# Non-degenerate Priors for Arbitrarily Deep Networks

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## Abstract

A good latent representation captures all the relevant degrees of freedom of the manifold on which the data live. We show, for typical deep architectures, that as the number of layers increase, the representational capacity of the model tends to capture fewer degrees of freedom. In the limit, deep representations only retain a single degree of freedom locally. In addition, gradient-based learning becomes intractable. We propose two alternate priors on network structure which do not suffer from these pathologies: First, simply connecting the input layer to every other layer. Second, a more general prior of computation graphs based on the Aldous-Hoover graph representation. We also analyze kernels obtained by taking arbitrarily-many feature compositions.

## 1 Introduction

Deep networks have become an important tool for machine learning [cite]. However, training these models are difficult, Many arguments have been made for the need for deep architectures [cite Bengio]. However, it is hard to know what effect the deepness of an architecture has. Also, the weights don't necessarily move that much from their initialization.

### 1.1 Desirable properties of latent representations

Rifai et al. [2011a] make the point that a good latent representation is one that remains invariant when moving in directions orthogonal to the manifold that the data lie on. Conversely, a good latent representation must also change in directions tangential to the data manifold - otherwise we are losing information about the data. Figure 1 demonstrates this idea.

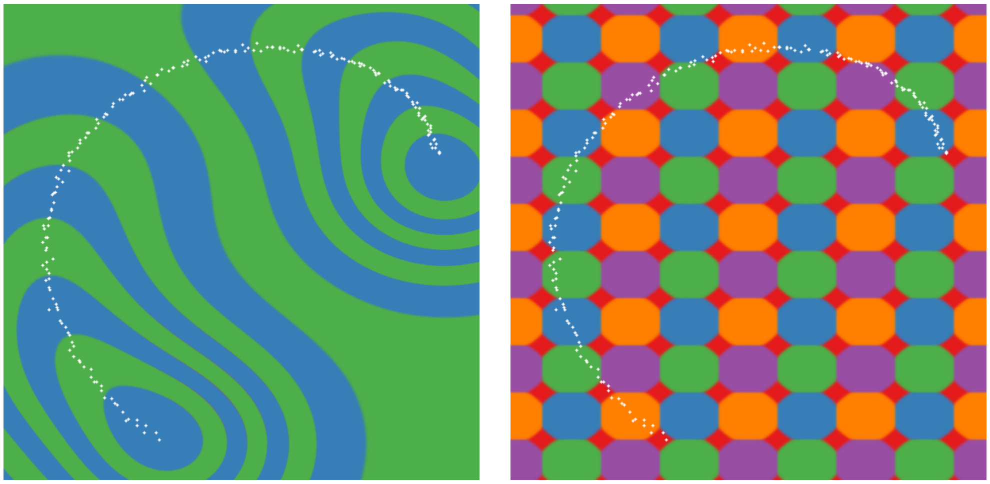
## 2 The Jacobian of Deep GPs

**Deep Gaussian Processes** We introduce a generative non-parametric model to address this problem. Our approach is based on the GP-LVM Lawrence [2004], Salzmann et al. [2008], Lawrence and Urtasun [2009], a flexible nonparametric density model. Deep Gaussian processes Damianou and Lawrence [2012].

**The derivatives of a function drawn from a GP prior with a product kernel are i.i.d. Normal** Because differentiation is a linear operator, the derivatives of a function drawn from a GP prior are also jointly Gaussian distributed, with covariance between derivatives w.r.t. different dimensions of $\mathbf{x}$ given by:

$$\operatorname{cov}\left(\frac{\partial f(\mathbf{x})}{\partial x_{d_1}}, \frac{\partial f(\mathbf{x})}{\partial x_{d_2}}\right) = \frac{\partial^2 k(\mathbf{x}, \mathbf{x}'))}{\partial x_{d_1} \partial x'_{d_2}}\Bigg|_{\mathbf{x}=\mathbf{x}'} \tag{1}$$

Solak et al. [2003]



A naive latent representation — A good latent representation

Figure 1: Comparing different latent representations of data on a manifold. A good latent representation is invariant in directions orthogonal to the data manifold, but changes along the manifold.

If our kernel is a product over individual dimensions $k(\mathbf{x}, \mathbf{x}') = \prod_d^D k_d(x_d, x'_d)$, as in the case of the isotropic squared-exp kernel, then the diagonal covariances are given by $\frac{\sigma_o^2}{\ell^2}$, and the off-diagonal entries are zero. This means that elements are independent and identically distributed.

**The elements of the Jacobian of a GP with an isotropic SE kernel are i.i.d. Gaussians** The Jacobian of the $\ell^{\text{th}}$function is:

$$J^{\ell}_{\mathbf{x}\to\mathbf{y}}(\mathbf{x}) = \begin{bmatrix} \frac{\partial f_1^{\ell}(\mathbf{x})}{\partial x_1} & \cdots & \frac{\partial f_1^{\ell}(\mathbf{x})}{\partial x_D} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_D^{\ell}(\mathbf{x})}{\partial x_1} & \cdots & \frac{\partial f_D^{\ell}(\mathbf{x})}{\partial x_D} \end{bmatrix} \tag{2}$$

Because we've assumed that the GP on each output dimension $f_d(\mathbf{x}) \sim \mathcal{GP}$ is independent, it follows that for a given $\mathbf{x}$, each row of $J_{\mathbf{x}\to\mathbf{y}}(\mathbf{x})$ is independent. Above, we showed that the elements of each row are independent. This means that each entry in the Jacobian of a GP-distributed transformation is i.i.d. Normal.

**The Jacobian of a deep GP is a product of random normal matrices** By the multivariate chain rule, the derivative (Jacobian) of any compositions of functions is simply the product of the Jacobians of each function. and the Jacobian of the composed (deep) function is:

$$J^{1:L}(x) = \prod_{\ell=1}^{L} J^{L}(x) \tag{3}$$

Combining these results, we can analyze the representational properties of a deep Gaussian process by simply examining the properties of products of i.i.d. Gaussian matrices.

We follow Rifai et al. [2011b] in characterizing the representational properties of a function by the singular value spectrum of the Jacobian. Figure 2 shows the spectrum for deep GPs of different depths. As the net gets deeper, the largest singular value dominates. This implies that there is only one effective degree of freedom in representation being computed.

Figure 3 demonstrates a related pathology that arises when composing functions to produce a deep latent-variable model. The density in observed space eventually becomes locally concentrated onto one-dimensional manifolds, or *filaments*.

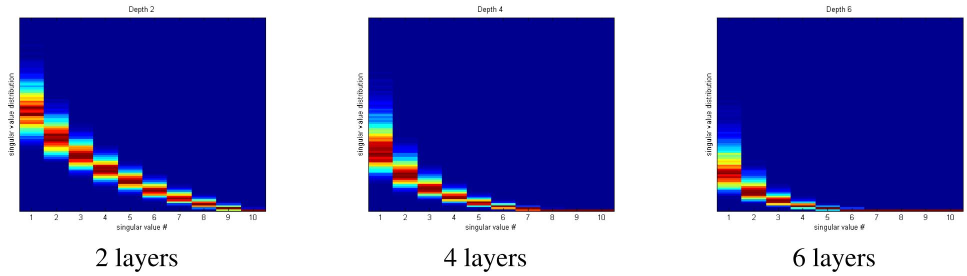



Figure 2: Singular value spectrum of the Jacobian of a deep GP. As the net gets deeper, the largest singular value dominates. This implies that there is only one effective degree of freedom in representation being computed.

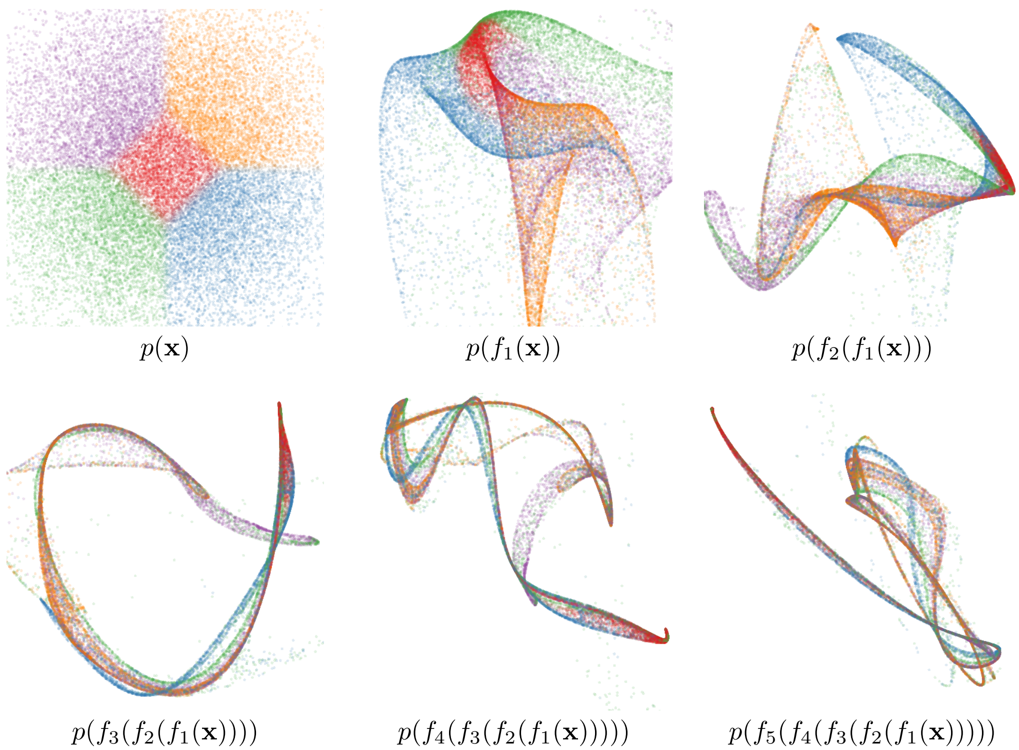



Figure 3: Draws from a deep GP. A distribution is warped by successive functions drawn from a GP prior. As the number of layers increases, the density exhibits a sort of filamentation.

To visualize this pathology in another way, figure 4 illustrates the value computed at each point in the input space, after successive warpings. After 40 warpings, we can see that locally, there is usually only one direction that one can move in $\mathbf{x}$-space in order to change the value of the function.

### 2.1 Formalizing the pathology

### 2.2 Fixing the pathology

Follow a suggestion in Neal [1995], we can fix the pathologies exhibited in figures 3 and 4 by simply making each layer of computation depend not only on the output of the previous layer, but also on the original input $\mathbf{x}$. Draws from the resulting priors are shown in figures 5 and 6.

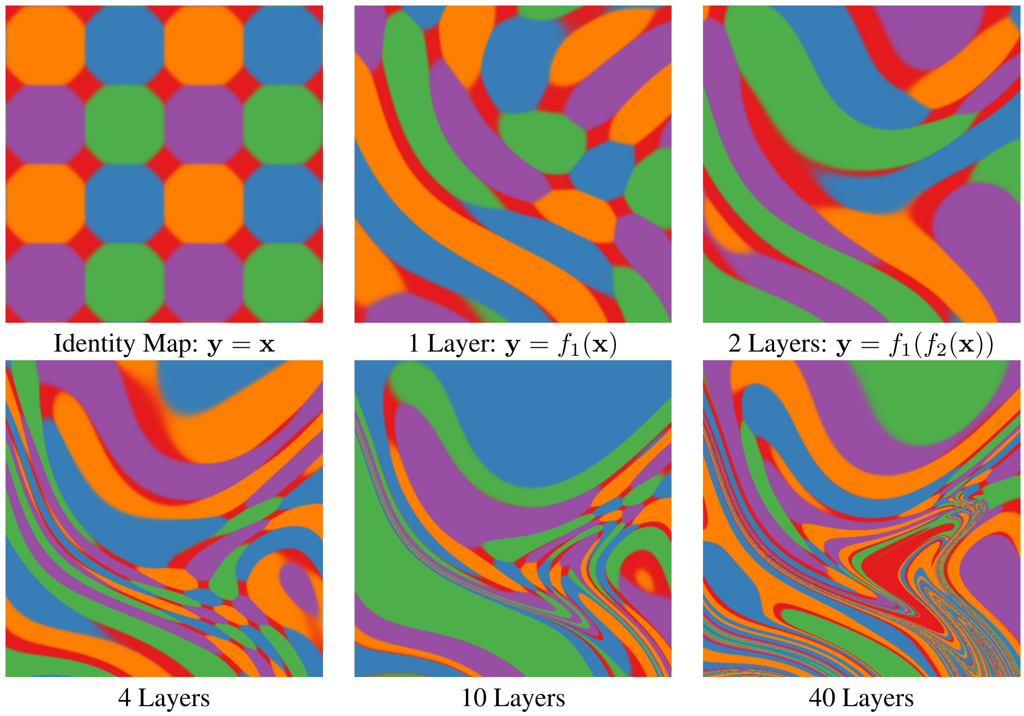



Figure 4: Feature Mapping of a deep GP. Shown here are the colors corresponding to the location $\mathbf{y} = f(\mathbf{x})$ that each point is mapped to after being warped by a deep GP. This figure can be seen as the inverse of figure 3. Just as the densities in 3 became locally one-dimensional, there is locally only one direction that one can move $\mathbf{x}$ in to change $\mathbf{y}$.

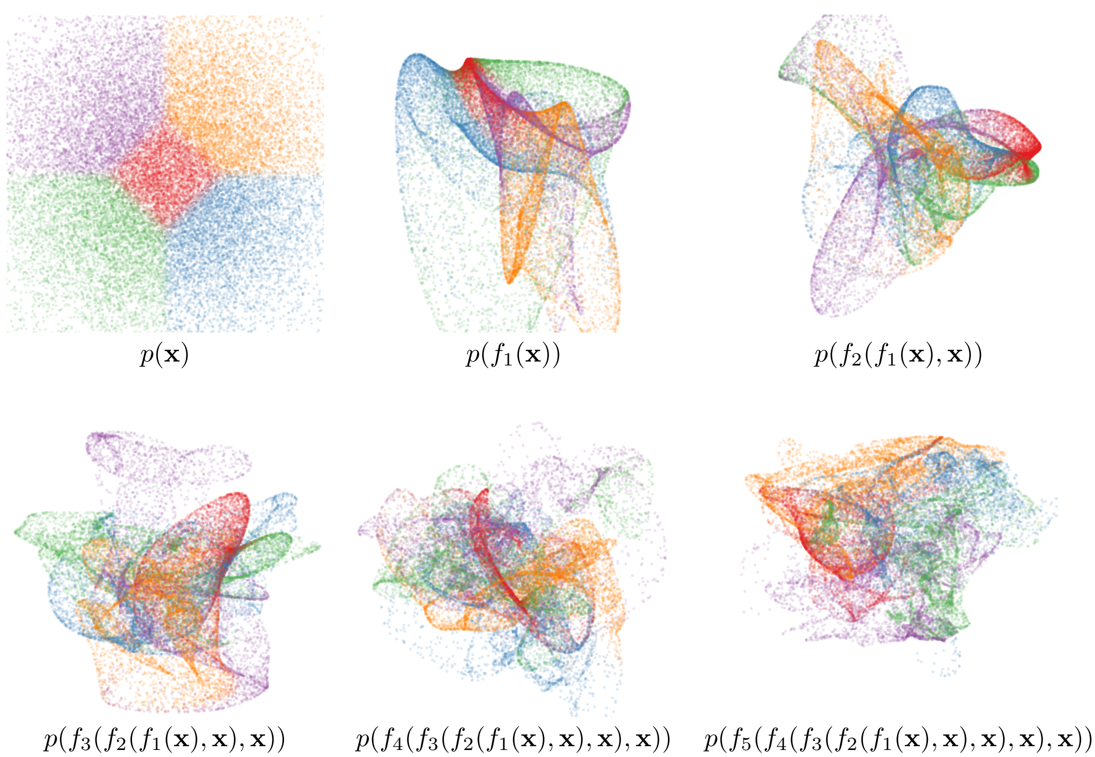



Figure 5: Draws from a deep GP, with each layer connected to the input $\mathbf{x}$. By always depending on the original input, the density becomes more complex without concentrating along filaments.

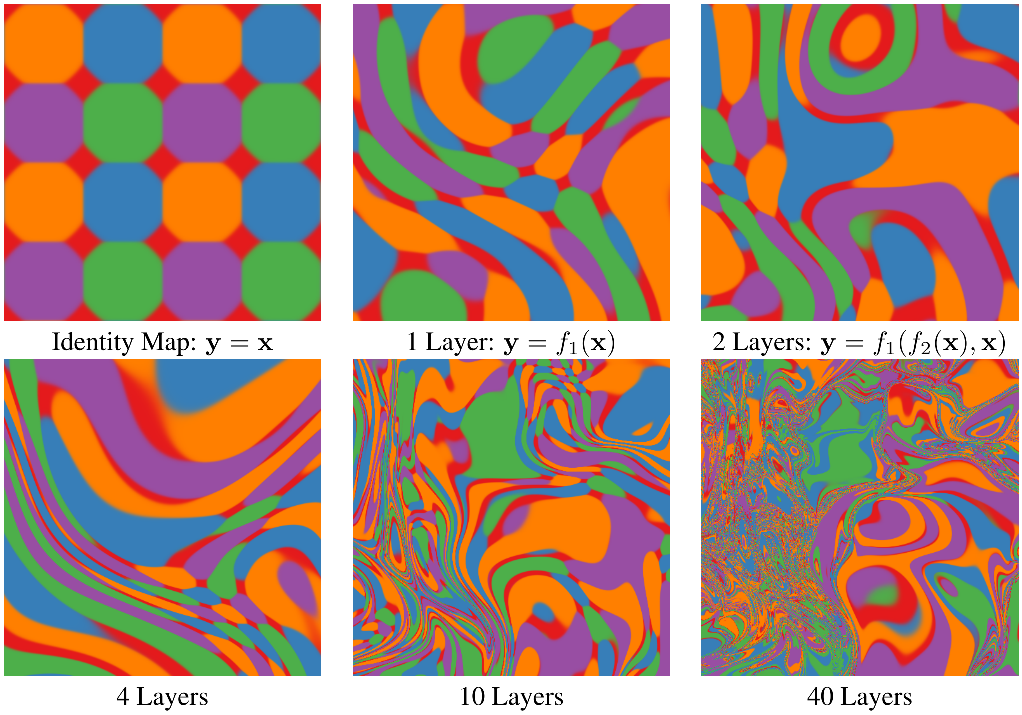



Figure 6: Feature Mapping of a deep GP with each layer connected to the input $\mathbf{x}$. Just as the densities in 5 became remain locally two-dimensional even after many transformations, in this mapping there are locally usually two directions that one can move $\mathbf{x}$ in to change $\mathbf{y}$.

## 3 Arbitarily Deep Kernels

These types of kernels were originally investigated by Cho [2012]. In this section, we take the infinite limits of these compositions, and propose a new variant.

One can derive a Gaussian process as a neural network: $f(x) = \alpha^T \Phi(x) = \sum_{i=i}^{K} \alpha_i \phi_i(x)$. We can consider applying the feature transform $\Phi(\cdot)$ to the features themselves: $\Phi_2 = \Phi(\Phi(\mathbf{x}))$,

In this section, we derive a kernel which corresponds to arbitrarily many compositions of the feature vectors corresponding to the squared-exp kernel:

$$k_2(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2}||\Phi(\mathbf{x}) - \Phi(\mathbf{x}')||_2^2\right) \tag{4}$$

$$k_2(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2}\sum_i \left[\phi_i(\mathbf{x}) - \phi_i(\mathbf{x}')\right]^2\right) \tag{5}$$

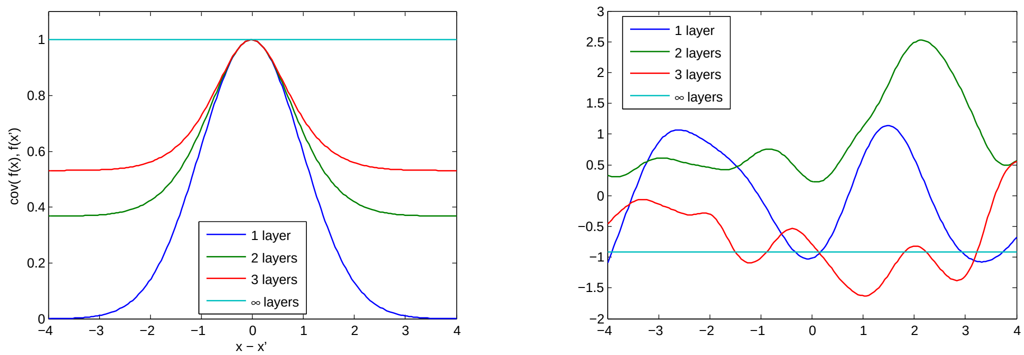
$$k_2(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2}\sum_i \left[\phi_i(\mathbf{x})^2 - 2\phi_i(\mathbf{x})\phi_i(\mathbf{x}') + \phi_i(\mathbf{x}')^2\right]\right) \tag{6}$$

$$k_2(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2}\left[\sum_i \phi_i(\mathbf{x})^2 - 2\sum_i \phi_i(\mathbf{x})\phi_i(\mathbf{x}') + \sum_i \phi_i(\mathbf{x}')^2\right]\right) \tag{7}$$

$$k_2(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2}\left[k_1(\mathbf{x}, \mathbf{x}) - 2k_1(\mathbf{x}, \mathbf{x}') + k_1(\mathbf{x}', \mathbf{x}')\right]\right) \tag{8}$$

$$k_2(\mathbf{x}, \mathbf{x}') = \exp\left(k_1(\mathbf{x}, \mathbf{x}') - 1\right) \tag{9}$$

Thus if $k_1(x, y) = e^{-||x-y||2}$, then the two-layer kernel is simply $k_2(x, y) = e^{k_1(x,y)-1}$. This formula is true for every layer: $k_{n+1}(x, y) = e^{k_n(x,y)-1}$. Note that nothing in this derivation depends on details of $k_1$, except that $k_1(\mathbf{x}, \mathbf{x}) = 1$. Because this is true for $k_2$ as well, this recursion




Kernel derived from iterated feature transforms | Draws from the corresponding kernel

Figure 7: A degenerate kernel produced by repeatedly applying a feature transform.

holds in general, and we have that $k_{n+1}(x, y) = e^{k_n(x,y)-1}$. In the infinite limit, this recursion converges to $k(x, y) = 1$ for all inputs.

Figure 7 shows this kernel at different depths, including the degenerate limit. One interpretation of why repeated feature transforms lead to this degenerate prior is that each layer can only lose information about the previous set of features. In the limit, the transformed features contain no information about the original input $\mathbf{x}$. Since the function doesn't depend on its input, it must be the same everywhere.

### 3.1 Fixing the deep kernel

Follow a suggestion from Radford Neal's thesis Neal [1995], we connect the inputs to each layer of features. We do this simply by augmenting the feature vector $\Phi_n(\mathbf{x})$ with the extra features $\mathbf{x}$ at every layer:

$$k_{n+1}(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2}\left|\left|\begin{bmatrix}\Phi_n(\mathbf{x})\\ \mathbf{x}\end{bmatrix} - \begin{bmatrix}\Phi_n(\mathbf{x}')\\ \mathbf{x}'\end{bmatrix}\right|\right|_2^2\right) \tag{10}$$

$$k_{n+1}(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2}\sum_i \left[\phi_i(\mathbf{x}) - \phi_i(\mathbf{x}')\right]^2 - \frac{1}{2}||\mathbf{x} - \mathbf{x}'||_2^2\right) \tag{11}$$

$$k_{n+1}(\mathbf{x}, \mathbf{x}') = \exp\left(k_1(\mathbf{x}, \mathbf{x}') - 1 - \frac{1}{2}||\mathbf{x} - \mathbf{x}'||_2^2\right) \tag{12}$$

Thus, this kernel satisfies the recurrence $k - \log(k) = 1 + \frac{1}{2}||\mathbf{x} - \mathbf{x}'||_2^2$.

**Properties of this kernel** The solution to this recurrence has no closed form, but it is continuous and differentiable everywhere except at $\mathbf{x} = \mathbf{x}'$.

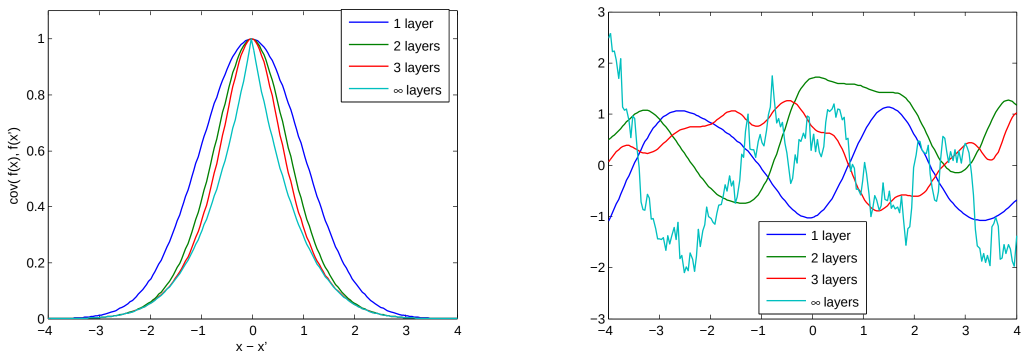
Conjectures:

- Samples from a GP with this prior are not differentiable.
- This kernel has smaller covariance than the squared-exp everywhere except at $\mathbf{x} = \mathbf{x}'$.
- Samples from this kernel are fractal.

## 4 Related Work

### 4.1 A Survey of deep architectures

**Deep Density Networks**




Kernel derived from iterated feature transforms with all layers connected to the input

Draws from the corresponding kernel

Figure 8: A non-degenerate version of the infinitely deep feature transform kernel. By connecting the inputs $\mathbf{x}$ to each layer, the function can still depend on its input even after arbitrarily many layers of computation.

**Bayesian Deep Networks** Adams et al. [2010] developed a prior on finite but unboundedly deep neural networks, each layer having a finite but unbounded number of hidden units.

**Sum-product networks** introducted by Poon and Domingos [2011].

**Feature Composition Kernels** Cho [2012] developed kernels of the type discussed in section 3, and investigated them experimentally.

**Recurrent Neural Networks**

**Dynamical Systems** These architectures are all constructed in a stacked manner, with connections only between adjacent layers.

[Warping a 1d uniform distribution]

### 4.2 Related Analyses

Montavon et al. [2010] note that performance of a MLP degrades as the number of layers with random weights increases.

## 5 Discussion

**To what extent are these pathologies present in nets being used today?** In simulations, we found that for deep functions with a fixed latent dimension $D$, that the singular value spectrum remained relatively flat for hundreds of layers as long as $D > 100$.

## 6 Conclusions

**Deep neural networks and deep Gaussian processes are analyzable using random matrix theory.** After proving that the Jacobian is an i.i.d. Gaussian matrix, many other forms of

**If you want to use very deep nets, you won't be able to do so if you initialize/regularize all your weights independently** We might want to think about different ways of

**If you initialize independently, the density becomes fractal** Points close in $x$-space can be very far in $y$-space, and vice versa.

**A spikey eigenspecturm will lead to saturation** Maybe we should initialize differently in order to avoid such saturation, like Martens' sparse initialization: `http://www.cs.toronto.edu/~jmartens/docs/Deep_HessianFree.pdf`


### Acknowledgments

We would like to thank Andrew McHutchon, Neil Lawrence, Josh Tenenbaum, Andreas Diamanadou, James Lloyd, and Mark van der Wilk for helpful discussions.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