Avoiding Pathologies in Very Deep Networks

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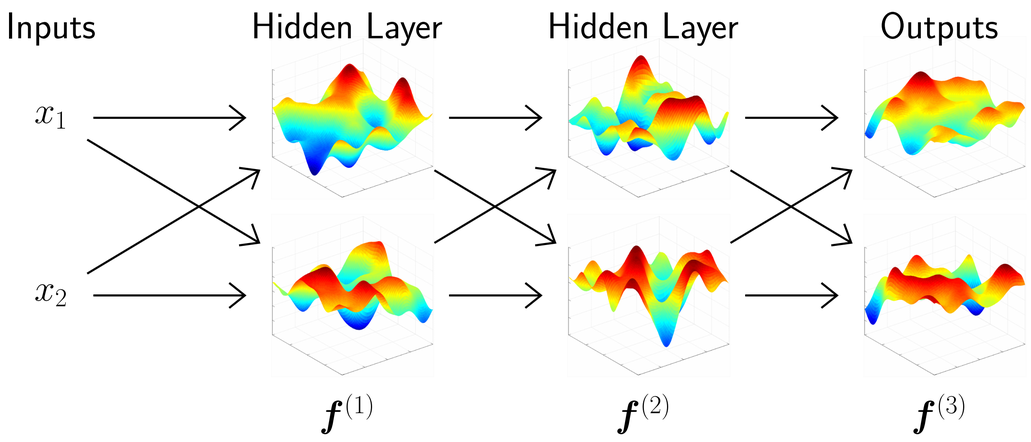
Let's Examine Priors on Deep Neural Networks

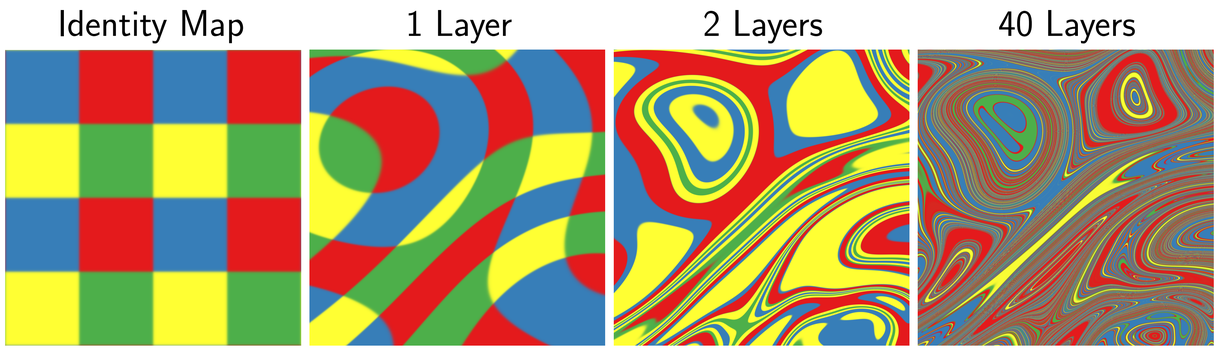


Deep GPs are compositions of functions, each $f^{(\ell)} \overset{\text{ind}}{\sim} \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}'))$.

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

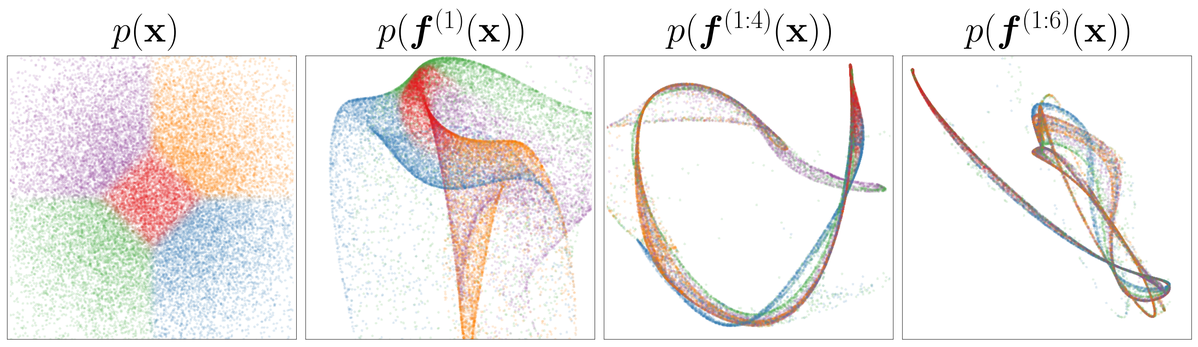
Random Deep Nets Capture Few Degrees of Freedom

Sampled mappings illustrate properties of this prior on functions:



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

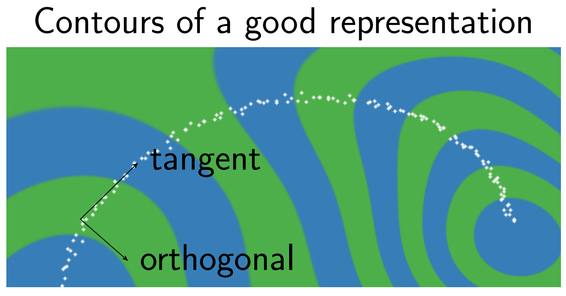
A distribution warped by successive functions drawn from a GP prior:



As depth increases, the density concentrates along one-dimensional filaments.

Good Representations Change Along All Tangents

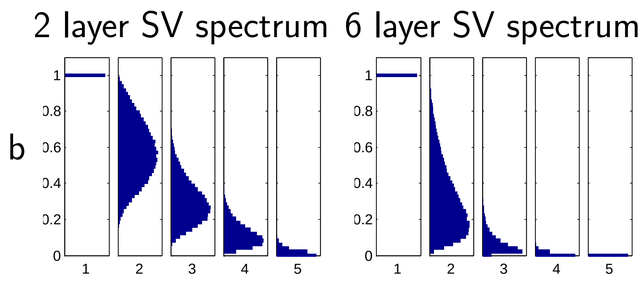
Contours of a good representation



- Representation $\mathbf{y} = \boldsymbol{f}(\mathbf{x})$ should capture relevant degrees of freedom of $\mathbf{x}$.
- Representation must change in directions tangent to the data manifold, to preserve information.

Explaining the Pathology

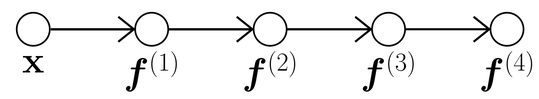
- Jacobian of a deep GP is a product of independent Gaussian matrices.
- Singular value spectrum shows relative size of derivatives.
- As net deepens, one direction has much larger derivative than others.



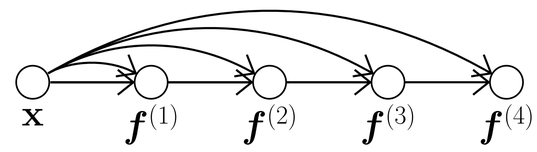
Fixing the pathology

- Following (Neal, 1995), we connect the input to every layer:

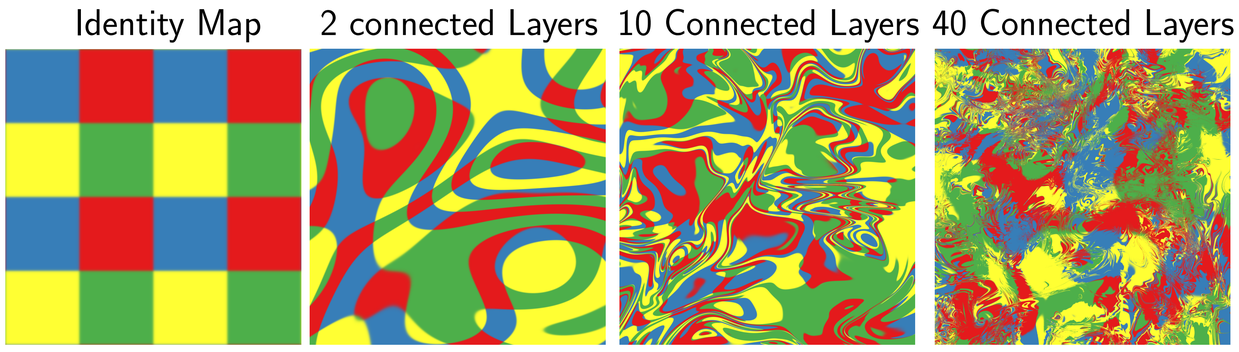
Standard deep net architecture



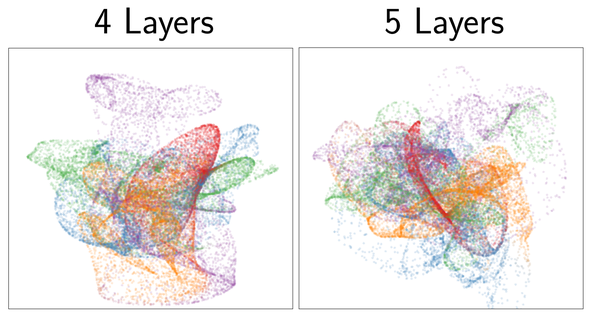
Input-connected architecture



- This fixes the problem: Locally up to D degrees of freedom, at any depth:



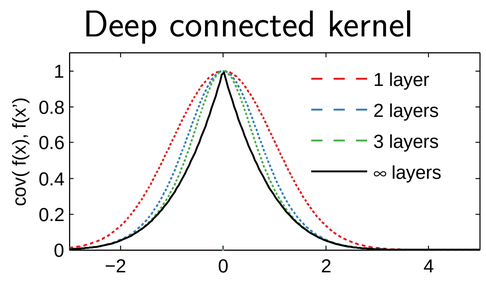
Pathology is also resolved in deep density models: Density does not concentrate along filaments when input connects to all layers.



Dropout in Gaussian Processes

Infinitely Deep Kernels

- If $k_1(\mathbf{x}, \mathbf{x}') = \mathbf{h}(\mathbf{x})^\mathsf{T}\mathbf{h}(\mathbf{x}')$,
  $k_2(\mathbf{x}, \mathbf{x}') = \mathbf{h}(\mathbf{h}(\mathbf{x}))^\mathsf{T}\mathbf{h}(\mathbf{h}(\mathbf{x}'))$.
- Recurrent limit for squared-exp kernel:
- $k_\infty - \log(k_\infty) = 1 + \frac{1}{2}||\mathbf{x} - \mathbf{x}'||_2^2$



Conclusions

- Random networks capture fewer degrees of freedom as they get deeper
- Connecting the input to each layer resolves this pathology
- Can build arbitrarily deep kernels

Code at `github.com/duvenaud/deep-limits`

Paper at `mlg.eng.cam.ac.uk/duvenaud/papers/verydeep.pdf`