization cannot be improved.

Our result is not as good as the accuracy (98.06%) of nonzero-mean DGPs reported in (Salimbeni and Deisenroth 2017). However, we emphasize that the main contribution of our work is not to demonstrate the classifier performance but to show the importance of incorporating the theoretical insights into practice. This shows that learning zero-mean DGPs is potentially possible.

### 7 Conclusion

We have presented a new analysis of the existing issue of DGP for a number of kernel functions via analyzing the chaotic properties of corresponding nonlinear systems which models the state of magnitudes between layers. We believe that such analysis can be beneficial in kernel structure discovery tasks (Duvenaud et al. 2013; Ghahramani 2015) for DGP. Our analysis not only provides a better understanding of the rate of convergence to fixed points but also considers a number of kernel types. Finally, our findings are verified by numerical experiments.
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Table 2: Summary of the recurrence relations

| Kernel Type                  | Recurrence Relation                                                                 |
|-----------------------------|--------------------------------------------------------------------------------------|
| Squared exponential (SE)    | \( \sigma^2 \exp \left( -\frac{\|x - x'\|^2}{2\ell^2} \right) u_n = 2m\sigma^2 \left( 1 - \left( 1 + u_{n-1}/m\ell^2 \right)^{-m/2} \right) \) |
| Rational quadratic (RQ)     | \( \left( 1 + \frac{\|x - x'\|^2}{(2\alpha\ell^2)} \right)^{-\alpha} u_n = 2m(1 - 2F_0(\alpha; \frac{m}{2}; \frac{-u_{n-1}}{\alpha\ell^2})) \) |
| Cosine (COS)                | \( \sigma^2 \cos \left( \pi \|x - x'\|/p \right) u_n = 2\sigma^2 \left( 1 - 1F_1(\frac{m}{2}; \frac{1}{2}; \frac{-2\pi^2}{p^2} u_{n-1}) \right) \) |
| Periodic (PER)              | \( \sigma^2 \exp \left( -\frac{2\sin^2(\pi \|x - x'\|/p)}{\ell^2} \right) u_n = 2m\sigma^2 \left( 1 - 1F_1(\frac{m}{2}; \frac{1}{2}; \frac{-2\pi^2}{p^2} u_{n-1}) \right) \) |
| Spectral mixture (SM)       | \( \exp(-2\pi^2\sigma^2 r^2) \cos(2\pi \mu r) \) \( u_n = 2m \left\{ 1 - \exp \left( -\frac{2m\pi^2 \mu^2 u_{n-1}}{1 + 4\pi^2 \sigma^2 u_{n-1}} \right) \right\} \) |

A Mathematical background

This section contains supporting theorems and results needed for proofs in the main text.

A.1 Some probability background

Lemma 1 (First Borel-Cantelli lemma). Let \( E_1, E_2, ... \) be a sequence of events in some probability space. If the sum of the probability of \( E_n \) is finite

\[
\sum_{n=1}^{\infty} \mathbb{P}(E_n) < \infty,
\]

then the probability that finitely many of them occur is 0, that is,

\[
\mathbb{P} \left( \limsup_{n \to \infty} E_n \right) = 0.
\]

A.2 Generalized hypergeometric function

A generalized hypergeometric function is in the form of

\[
_{p}F_{q}(a_1, a_2, \ldots, a_p; b_1, b_2, \ldots, b_q; z) = \sum_{n=0}^{\infty} \frac{a_1^n a_2^n \ldots a_p^n \cdot z^n}{b_1^n b_2^n \ldots b_q^n \cdot n!}.
\]

Here, \( x^n \) is the rising factorial defined as

\[
x^n = \prod_{k=0}^{n-1} (x + k).
\]

The function \( _1F_1(a_1, a_2; z) \) is used in the case of cosine kernel.

The function \( _2F_0(a_1, a_2; z) \) is used in the case of rational quadratic kernel.

B The recurrence relation for the case of PER

The periodic kernel (PER) resembles COS kernel, and is written in the form of

\[
\text{PER}(x, x') = \sigma^2 \exp \left( -\frac{2\sin^2(\pi \|x - x'\|/p)}{\ell^2} \right).
\]

In this case, we do not have an exact recurrence under equality. Instead, we find the lower bound of \( \mathbb{E}[Z_n] \). It is done by using \( e^x \geq 1 + x \):

\[
\exp \left( -\frac{2\sin^2(\pi r/p)}{\ell^2} \right) \geq g(\cos(2\pi r/p)).
\]

where \( r = \|x - x'\|_2 \), and \( g(\cos(2\pi r/p)) = 1 - (1 - \ell^2 + \ell^{-2} \cos(2\pi r/p)) \). We can see that the PER kernel now is bounded in terms of COS kernels and use the readily obtained result of COS kernel to get the recurrence.
The function \( g \) is obtained based on \( \exp(x) \geq 1 + x \):
\[
g(\cos(\frac{2\pi r}{p})) = 1 - \frac{1}{\ell^2} + \frac{1}{\ell^2} \cos(\frac{2\pi r}{p}).
\]

The bound of \( \mathbb{E}[Z_n] \) is recursively computed from \( \mathbb{E}[Z_{n-1}] \):
\[
\mathbb{E}[Z_n] \leq h(\mathbb{E}[Z_{n-1}]),
\]
where
\[
h(\mathbb{E}[Z_{n-1}]) = \frac{2\alpha^2}{\beta^2} \left( 1 - 4F_1 \left( \frac{m}{2}, 1, \frac{2\alpha^2}{p^2} \mathbb{E}[Z_{n-1}] \right) \right).
\]

## C Spectral mixture kernel

We consider the case the spectral mixture kernel has one-dimensional inputs and one mixture. We rewrite the kernel function as:
\[
\exp(-2\pi^2 \sigma^2 r^2) \cos(2\pi \mu r) = \frac{1}{2} \left\{ \exp(-2\pi^2 \sigma^2 r^2 + 2\pi \mu r) + \exp(-2\pi^2 \sigma^2 r^2 - 2\pi \mu r) \right\}
\]
\[
= \frac{1}{2} \exp\left( -\frac{\mu^2}{2\sigma^2} \right) \left\{ \exp\left( -2\pi^2 \sigma^2 (r - \frac{i\mu}{2\pi \sigma^2})^2 \right) + \exp\left( -2\pi^2 \sigma^2 (r + \frac{i\mu}{2\pi \sigma^2})^2 \right) \right\}.
\]

This leads to our change in variables in the main text where we denote
\[
w^2 = \exp(-\frac{\mu^2}{2\sigma^2}), \quad u^2 = 2\pi^2 \sigma^2, \quad u = \frac{i\mu}{2\pi \sigma^2}.
\]

Because \( \sqrt{Z_{n-1} \pm \mu/(2\pi \sigma^2)} \) is distributed according to a non-central Chi-square distribution with degree of freedom 1 and the noncentrality parameter \( \lambda = \mu^2/(4\pi^2 \sigma^4 s_{n-1}) \). The moment-generating function is
\[
M_{X^2}(t) = \mathbb{E} \left[ \exp \left( t \sqrt{Z_{n-1} \pm \mu/(2\pi \sigma^2)} \right) \right] = (1 - 2t)^{-1/2} \exp\left( \frac{\lambda t}{1 - 2t} \right).
\]

Choosing \( t = -2\pi^2 \sigma^2 s_{n-1} \), we have
\[
\mathbb{E} \left[ \exp \left( -2\pi^2 \sigma^2 (\sqrt{Z_{n-1}} \pm \frac{i\mu}{2\pi \sigma^2})^2 \right) \right] = (1 + 4\pi^2 \sigma^2 s_{n-1})^{-1/2} \exp\left( \frac{\mu^2}{2\pi \sigma^2} \right).
\]

We can obtain the recurrence relation as
\[
u_n = 2 \left\{ 1 - \exp\left( -\frac{\mu^2}{2\sigma^2} \right) \exp\left( \frac{\mu^2}{2\pi \sigma^2} \right) \right\} (1 + 4\pi^2 \sigma^2 s_{n-1})^{-1/2}
\]
\[
= 2 \left\{ 1 - \exp\left( -\frac{2\pi^2 \mu^2 s_{n-1}}{1 + 4\pi^2 \sigma^2 s_{n-1}} \right) \right\} (1 + 4\pi^2 \sigma^2 s_{n-1})^{-1/2}.
\]

In the case of high-dimensional DGPs, the SM kernel takes \( m \)-dimensional inputs. Because all dimensions are independent, we can obtain the expectation rely on the probabilistic independence between input dimensions to obtain the expectation as the product of the expectation in each dimension. Hence, we can have the recurrence in the form:
\[
u_n = 2m \left\{ 1 - \exp\left( -\frac{2m\pi^2 \mu^2 s_{n-1}}{1 + 4\pi^2 \sigma^2 s_{n-1}} \right) \right\} (1 + 4\pi^2 \sigma^2 s_{n-1})^{-m/2}.
\]

Note that we assume all dimensions share the same parameter \( \sigma^2 \) and \( \mu \).

## D The recurrence relation for the case of rational quadratic kernel

Now, we study the rational quadratic (RQ) kernel. This kernel is obtained from the SE kernel by marginalizing the inverse lengthscale of SE kernel \cite{Rasmussen2005}:
\[
\text{RQ}(x, x') = \left( 1 + \|x - x'\|^2 / (2\alpha \ell^2) \right)^{-\alpha}.
\]
We use the power series expansion $(1 + x)^{-\alpha} = \sum_{k=0}^{\infty} (-\alpha)^k x^k$ for this kernel

$$E[Z_n] = 2\sigma^2 - 2\sigma^2 \sum_{k=0}^{\infty} (-\alpha)^k \frac{E[Z_{n-1}] f_{n-2}}{(2\alpha \ell^2)^k}.$$  

Next, we use the high-order moment of Chi-squared distribution. As $Z_{n-1} f_{n-2} \sim \chi^2_m$, it is known that $E[Z_{n-1} f_{n-2}] = 2k \frac{\Gamma(k+m/2)}{\Gamma(m/2)}$. Then, we can obtain the corresponding recurrence relation as

$$E\left[ (1 + \frac{Z_{n-1}}{2\alpha \ell^2})^{-\alpha} | f_{n-2} \right] = \sum_{k=0}^{\infty} (-\alpha)^k \frac{E[Z_{n-1}] f_{n-2}}{(2\alpha \ell^2)^k}$$

(use high-order moment of Chi-squared)

$$= \sum_{k=0}^{\infty} \frac{(-1)^k \alpha^k \Gamma(k+m/2)}{k!} \frac{\Gamma(2\alpha \ell^2)}{(2\alpha \ell^2)^k} E[Z_{n-1} f_{n-2}]$$

(by a property of rising factorial)

$$= 2F_0(\alpha; m/2; -E[Z_{n-1} f_{n-2}])$$

(by definition of hypergeometric function)

Consequently, we obtain the recurrence between layers as

$$u_n = 2m(1 - 2F_0(\alpha; m/2; -u_{n-1} \alpha \ell^2)),$$

where $2F_0(\cdot; \cdot; \cdot)$ is one of the hypergeometric functions (see Definition in Appendix A.2). This $2F_0(\cdot; \cdot; \cdot)$ function has a close connection to the exponential integral function $Ei(x) = \int_{-x}^{+\infty} \frac{e^t}{t} dt$. This is related to the way of constructing the RQ kernel from SE kernel.

### E More on bifurcation plots

Figure 13 shows the bifurcation plots of SE kernel in high-dimensional cases ($m = 2, 3$).

Figure 14 shows the bifurcation plots of PER kernel.

Figure 15 shows the contour plots of RQ kernel for two cases of $\alpha$, indicating that changing $\alpha$ does not affect the condition to escape the pathology.

### F More on experiment

#### F.1 High-dimensional DGPs with SE

In this experiment, we track the RMSDs at layer 100 with different settings of dimension (number of units) at a layer, $m$, and the ratio $\ell^2/\sigma^2$. Figure 16 shows the values of RMSDs, illustrating that choosing $m > \ell^2/\sigma^2$ will help DGP overcome the pathology.

#### F.2 Correctness of recurrence relations

Figure 17 and 18 contain the comparisons between the true $E[Z_n]$ versus its empirical estimation.
Figure 14: Bifurcation plot of the recurrence of periodic kernel for $m = 1$. First row: From left to right, $\ell$ is varied. Second row: $\sigma^2$ is varied.

Figure 15: RQ: Contour plots of $E[Z_n]$ at $n = 300$. The two contour plots share the same zero-value level. So that $\alpha$ does not decide the condition overcome the pathology.

F.3 Monitoring DGP for Boston housing and diabetes data set

The Boston housing data set concerns housing values in suburbs of Boston, consisting of 506 instances with 14 attributes. The diabetes data set (Efron et al. 2004) measuring disease progression contains 442 instances with 10 attributes. Figure 19 contains the results from the Boston housing data set with standard zero-mean DGPs. Figure 20 contains the results from the Boston housing data set with constrained zero-mean DGPs where $c_0 = 0.2$. Figure 21 contains the results from the diabetes data set with standard zero-mean DGPs. Figure 22 contains the results from the diabetes data set with constrained zero-mean DGPs where $c_0 = 0.1$. 
Figure 16: Plot of RMSDs at layer 100 as the dimension $m$ and $\ell^2/\sigma^2$ change.

Figure 17: High-dimensional SE: $E[Z_n]$ computed from recurrence vs. empirical estimation of $E[Z_n]$.

Figure 18: SM kernel: $E[Z_n]$ computed from recurrence vs. empirical estimation of $E[Z_n]$.

Figure 19: Standard zero-mean DGPs: Results of Boston housing data set
Figure 20: Constrained DGPs Results of Boston housing data set

Figure 21: Standard zero-mean DGPs: Results of diabetes data set

Figure 22: Constrained DGPs: Results of diabetes data set