Avoiding Pathologies in Very Deep Networks

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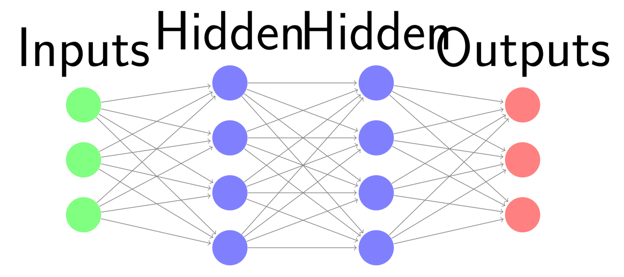
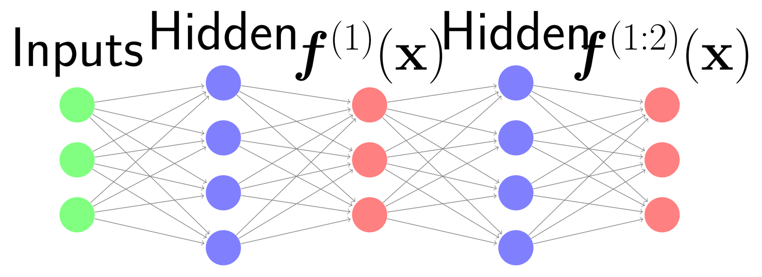
Abstract

- We analyze deep Gaussian processes, a type of infinitely-wide, deep neural net.
- We study distributions of deep GPs and a find a pathology, then show a simple fix.
- We also derive kernels corresponding to infinitely deep nets.

Deep Nets and Deep Gaussian processes



Two-hidden layer MLP



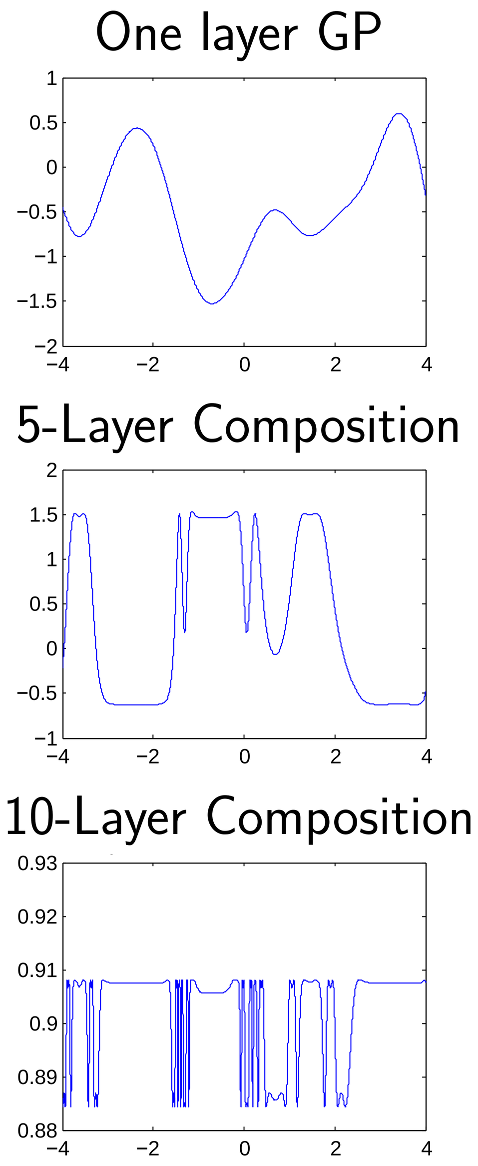
Two-layer GP: $\mathbf{y} = \boldsymbol{f}^{(2)}(\boldsymbol{f}^{(1)}(\mathbf{x}))$

Deep GPs are priors on compositions of functions:

$$\boldsymbol{f}^{(1:L)}(\mathbf{x}) = \boldsymbol{f}^{(L)}(\boldsymbol{f}^{(L-1)}(\ldots \boldsymbol{f}^{(2)}(\boldsymbol{f}^{(1)}(\mathbf{x}))\ldots))$$

Each $f^{(\ell)} \overset{\text{ind}}{\sim} \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}'))$. Can be viewed as either

1. MLPs with nonparametric activation functions
2. MLPs with infintely-many parametric hidden nodes

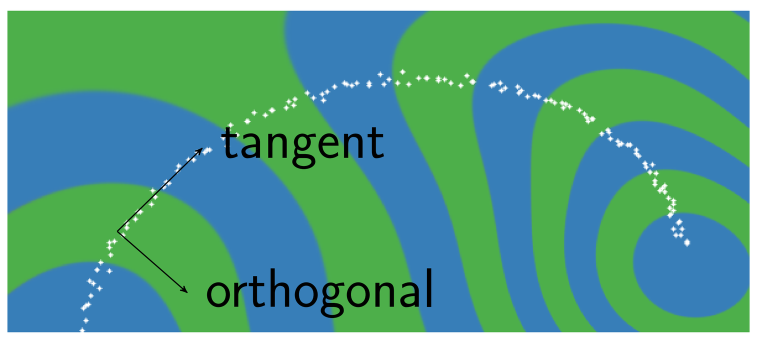


One-dimensional asymptotics

- Can examine deep GPs through distribution of derivatives.
- Size of derivative has log-normal limiting distribution.
- Derivative becomes almost zero everywhere, with large jumps.

Degrees of Freedom of a Neural Network

- Neural net computes a representation $\mathbf{y} = f(\mathbf{x})$ of data $\mathbf{x}$.
- $\mathbf{y}$ needs to capture relevant degrees of freedom of $\mathbf{x}$.

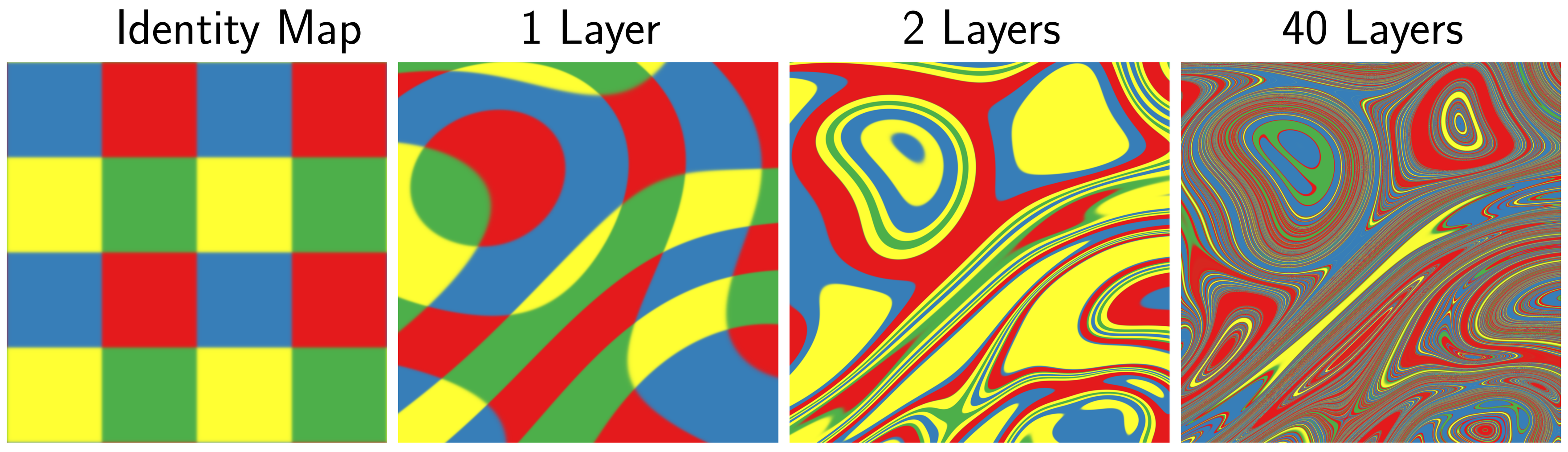


Contours show $f(\mathbf{x})$, a noise-tolerant representation of a data manifold (white)

- (Rifai et. al., 2011) argue that a good latent representation is invariant in directions orthogonal to the manifold on which the data lie.
- Conversely, a good latent representation must also change in directions tangent to the data manifold, in order to preserve relevant information.

Random deep nets have few degrees of freedom

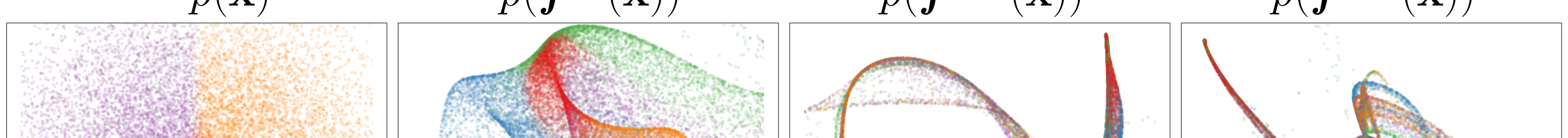
We visualize random mappings to show properties of this prior on functions:



$\mathbf{y} = \mathbf{x}$ $\quad \mathbf{y} = \boldsymbol{f}^{(1)}(\mathbf{x})$ $\quad \mathbf{y} = \boldsymbol{f}^{(1:2)}(\mathbf{x})$ $\quad \mathbf{y} = \boldsymbol{f}^{(1:40)}(\mathbf{x})$

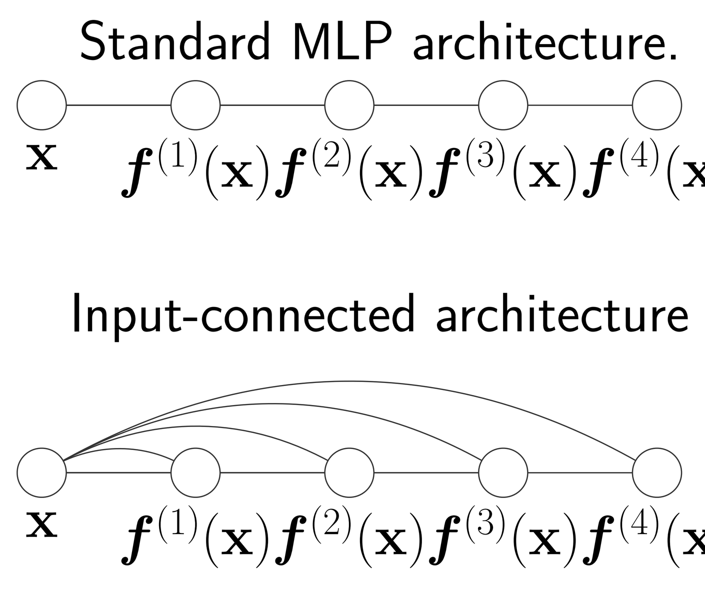
As depth increases, there is usually only one direction we can move $\mathbf{x}$ to change $\mathbf{y}$.

We also visualize a distribution warped by successive functions drawn from a GP prior:

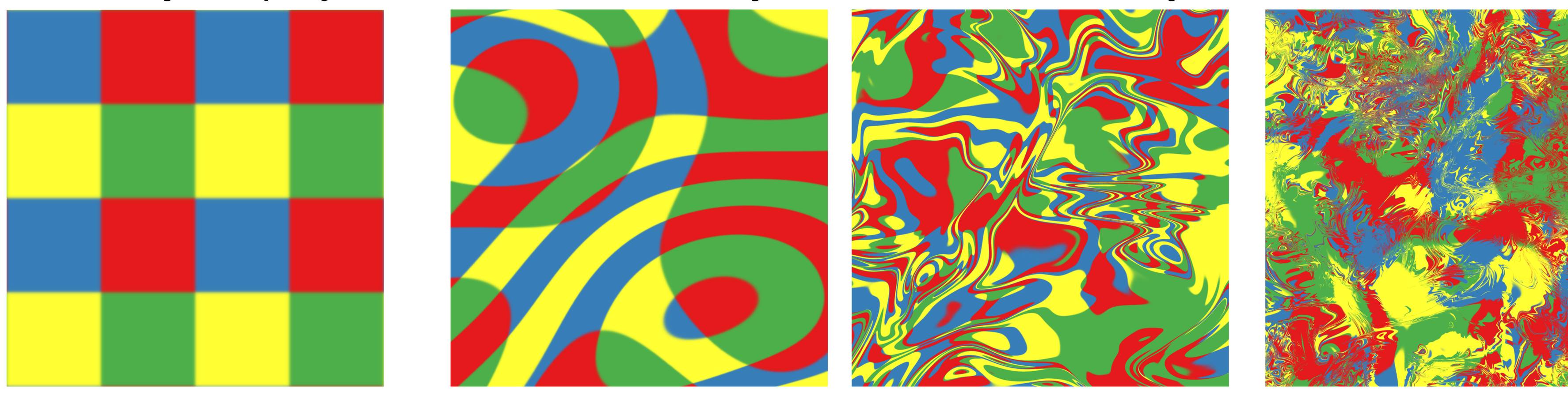


Fixing the pathology

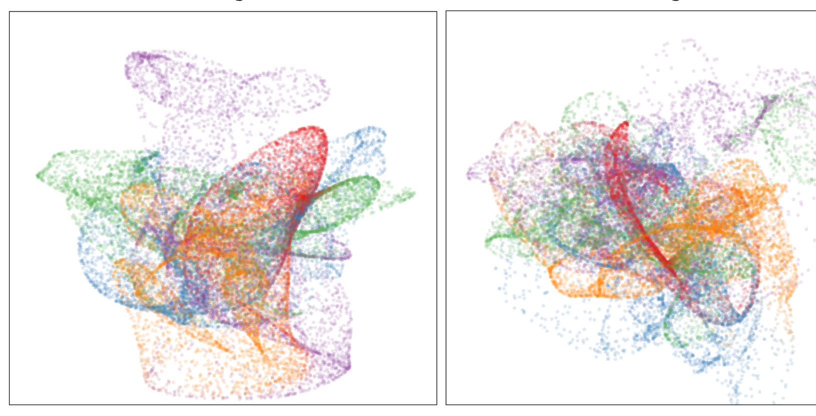
- Following a suggestion from (Neal, 1995), connect input to every layer:



- This fixes the problem: Locally there are usually D degrees of freedom, at any d

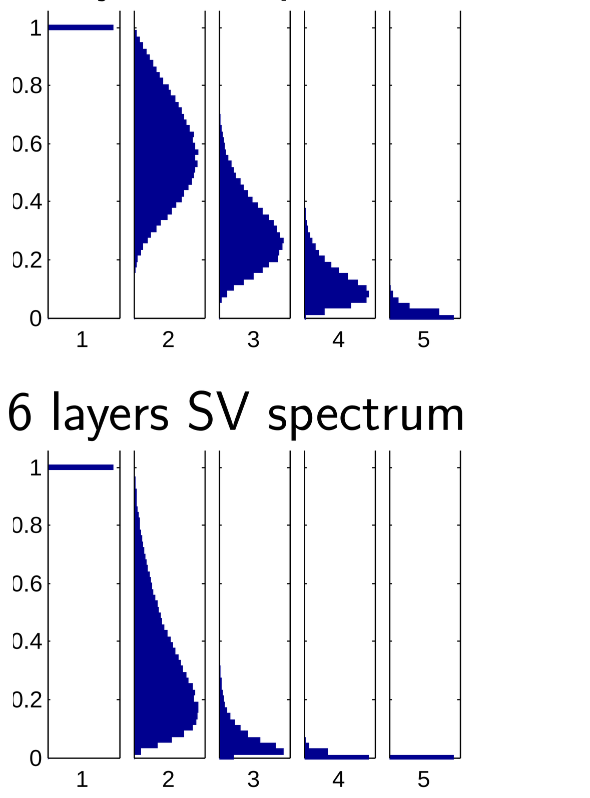


Pathology is also resolved in deep density models: Density does not concentrate along filaments when input connects to all layers.



Explaining the Pathology

- Jacobian of a deep GP is a product of independent Gaussian matrices.
- Singular values spectrum of Jacobian quantifies relative size of derivatives.
- As the net gets deeper, distribution of SVs becomes heavy-tailed, and the largest singular value dominates.
- Eventually, there is only one direction we can move $\mathbf{x}$, in order to change $\mathbf{y}$.



Infinitely Deep Kernels

- Can also analyze fixed deep feature mappings:
- (Cho, 2012) built kernels from multiple layers of feature mappings:
- If $k_1(\mathbf{x}, \mathbf{x}') = \Phi(\mathbf{x})^\mathsf{T}\Phi(\mathbf{x}')$, we can also build kernel $k_2(\mathbf{x}, \mathbf{x}') = k_2(\Phi(\mathbf{x}), \Phi(\mathbf{x}')) = \Phi(\Phi(\mathbf{x}))^\mathsf{T}\Phi(\Phi(\mathbf{x}'))$.
- For the squared-exp kernel, this composition operation has a closed form:

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

- This kernel satisfies $k_\infty - \log(k_\infty) = 1 + \frac{1}{2}||\mathbf{x} - \mathbf{x}'||_2^2$
- No closed form, but it is continuous and differentiable everywhere except at $\mathbf{x} = \mathbf{x}'$