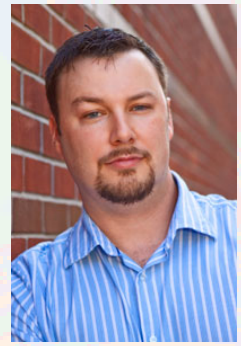
Avoiding Pathologies in Very Deep Networks



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Motivation 1: Deep Learning is Cool

- Don't you wish we were doing it?
- Zoubin (2011) "Do you guys ever wonder if this lab focuses too much on Gaussian processes? Like maybe we're going to miss the next big thing, like maybe, say, deep learning"
- But - GPs are just neural nets, we can make them deep!

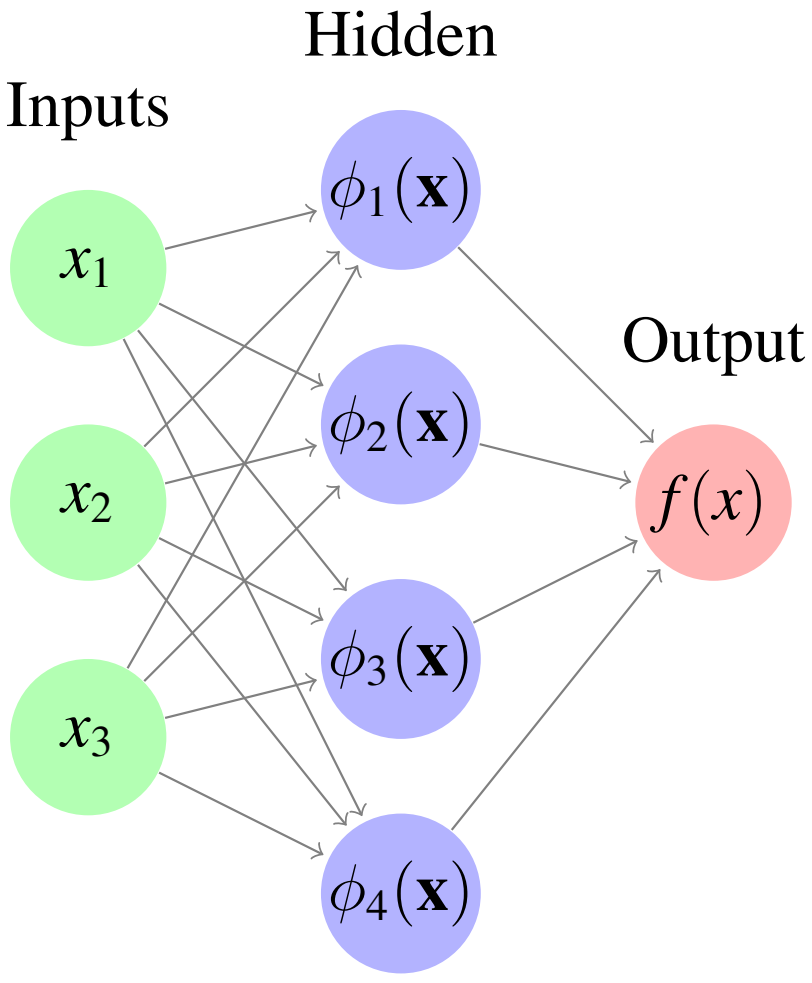
Motivation 2: Regularizing Nets

- Neural nets are getting larger
- How to regularize billions of parameters?
- Closely related to constructing priors
- Priors are easy to analyze - just sample from the prior and look and what sorts of things you get!
- Can we suggest new regularization schemes or network architectures?

OUTLINE

- Relation between GPs and neural nets
- Two ways to deepness:
  - Deep kernels
  - Deep GPs
- What kind of prior on functions do we want?
  - problems with lots of indepenent layers
  - a simple fix
- Dropout for GPs
  - Dropping out features
  - Dropping out inputs

GPs as Neural Nets



A weighted sum of features,

$$f(\mathbf{x}) = \frac{1}{K}\sum_{i=1}^{K} \alpha_i \phi_i(\mathbf{x})$$

with any weight distribution,

$$\mathbb{E}\left[\alpha_i\right] = 0, \quad \mathbb{V}\left[\alpha_i\right] = \sigma^2, \quad i.i.d.$$

by CLT, gives a GP as $K \to \infty$!

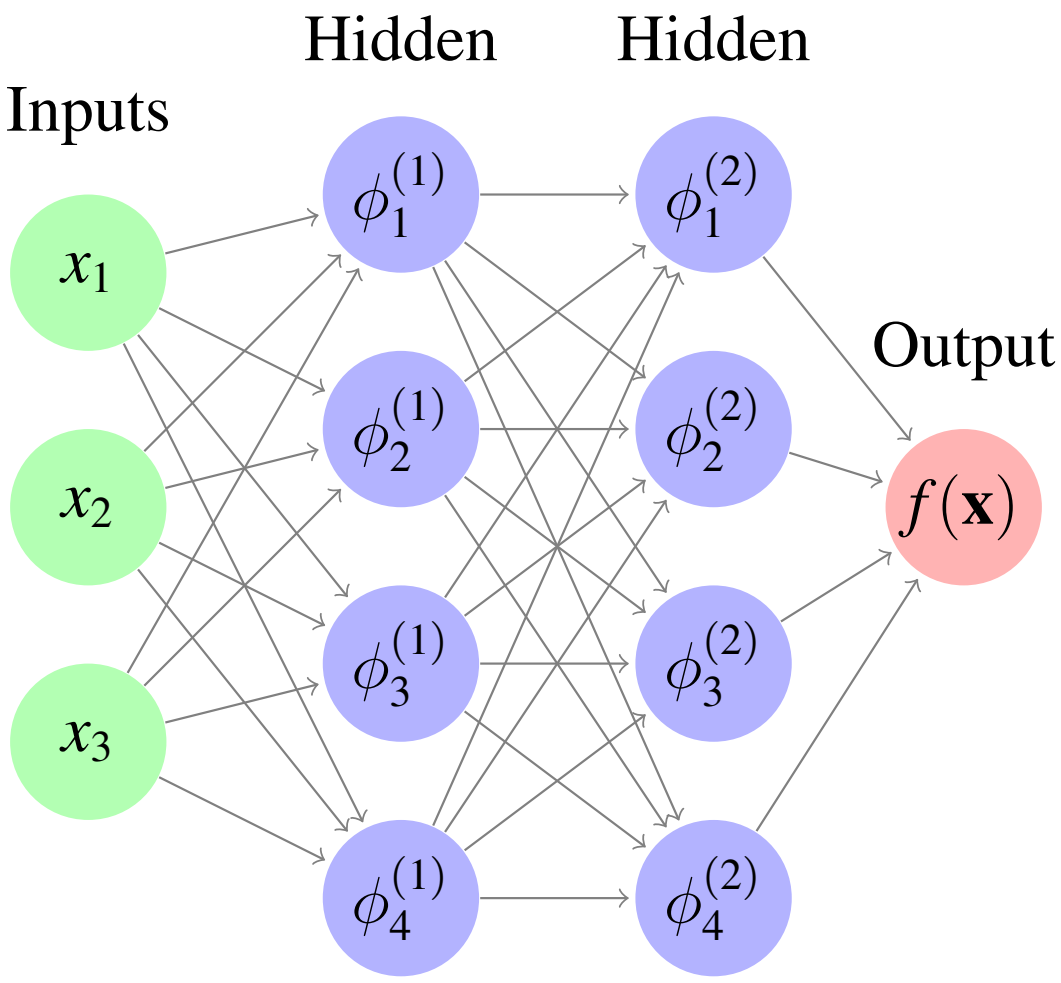
$$\mathrm{cov}\begin{bmatrix} f(\mathbf{x}) \\ f(\mathbf{x}') \end{bmatrix} \to \frac{\sigma^2}{K}\sum_{i=1}^{K} \phi_i(\mathbf{x})\phi_i(\mathbf{x}')$$

KERNEL LEARNING AS FEATURE LEARNING

- GPs have fixed features, integrate out feature weights.
- Mapping between kernels and features:
  $k(\mathbf{x}, \mathbf{x}') = \Phi(\mathbf{x})^\mathsf{T}\Phi(\mathbf{x}')$.
- Any PSD kernel can be written as inner product of features. (Mercer's Theorem)
- Kernel learning = feature learning

- What if we make the GP nueral network deep?

Deep nets, deep kernels



Now our model is:

$$f(\mathbf{x}) = \frac{1}{K}\sum_{i=1}^{K} \alpha_i \phi_i\left(\Phi^{(1)}(\mathbf{x})\right)$$
$$= \boldsymbol{\alpha}^\mathsf{T}\Phi^{(2)}\left(\Phi^{(1)}(\mathbf{x})\right)$$

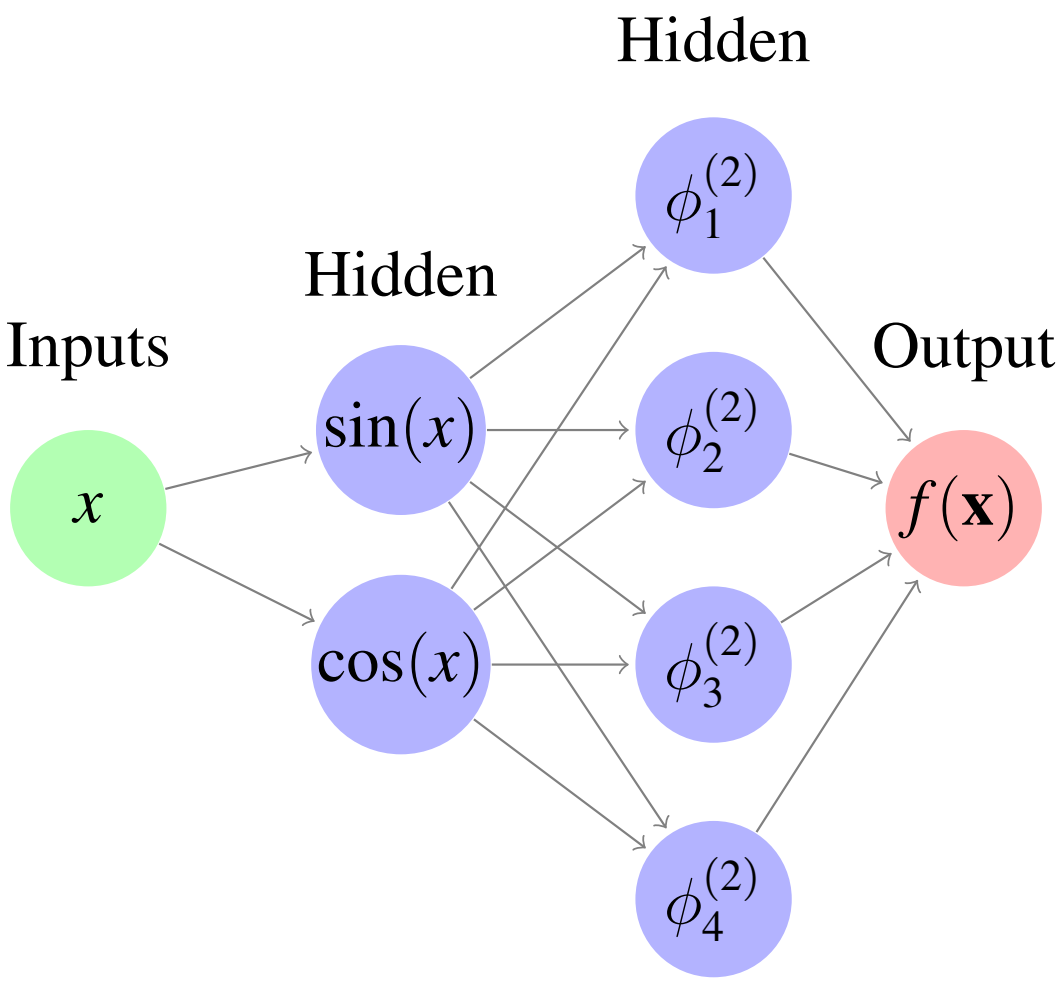
Instead of

$$k_1(\mathbf{x}, \mathbf{x}') = \Phi^{(1)}(\mathbf{x})^\mathsf{T}\Phi^{(1)}(\mathbf{x}'),$$

we have "deep kernel":

$$k_2(\mathbf{x}, \mathbf{x}')$$
$$= \Phi^{(2)}(\Phi^{(1)}(\mathbf{x}))^\mathsf{T}\Phi^{(2)}(\Phi^{(1)}(\mathbf{x}'))$$

EXAMPLE DEEP KERNEL: PERIODIC



Now our model is:

$$\Phi^1(x) = [\sin(x), \cos(x)]$$

we have "deep kernel":

$$k_2(\mathbf{x}, \mathbf{x}')$$

$$= \exp(-\frac{1}{2}\left(\Phi^1(\mathbf{x})) - \Phi^1(\mathbf{x}')\right)$$

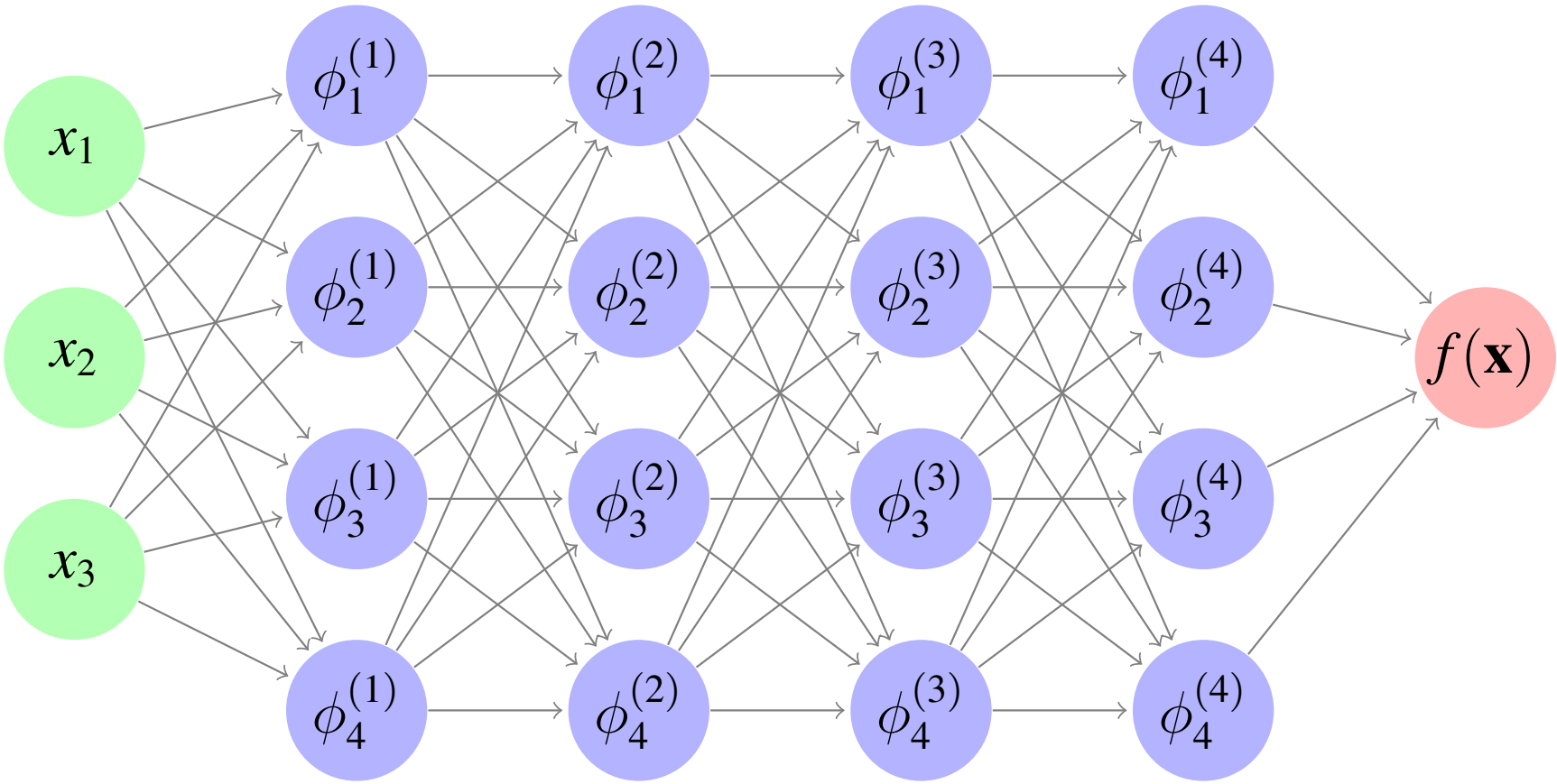
Deep Kernels

- (Cho, 2012) built kernels by composing feature mappings.
- Composing any kernel k_1 with a squared-exp kernel (SE):

$$
\begin{aligned}
& k_2(\mathbf{x}, \mathbf{x}') = \\
& = \left(\Phi^{SE}\left(\Phi^1(\mathbf{x})\right)\right)^{\mathsf{T}} \Phi^{SE}\left(\Phi^1(\mathbf{x}')\right) \\
& = \exp\left(-\frac{1}{2}||\Phi^1(\mathbf{x}) - \Phi^1(\mathbf{x}')||_2^2\right) \\
& = \exp\left(-\frac{1}{2}\left[\Phi^1(\mathbf{x})^{\mathsf{T}}\Phi^1(\mathbf{x}) - 2\Phi^1(\mathbf{x})^{\mathsf{T}}\Phi^1(\mathbf{x}') + \Phi^1(\mathbf{x}')^{\mathsf{T}}\Phi^1(\mathbf{x}')\right]\right) \\
& = \exp\left(-\frac{1}{2}\left[k_1(\mathbf{x}, \mathbf{x}) - 2k_1(\mathbf{x}, \mathbf{x}') + k_1(\mathbf{x}', \mathbf{x}')\right]\right)
\end{aligned}
$$

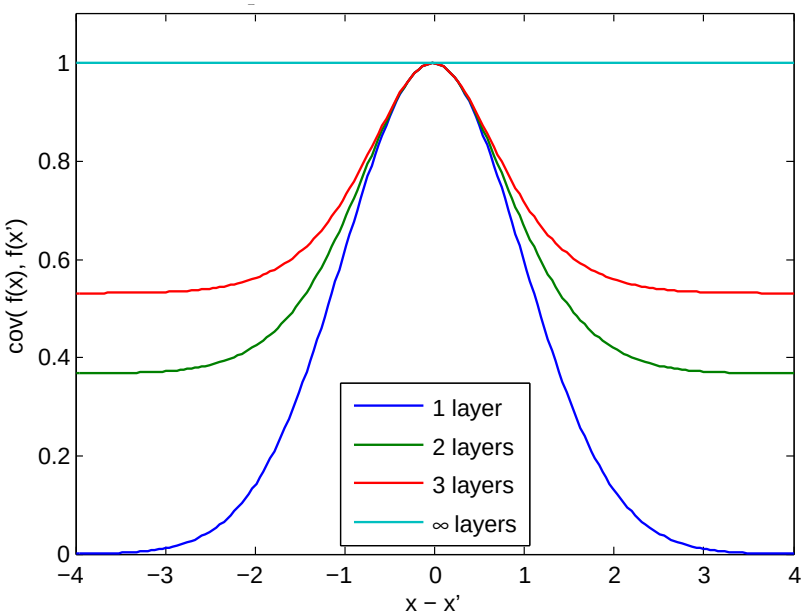
- A closed form... let's do it again!

We need to go deeper

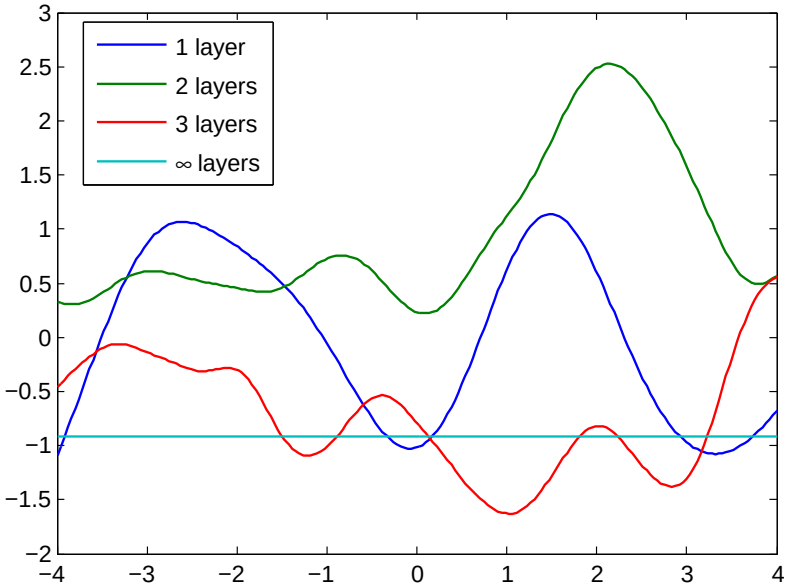


Infinitely Deep Kernels

- For SE kernel, $k_{L+1}(\mathbf{x}, \mathbf{x}') = \exp\left(k_L(\mathbf{x}, \mathbf{x}') - 1\right)$.
- What is the limit of composing SE features?



Kernel

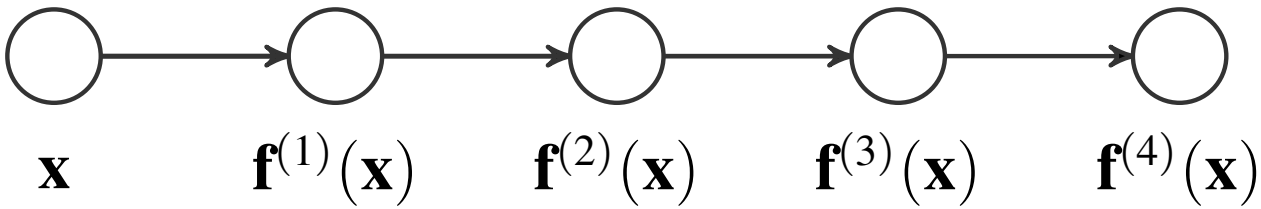


Draws from GP prior

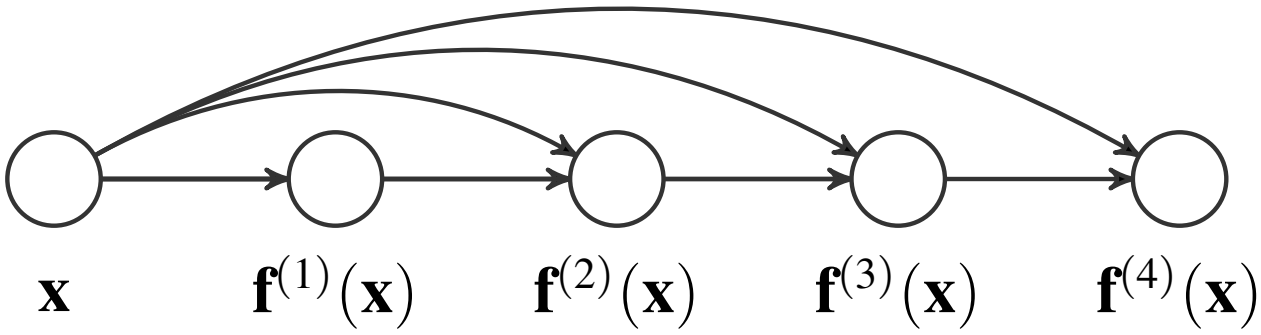
- $k_\infty(\mathbf{x}, \mathbf{x}') = 1$ everywhere. ☹

A SIMPLE FIX...

- Following a suggestion from Neal (1995), we connect the inputs $\mathbf{x}$ to each layer:



a) standard MLP architecture.



b) Input-connected architecture.

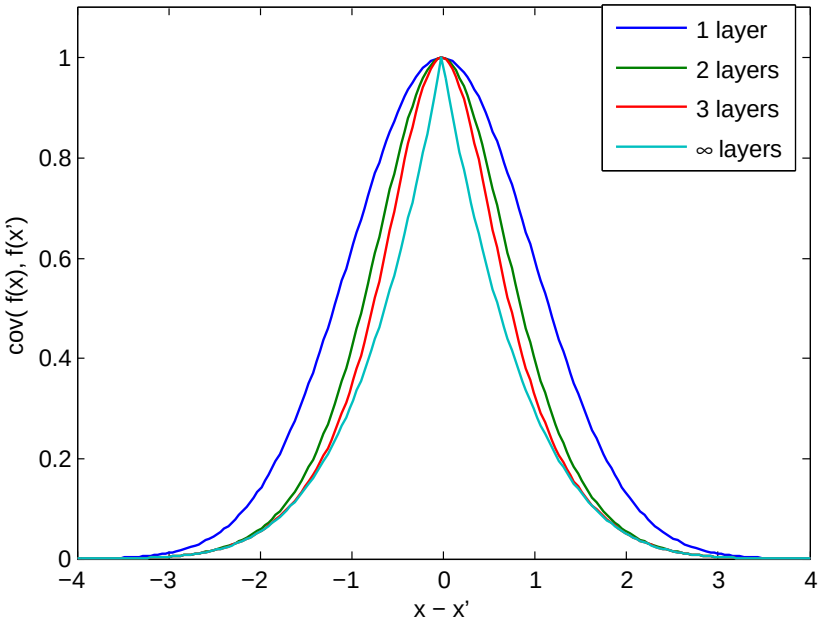
A SIMPLE FIX...

- Following a suggestion from Neal (1995), we connect the inputs $\mathbf{x}$ to each layer:

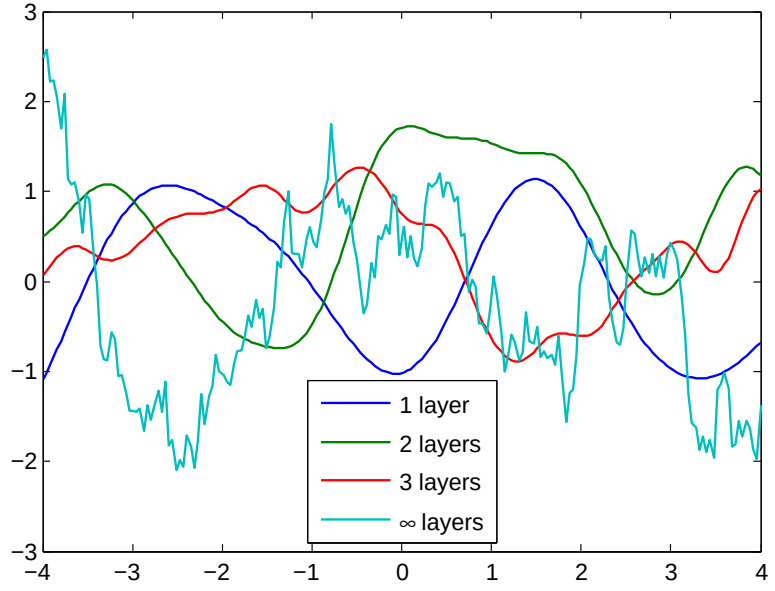
$$
\begin{aligned}
&k_{L+1}(\mathbf{x}, \mathbf{x}') = \\
&= \exp\left(-\frac{1}{2}\left|\left|\begin{bmatrix}\Phi^L(\mathbf{x}) \\ \mathbf{x}\end{bmatrix} - \begin{bmatrix}\Phi^L(\mathbf{x}') \\ \mathbf{x}'\end{bmatrix}\right|\right|_2^2\right) \\
&= \exp\left(-\frac{1}{2}\left[k_L(\mathbf{x}, \mathbf{x}) - 2k_L(\mathbf{x}, \mathbf{x}') + k_L(\mathbf{x}', \mathbf{x}')\right] - \frac{1}{2}||\mathbf{x} - \mathbf{x}'||_2^2\right)
\end{aligned}
$$

Infinitely Deep Kernels

- What is the limit of compositions of input-connected SE features?
- $k_{L+1}(\mathbf{x}, \mathbf{x}') = \exp\left(k_L(\mathbf{x}, \mathbf{x}') - 1 - \frac{1}{2}||\mathbf{x} - \mathbf{x}'||_2^2\right).$



Kernels



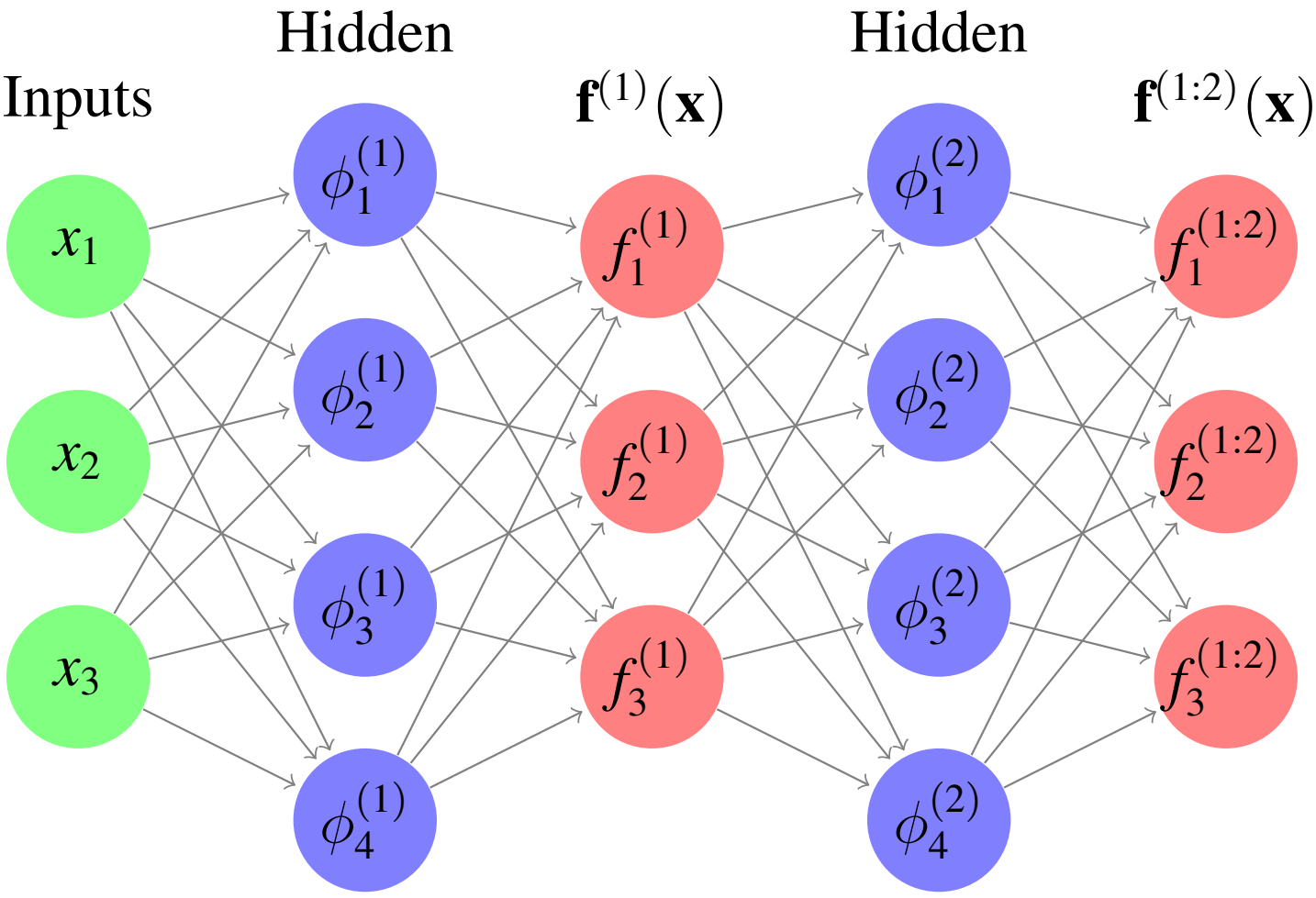
Draws from GP priors

- Like an Ornstein-Uhlenbeck process with skinny tails
- Samples are non-differentiable (fractal).

What went wrong?

- Fixed feature mapping, unlikely to be useful for anything
- power of neural nets comes from learning a custom representation
- Need to search over feature mappings!
- Can try to learn kernels, or even better, integrate over feature mappings

Deep Gaussian Processes



Deep Gaussian Processes

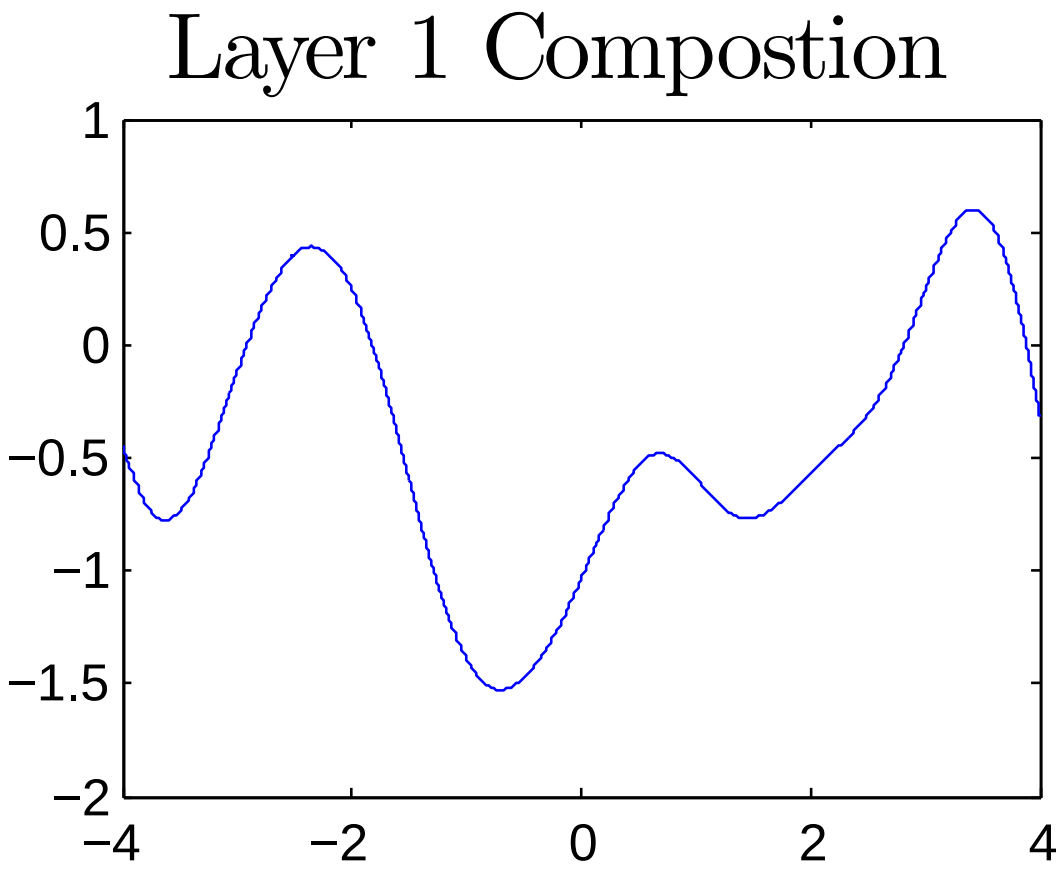
- a prior over compositions of functions:

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

  where each $\mathbf{f}_d^{(\ell)} \overset{\text{ind}}{\sim} \mathcal{GP}\left(0, k_d^{\ell}(\mathbf{x}, \mathbf{x}')\right)$.
- Analogous to neural nets, where each neuron's activation function is an independent draw from a GP.
- inference is really hard.
- maybe we can learn something just from looking at draws?

Deep Gaussian Processes

- Draws from one-dimensional deep GPs:



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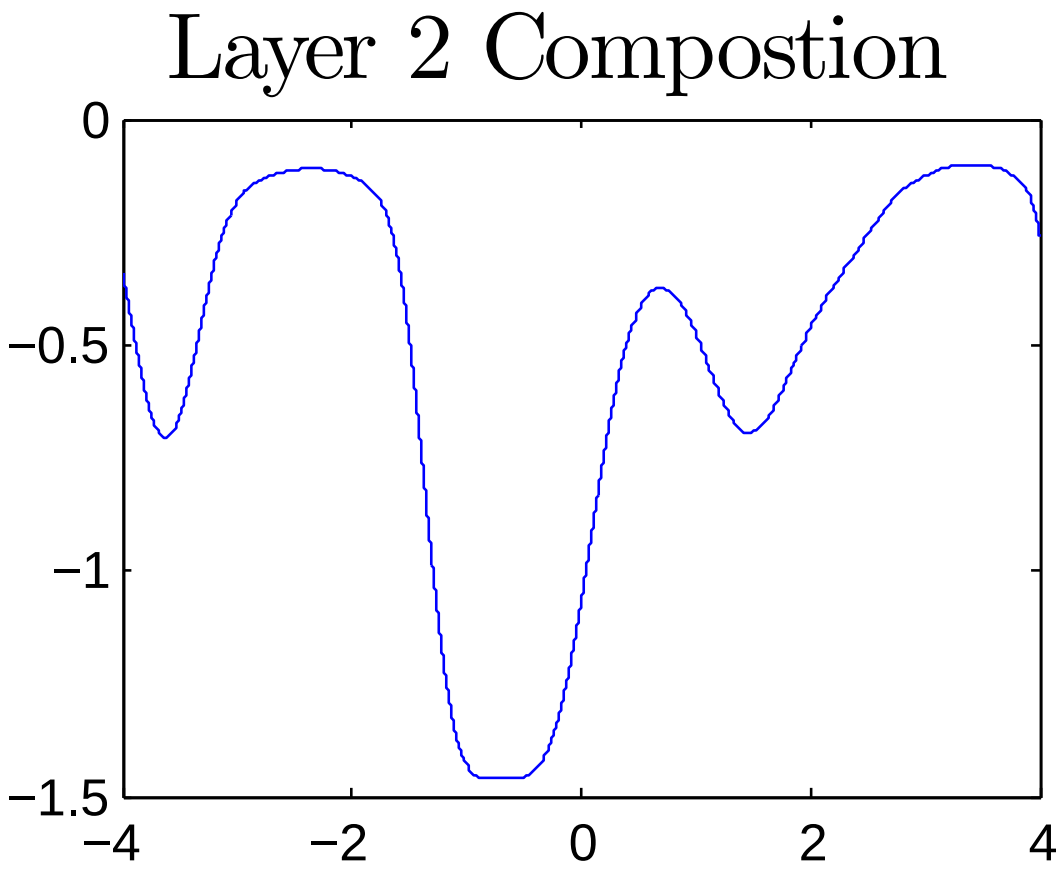

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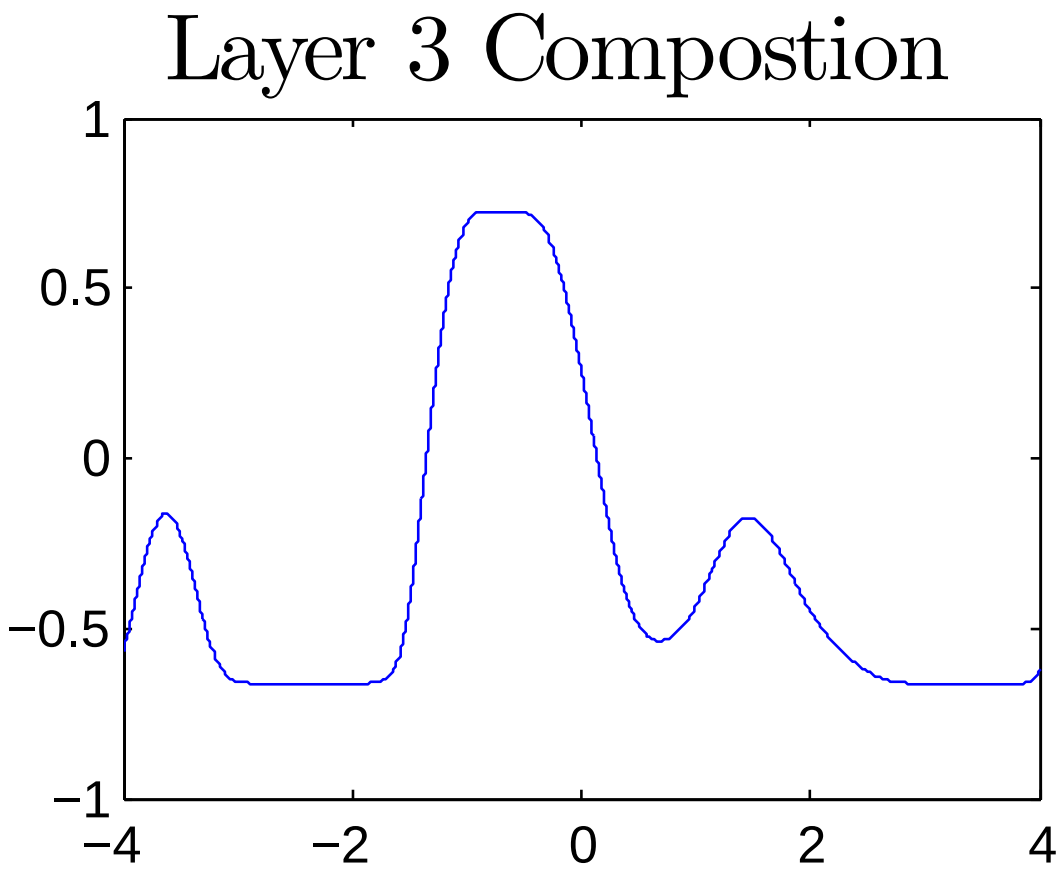

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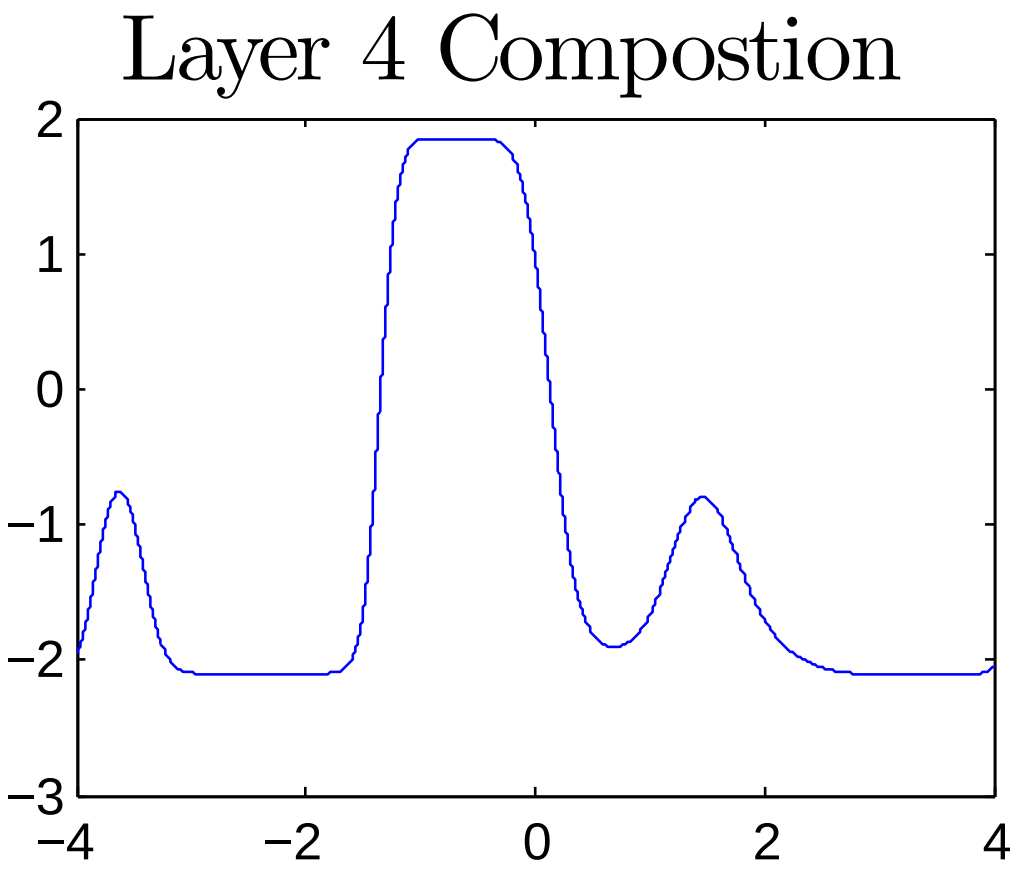

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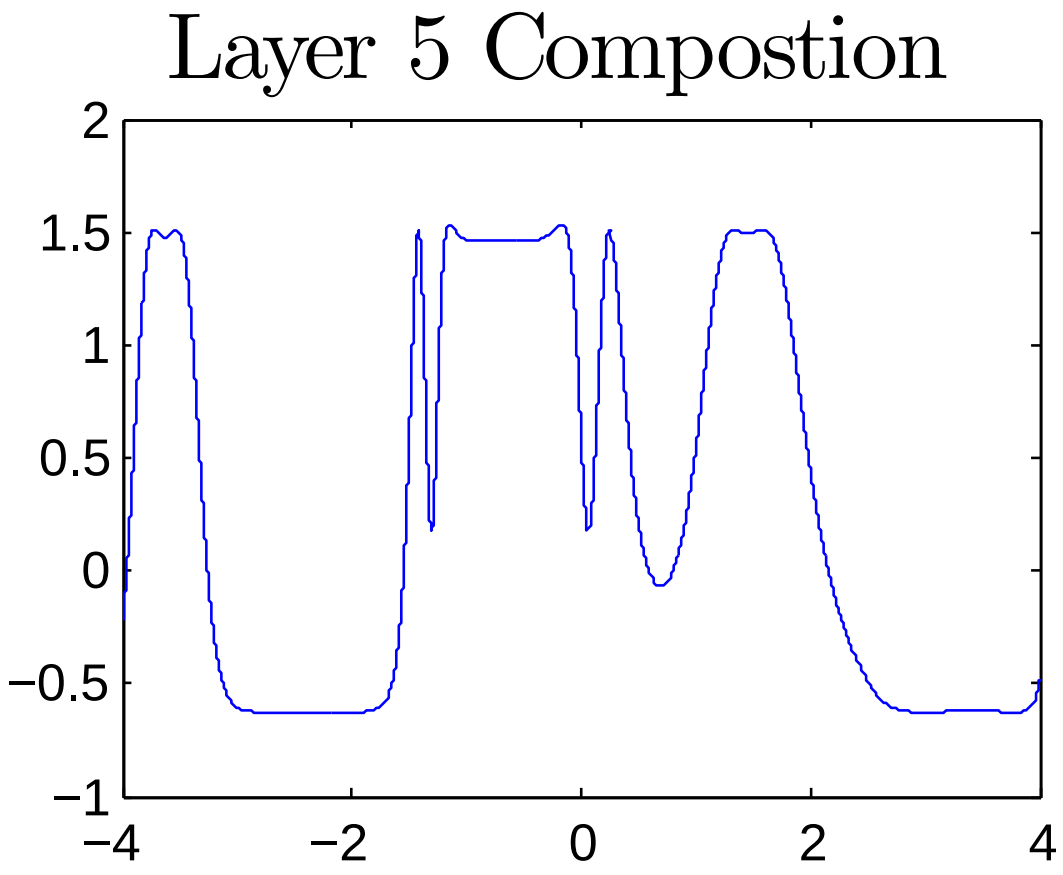

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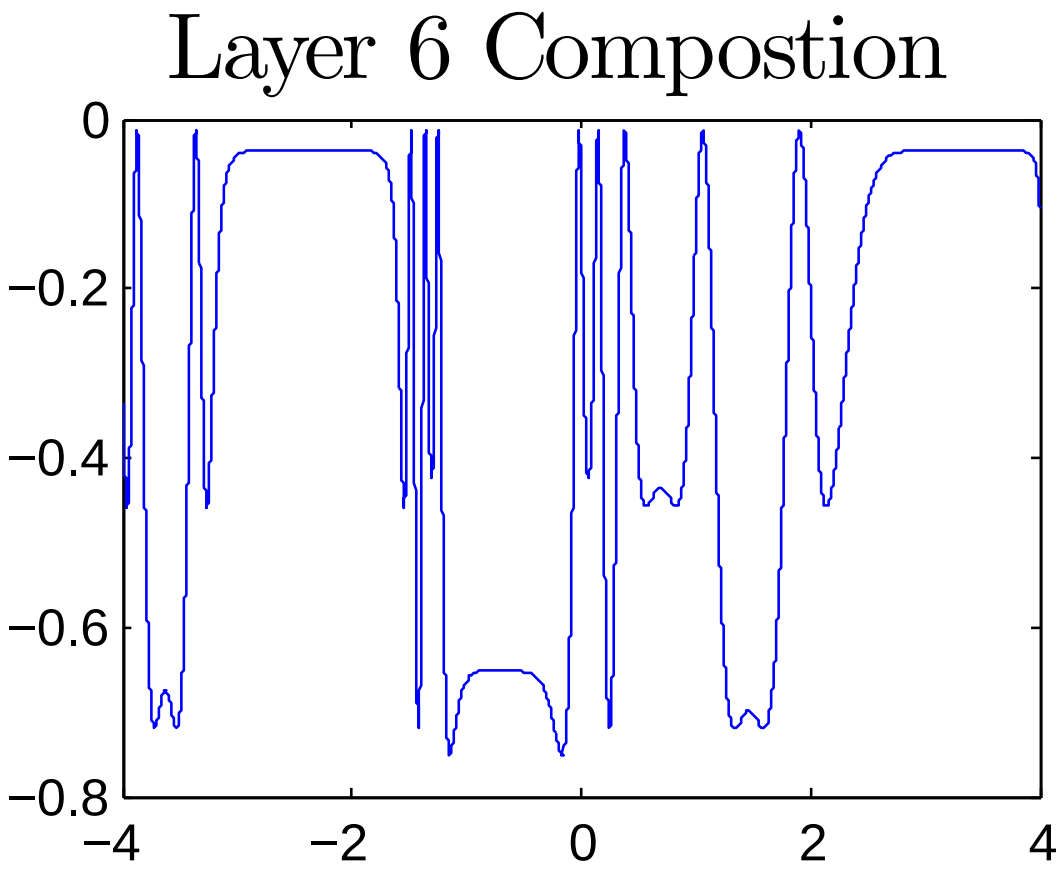

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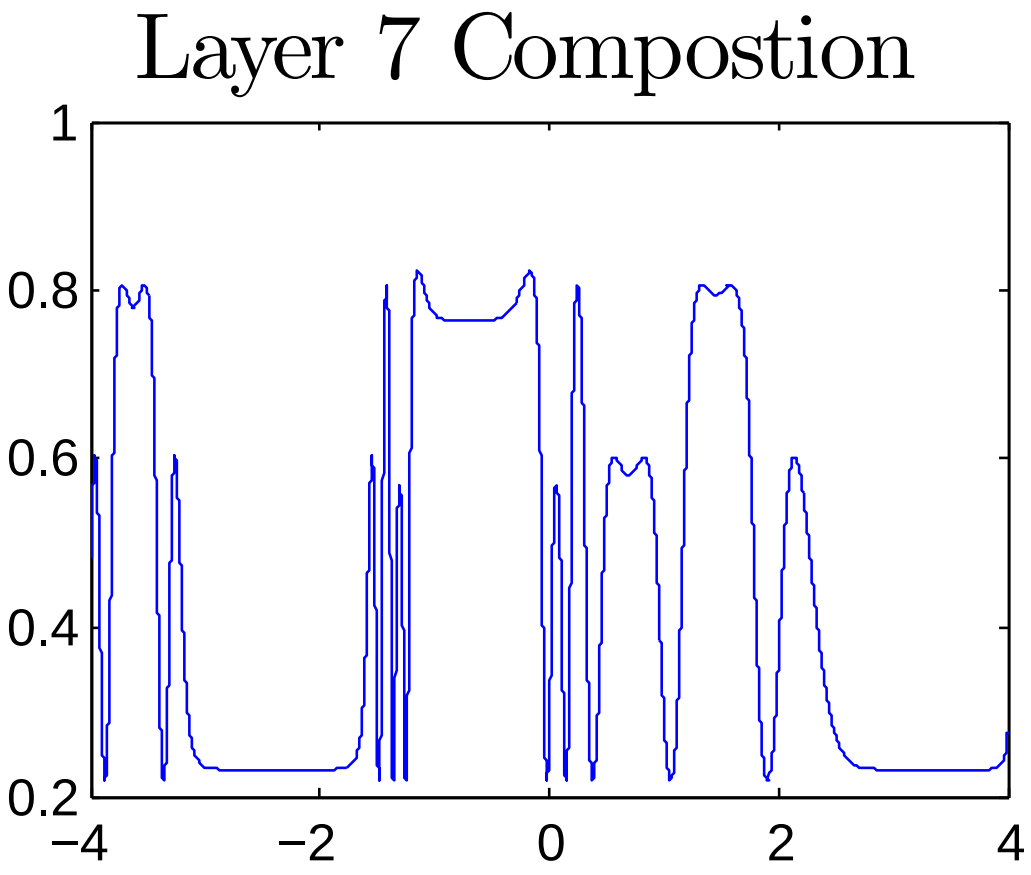

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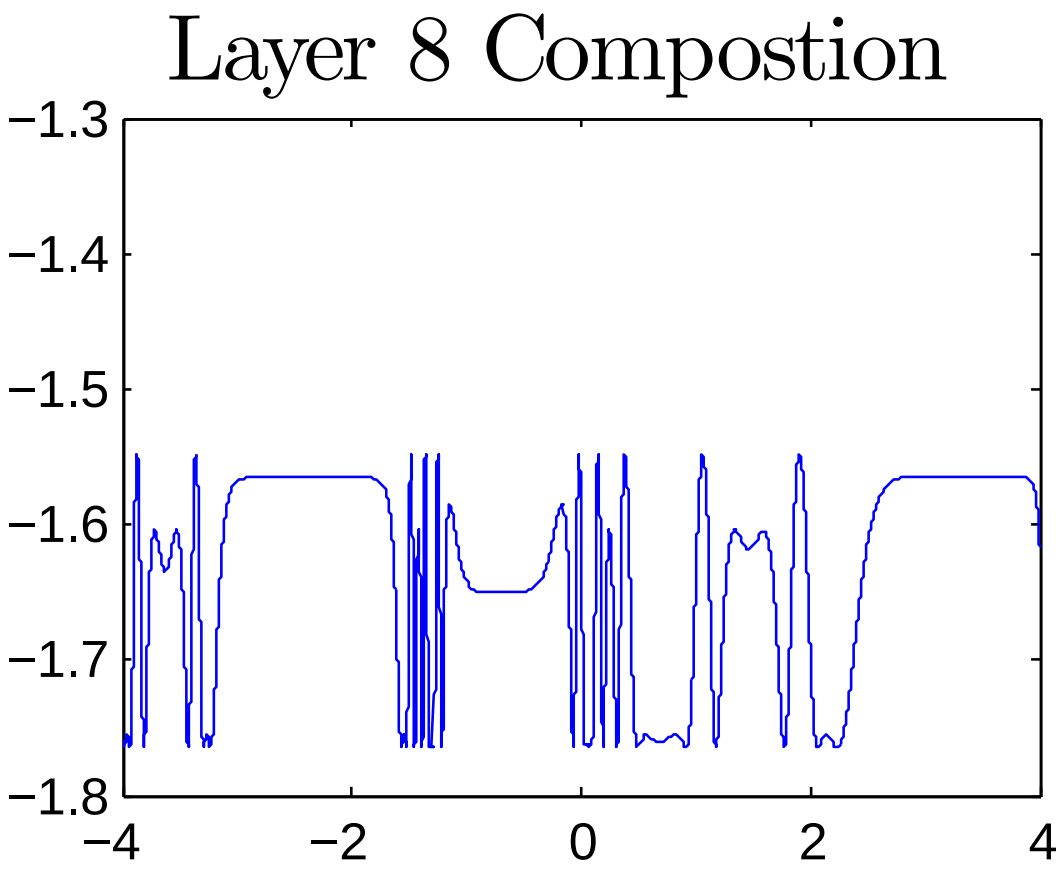

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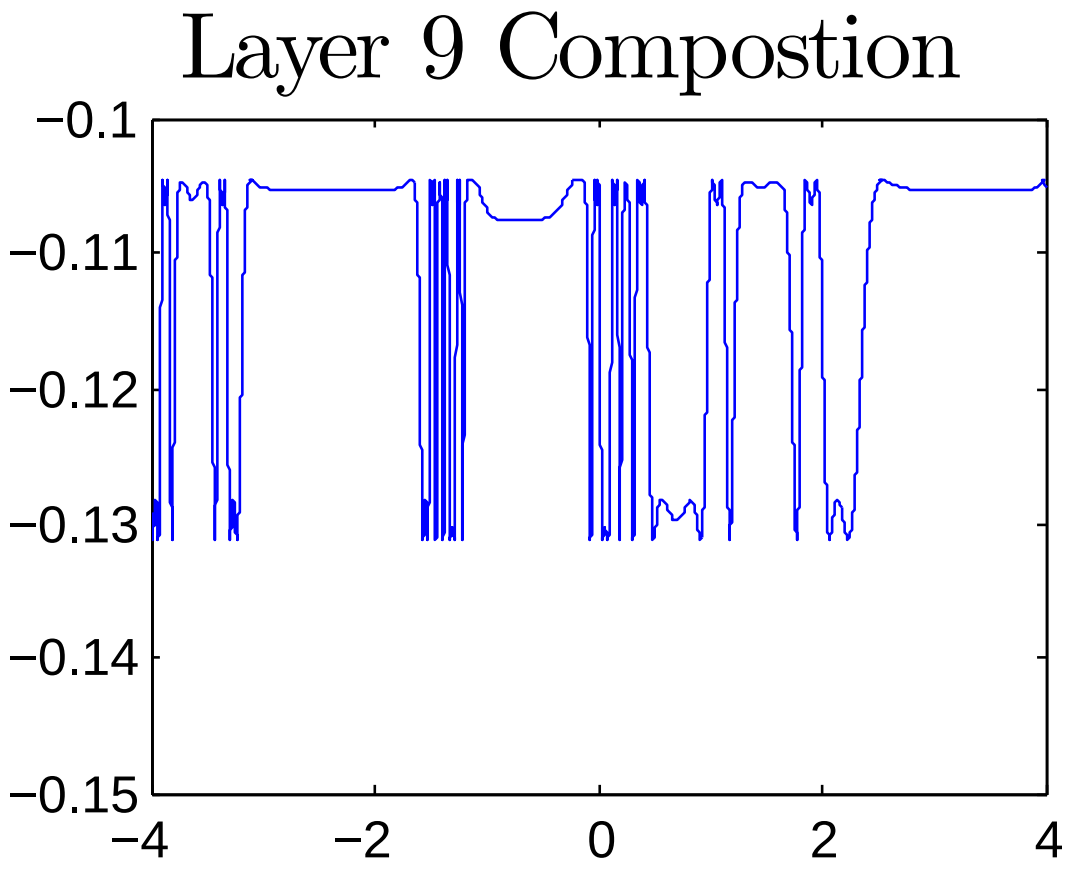

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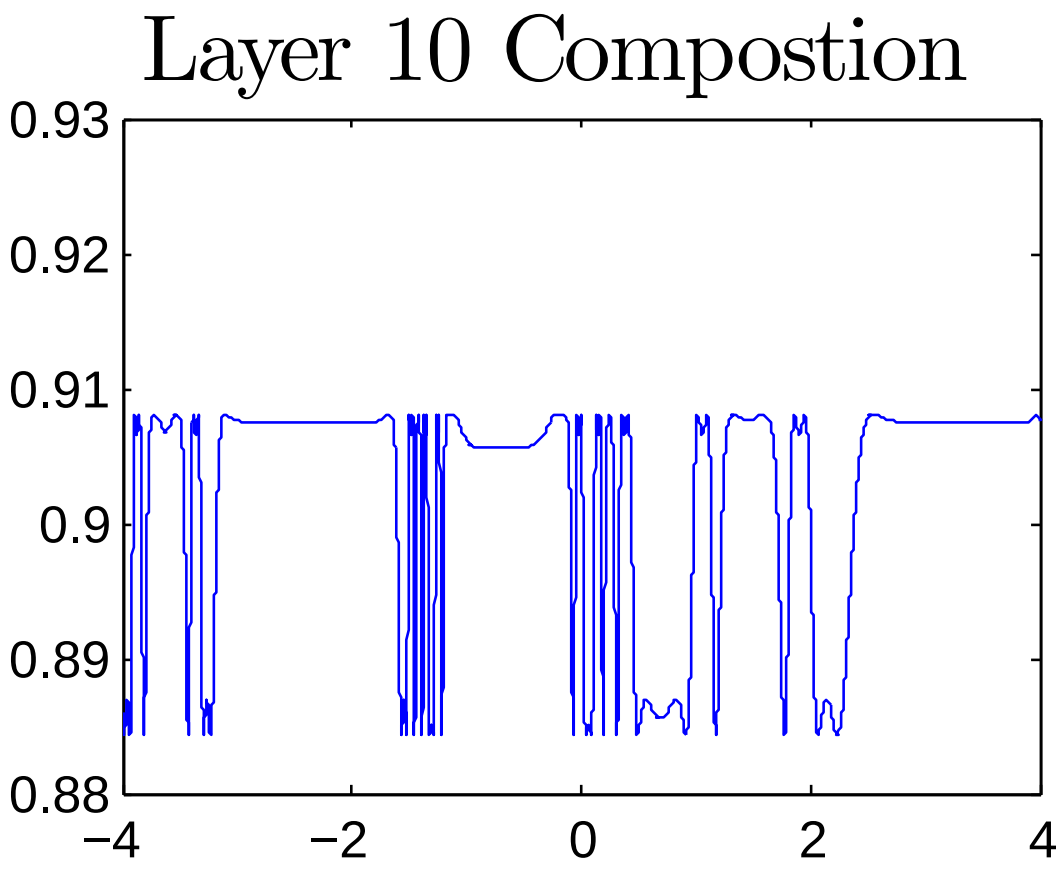
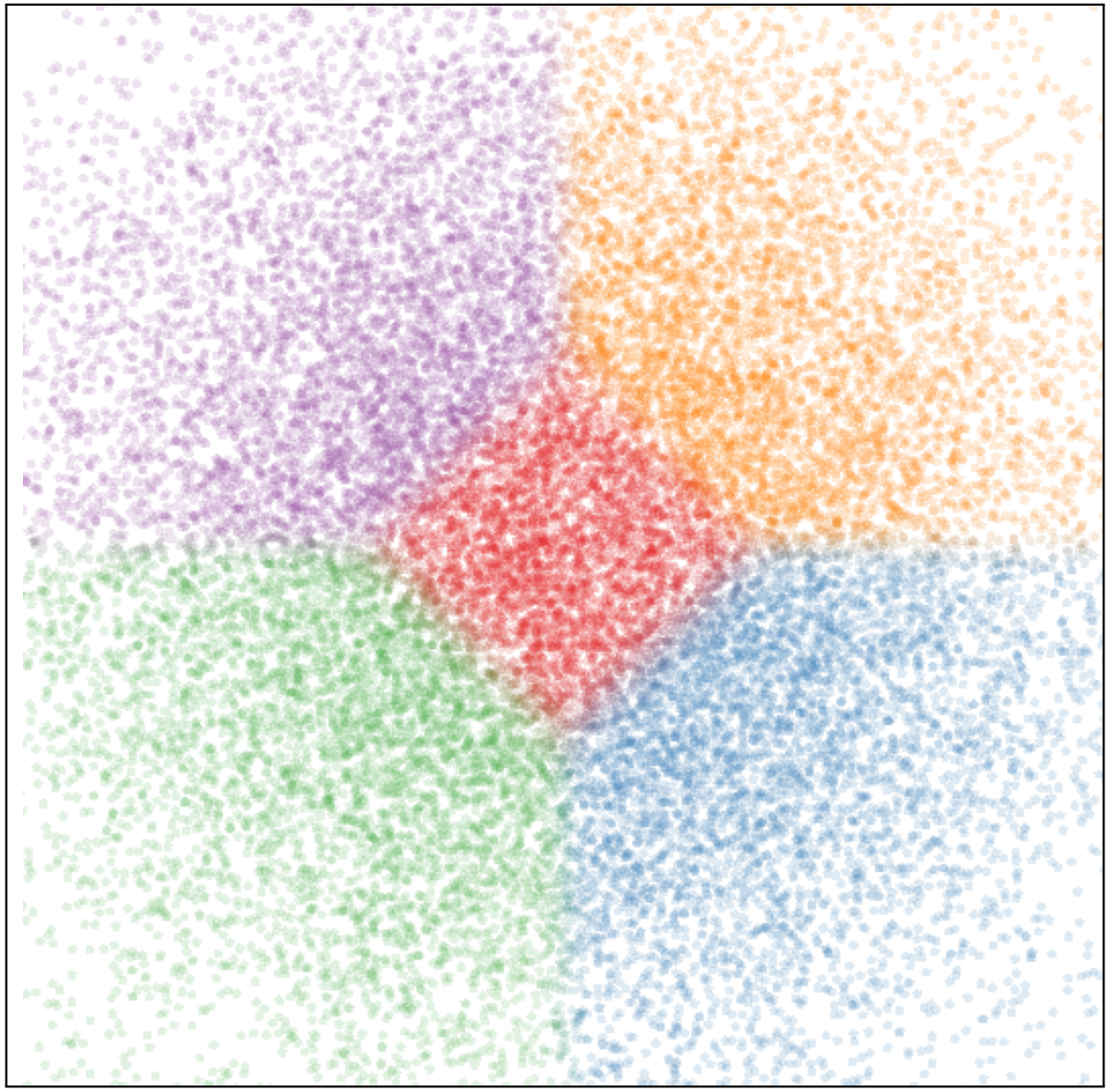


Deep Gaussian Processes

- 2D to 2D warpings of a Gaussian density:



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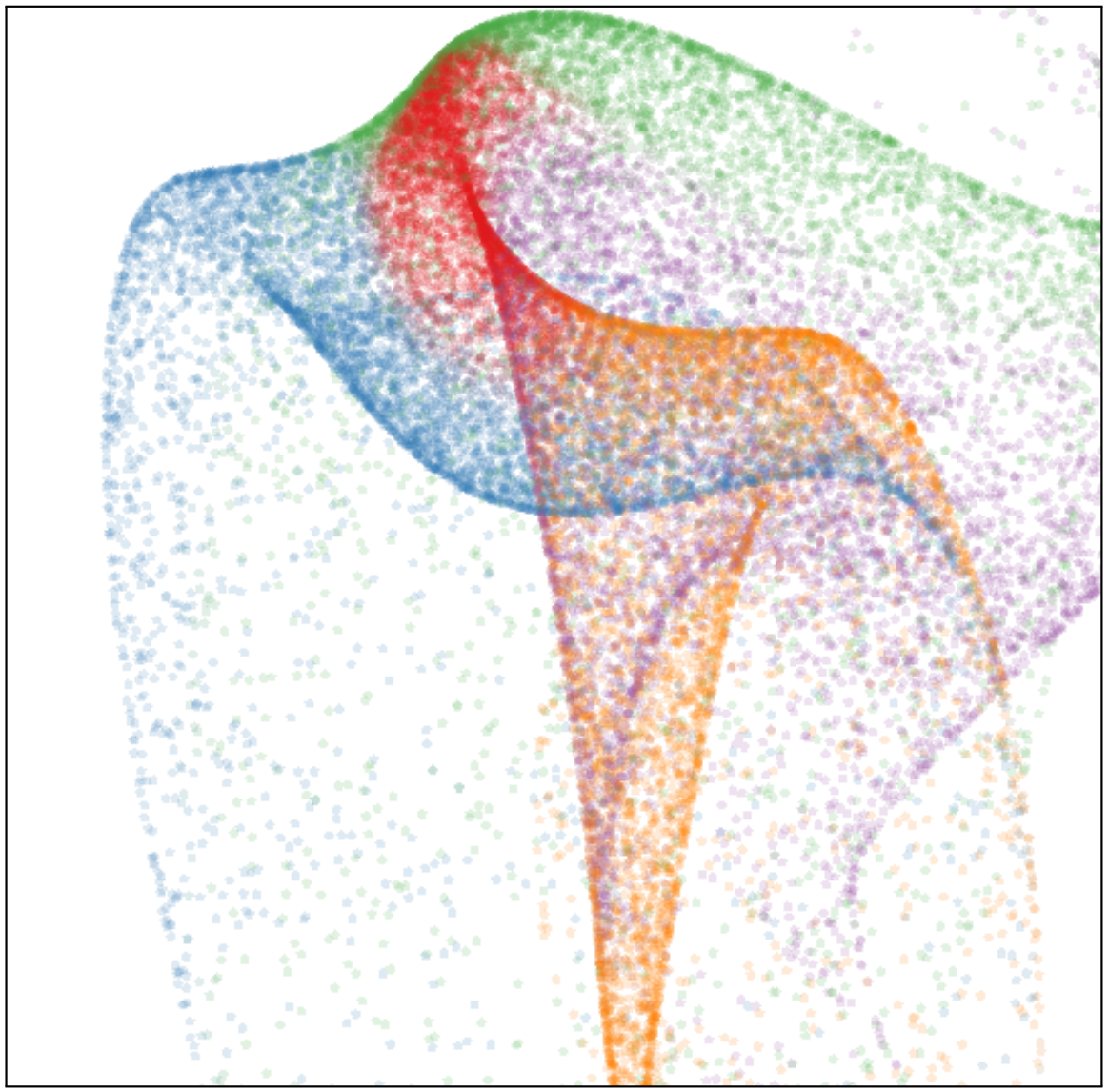

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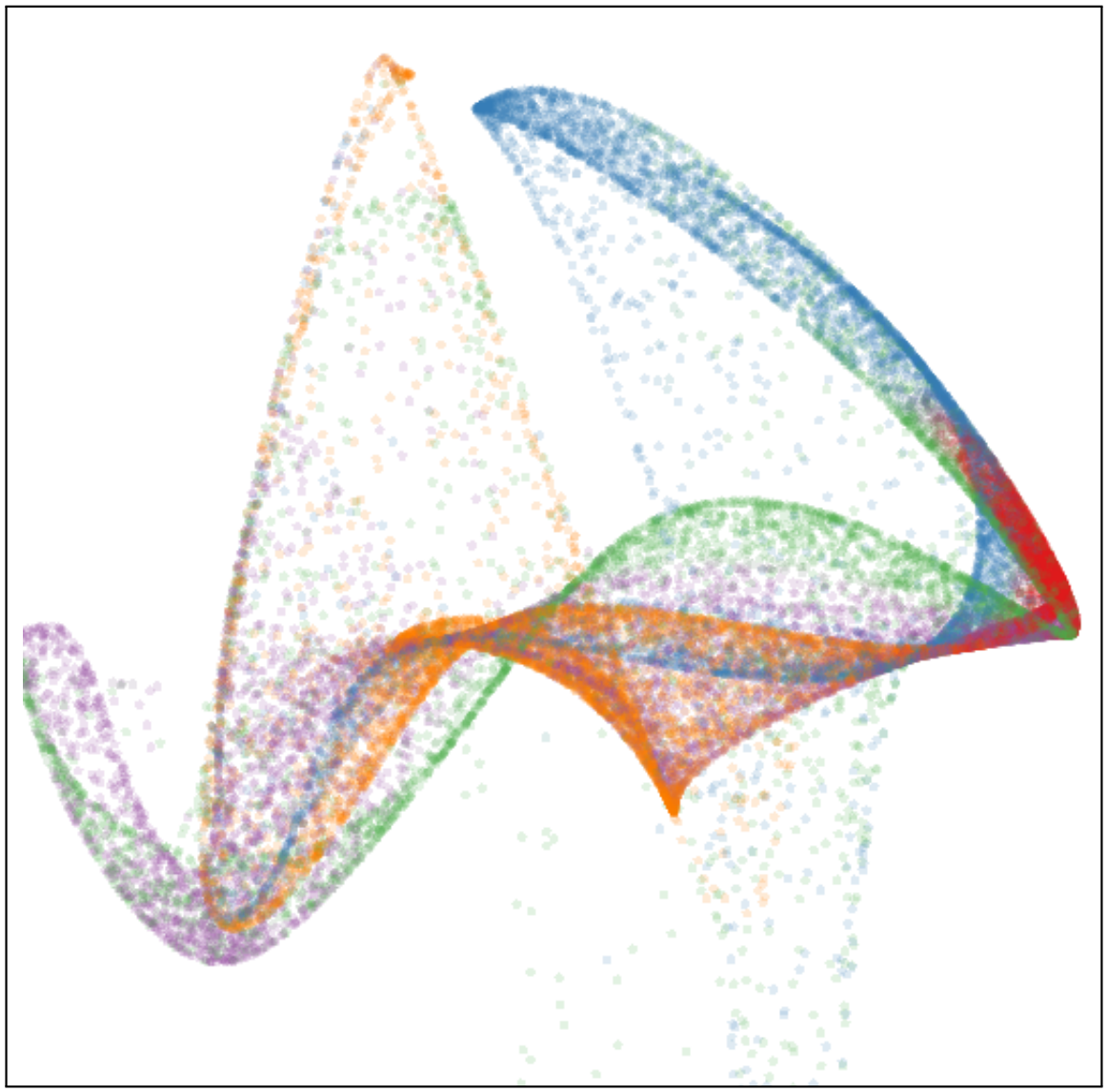

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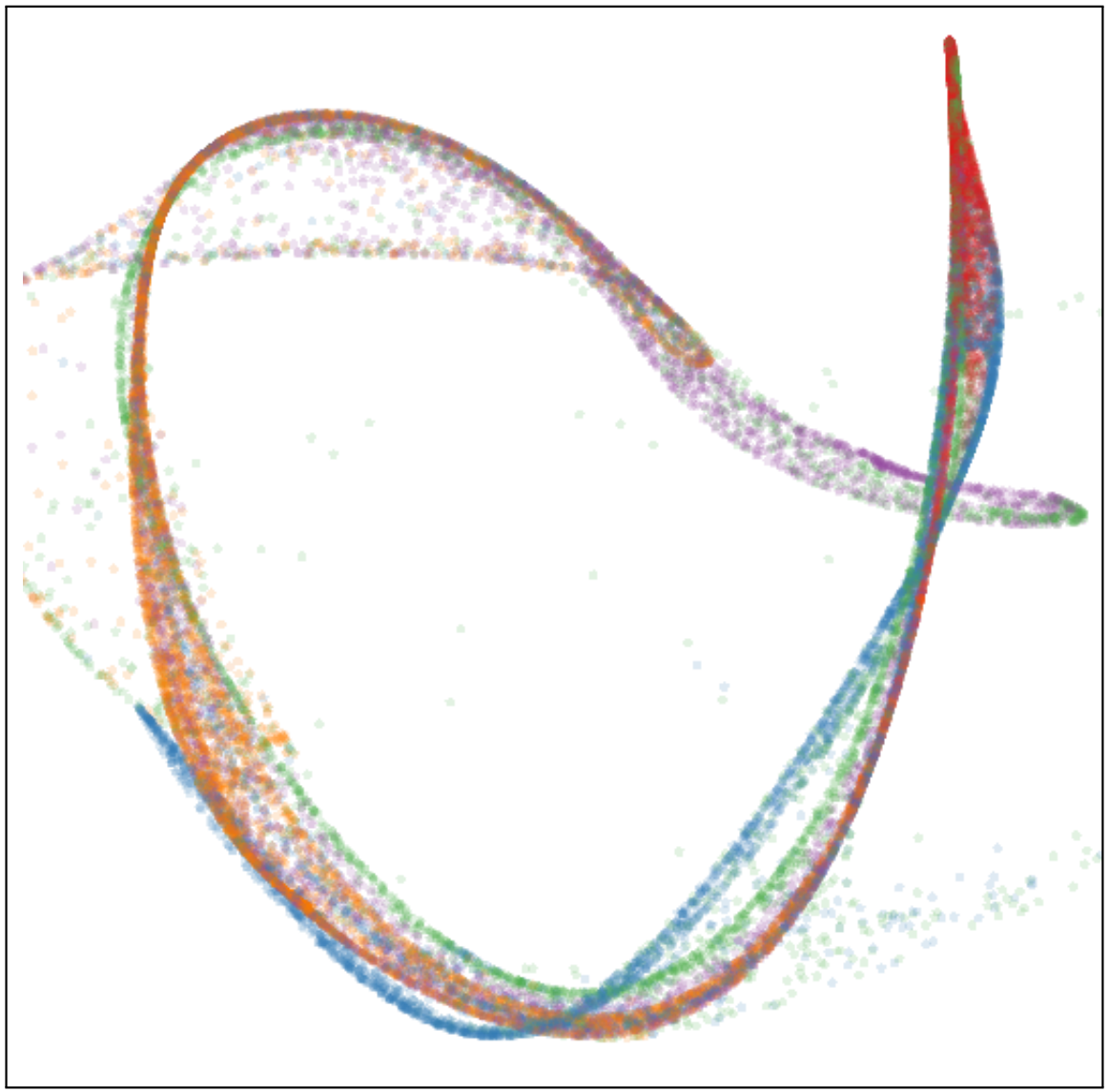

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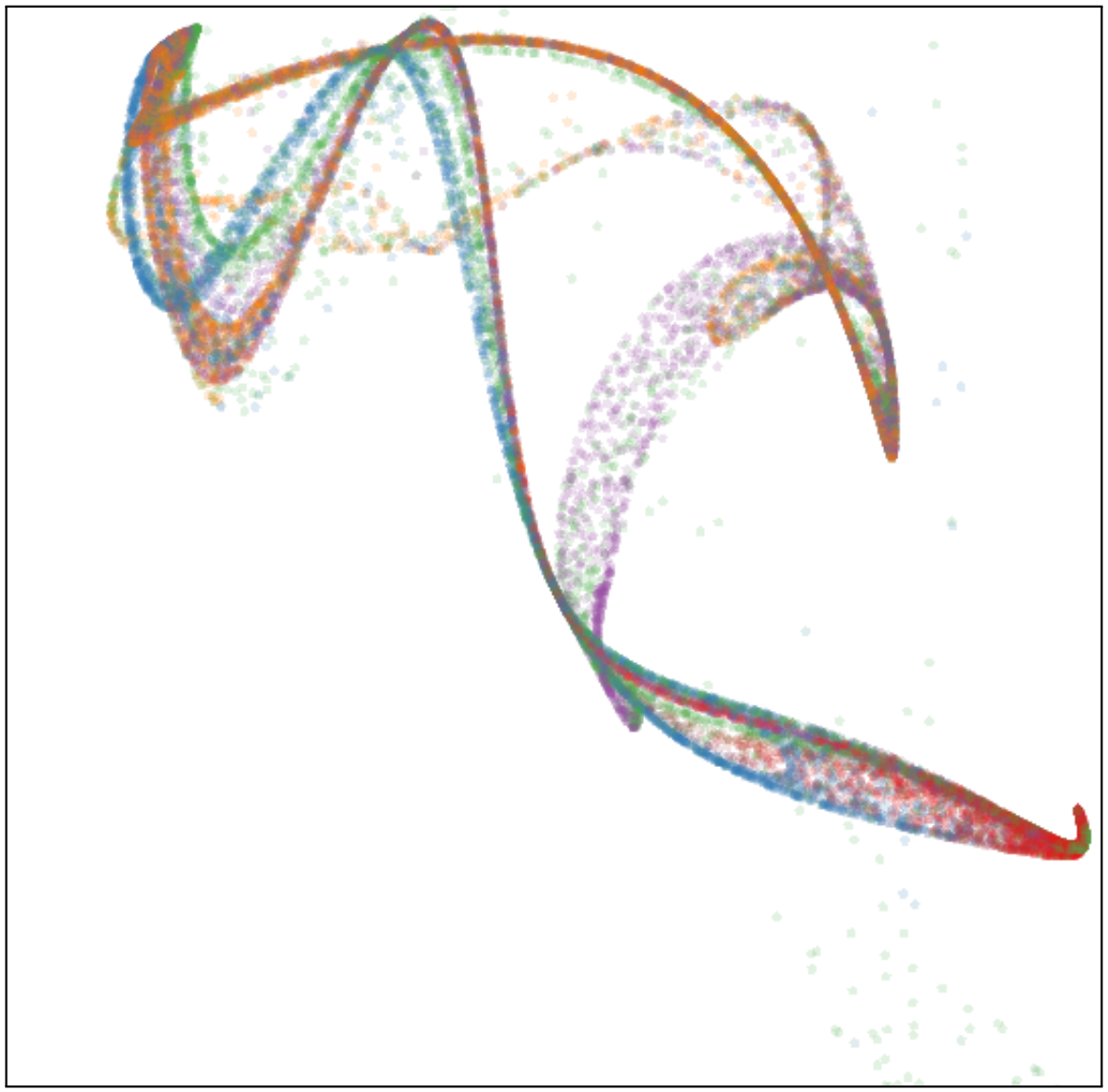

Deep Gaussian Processes

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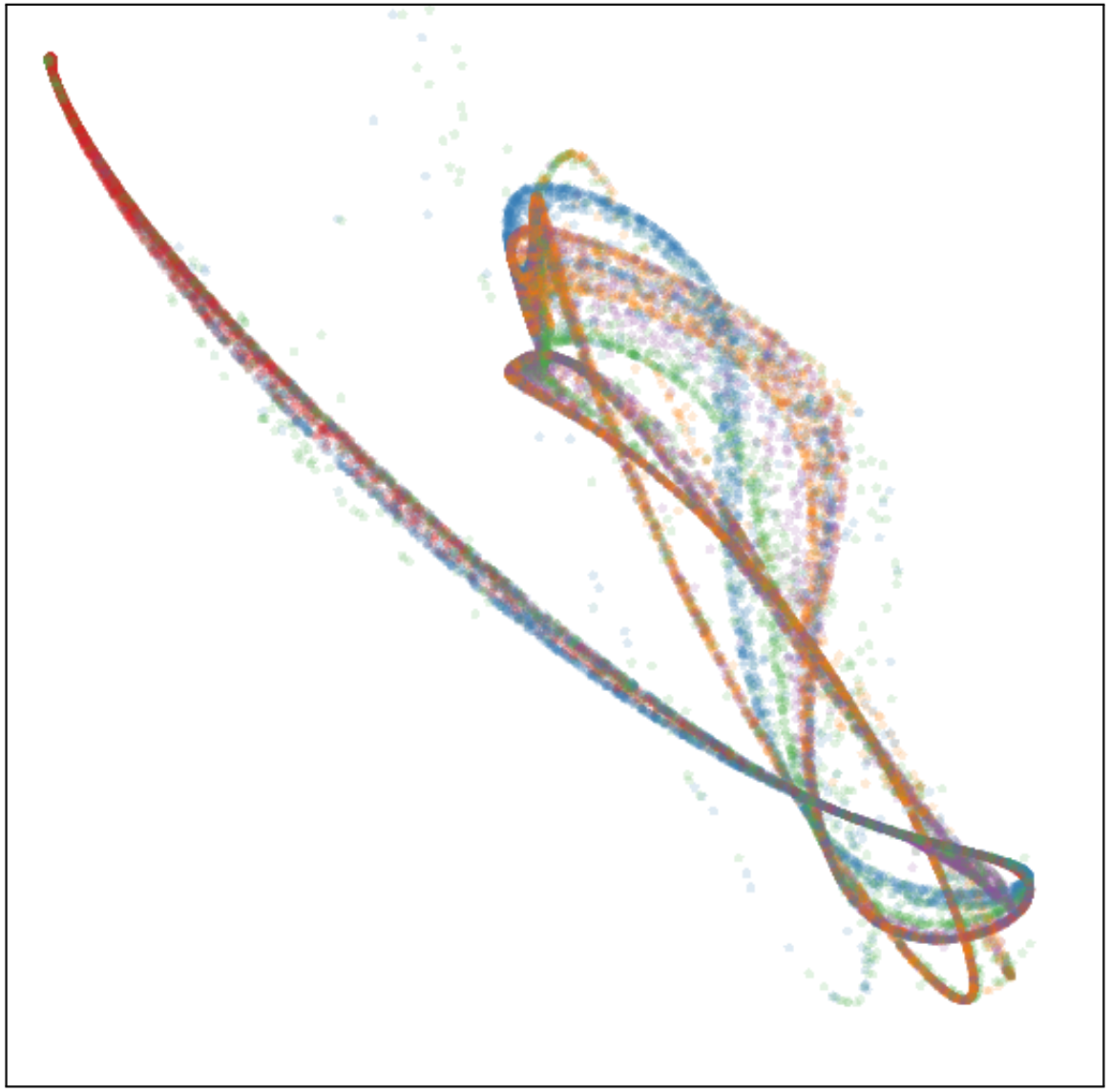
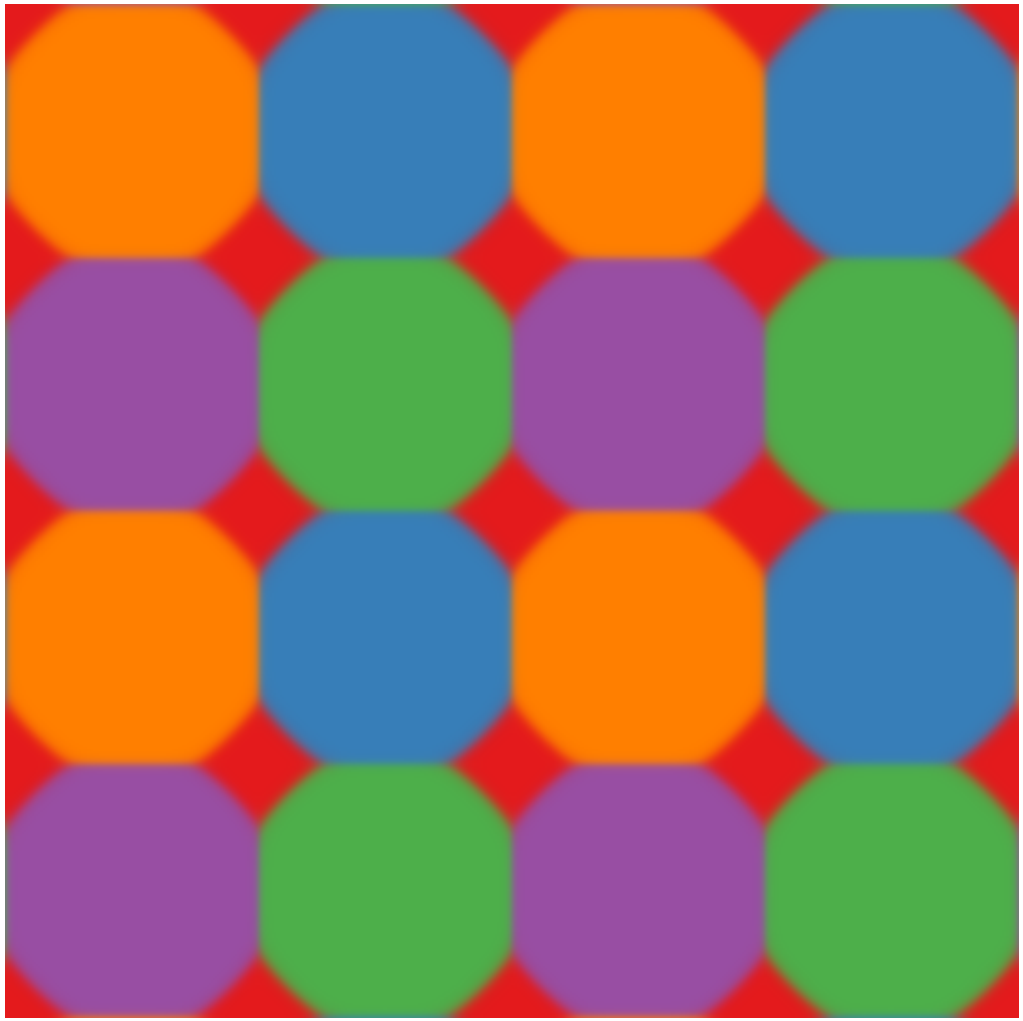


Deep Gaussian Processes

- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)



No warping

Deep Gaussian Processes

- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)

One Layers

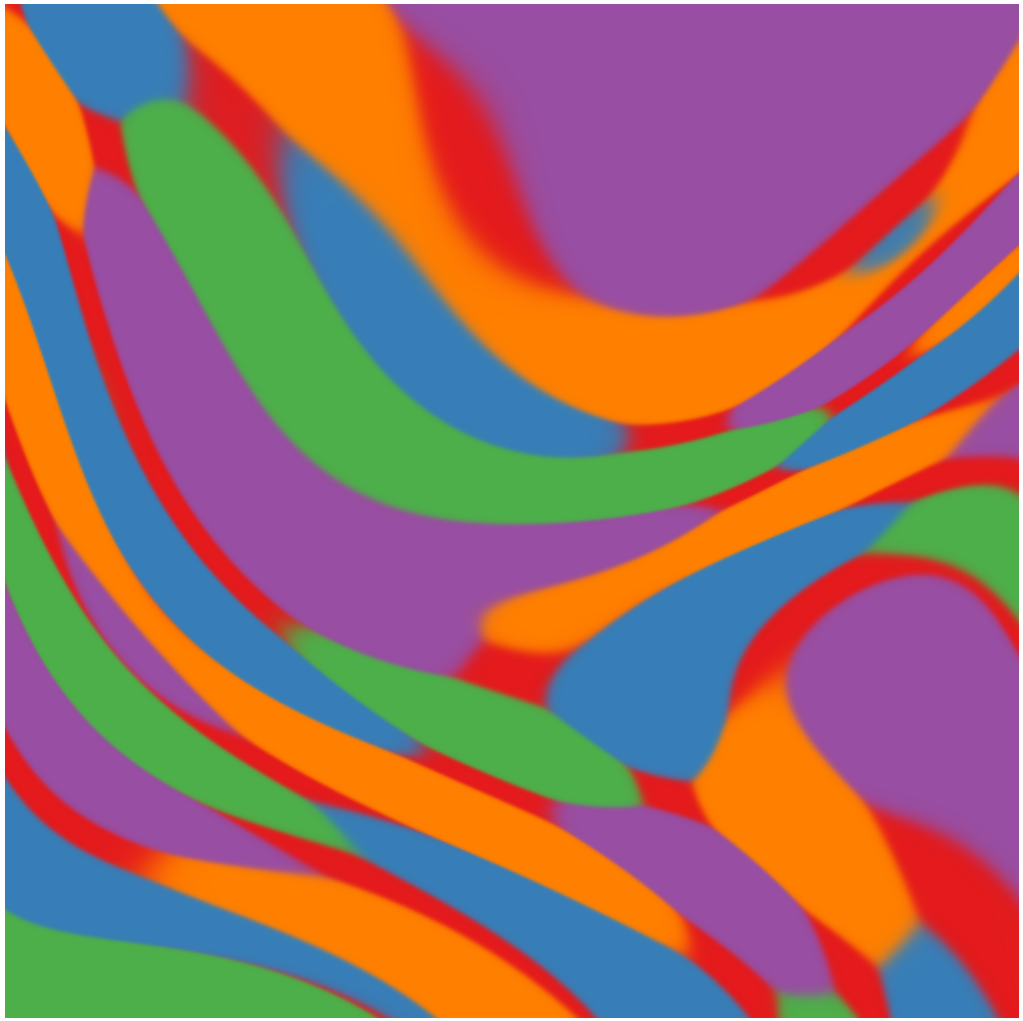
Deep Gaussian Processes

- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)

Two Layers

Deep Gaussian Processes

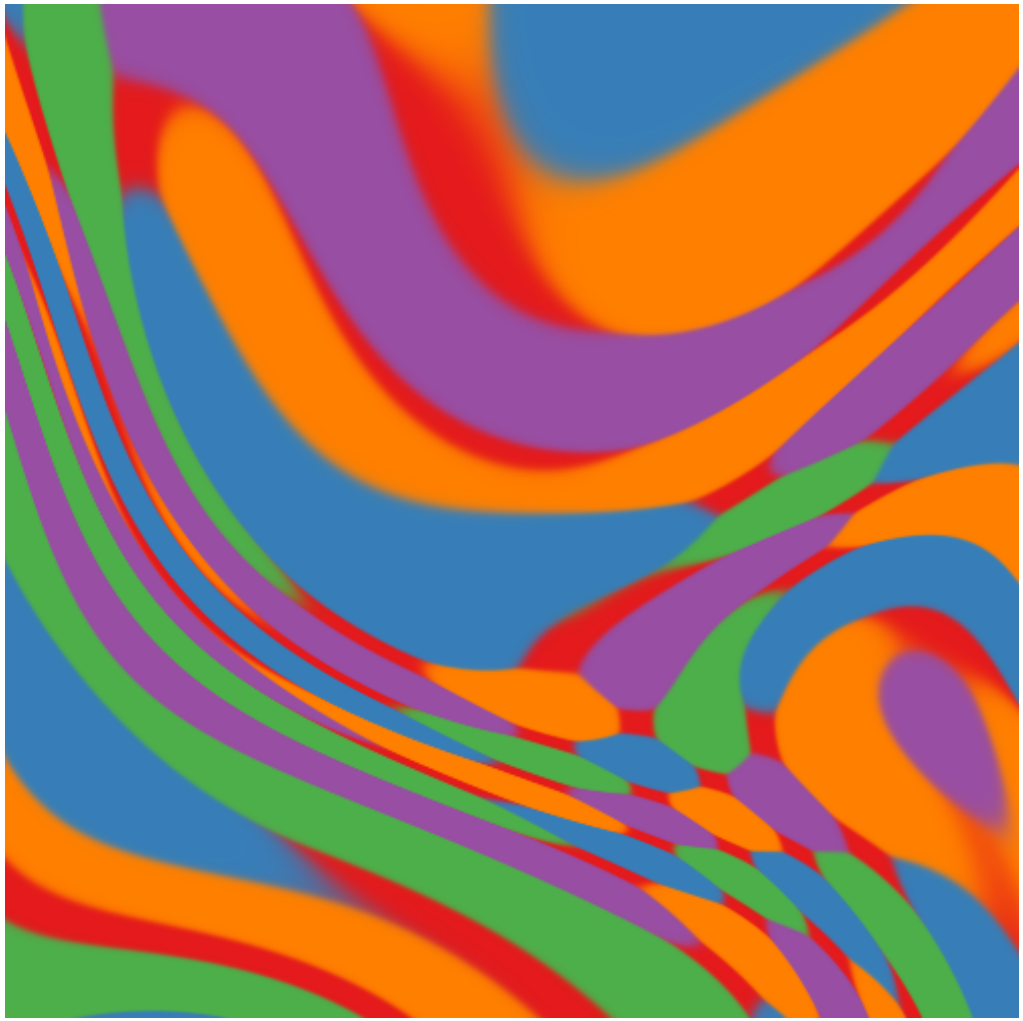
- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)



Three Layers

Deep Gaussian Processes

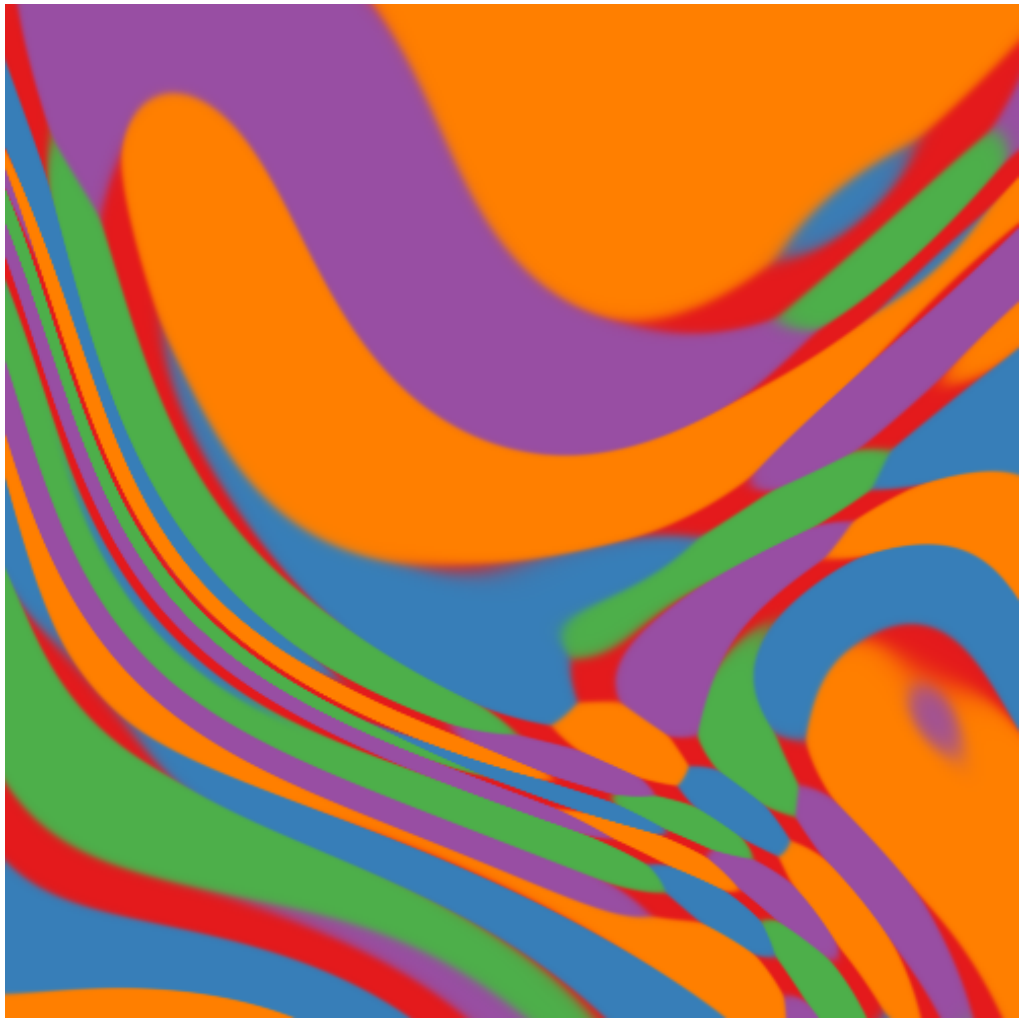
- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)



Four Layers

Deep Gaussian Processes

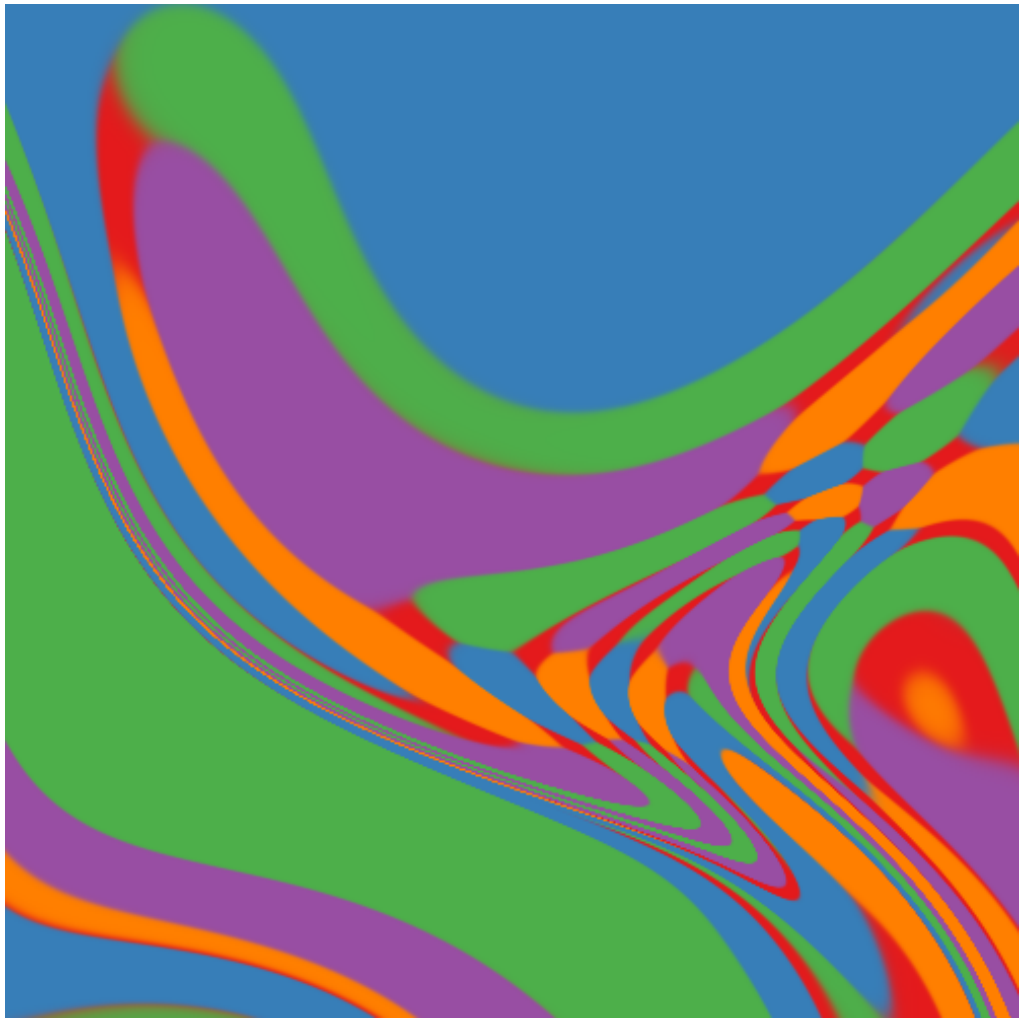
- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)



Five Layers

Deep Gaussian Processes

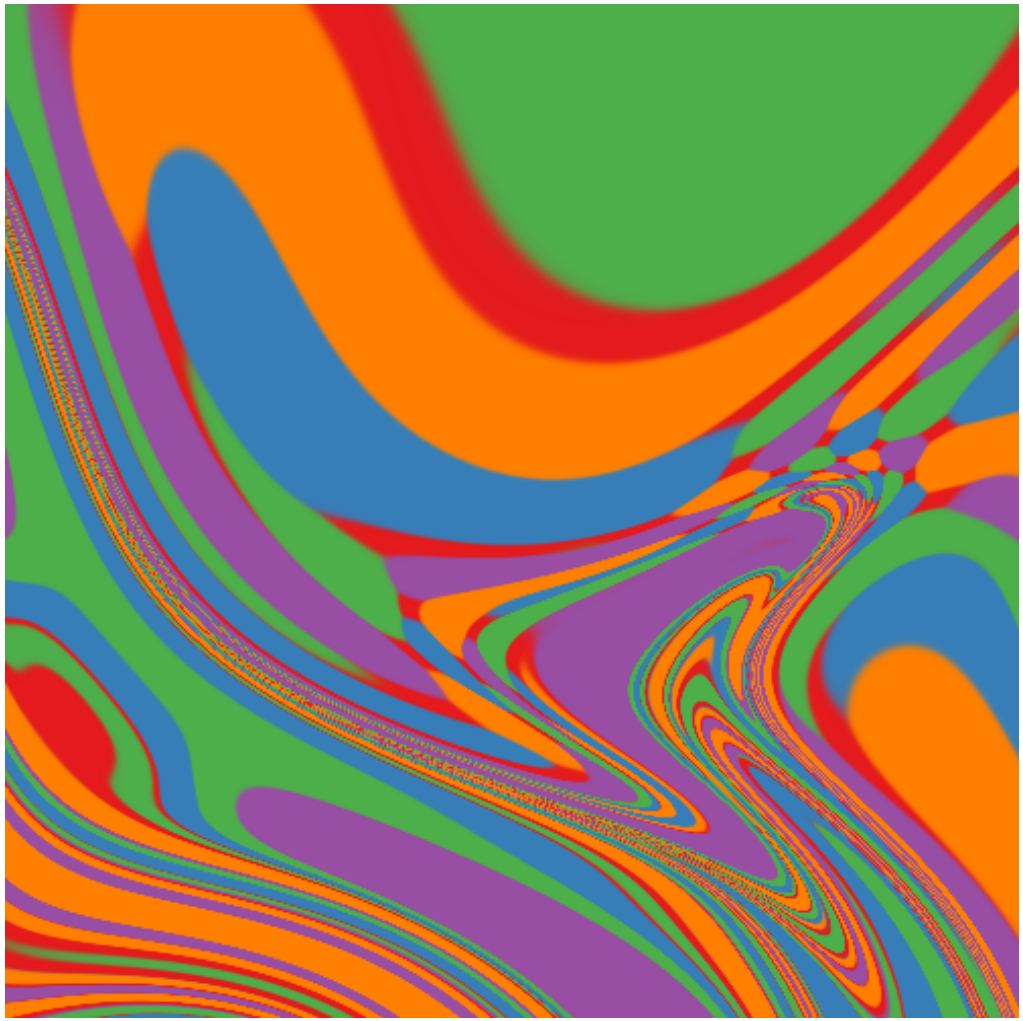
- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)



Ten Layers

Deep Gaussian Processes

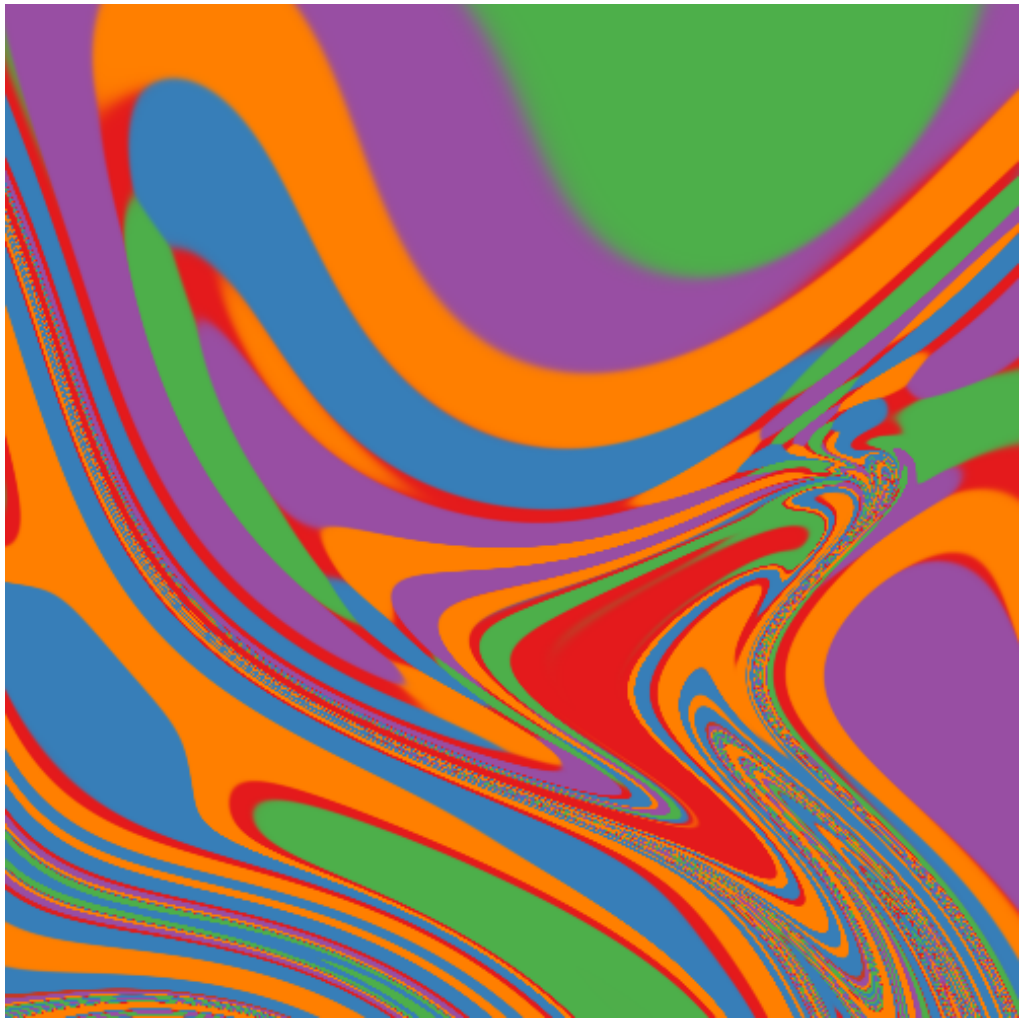
- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)



Twenty Layers

Deep Gaussian Processes

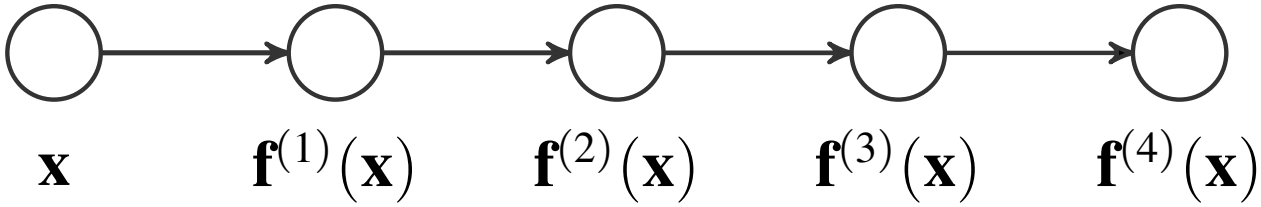
- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)



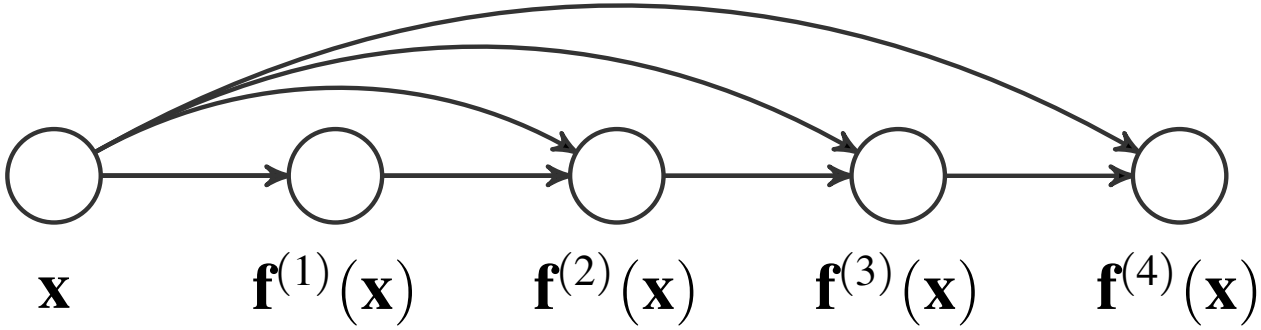
Forty Layers

Deep Gaussian Processes

- Only one degree of freedom in x is being captured!
- Again following Radford's thesis, connect every layer to input:



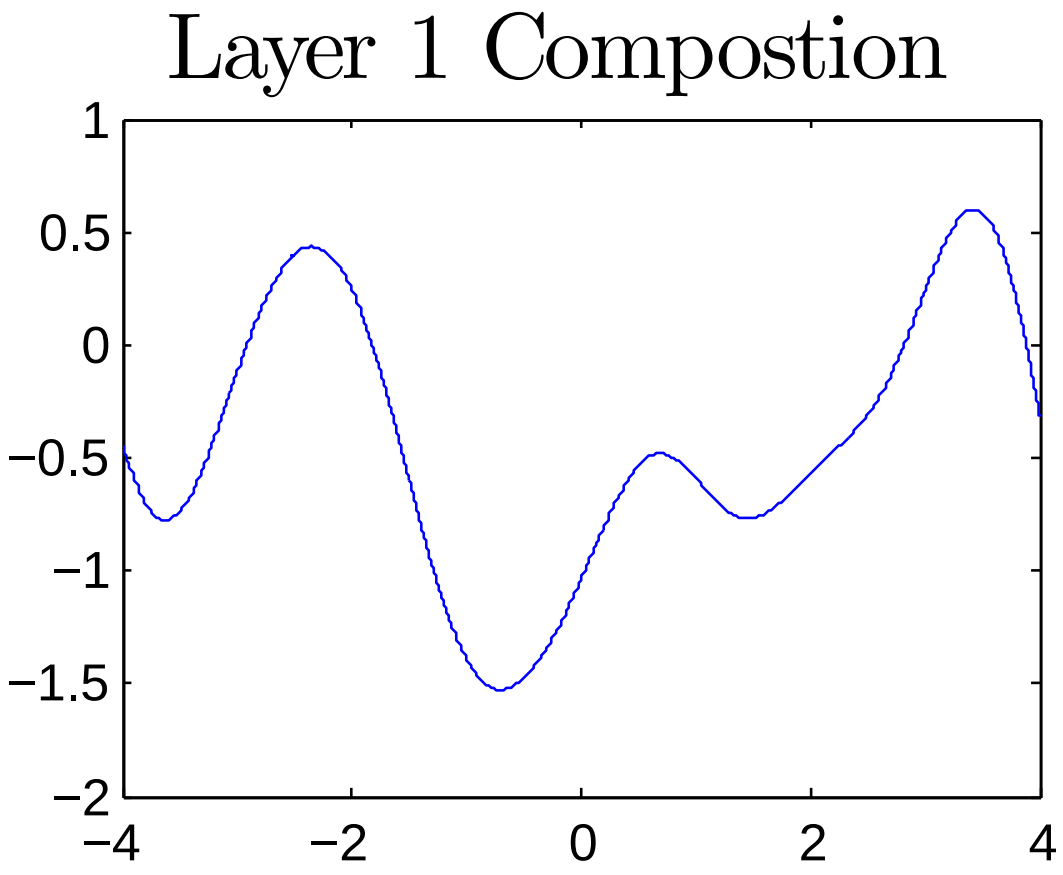
a) standard MLP architecture.



b) Input-connected architecture.

Deep Gaussian Processes

- Draws from input-connected one-dimensional deep GPs:



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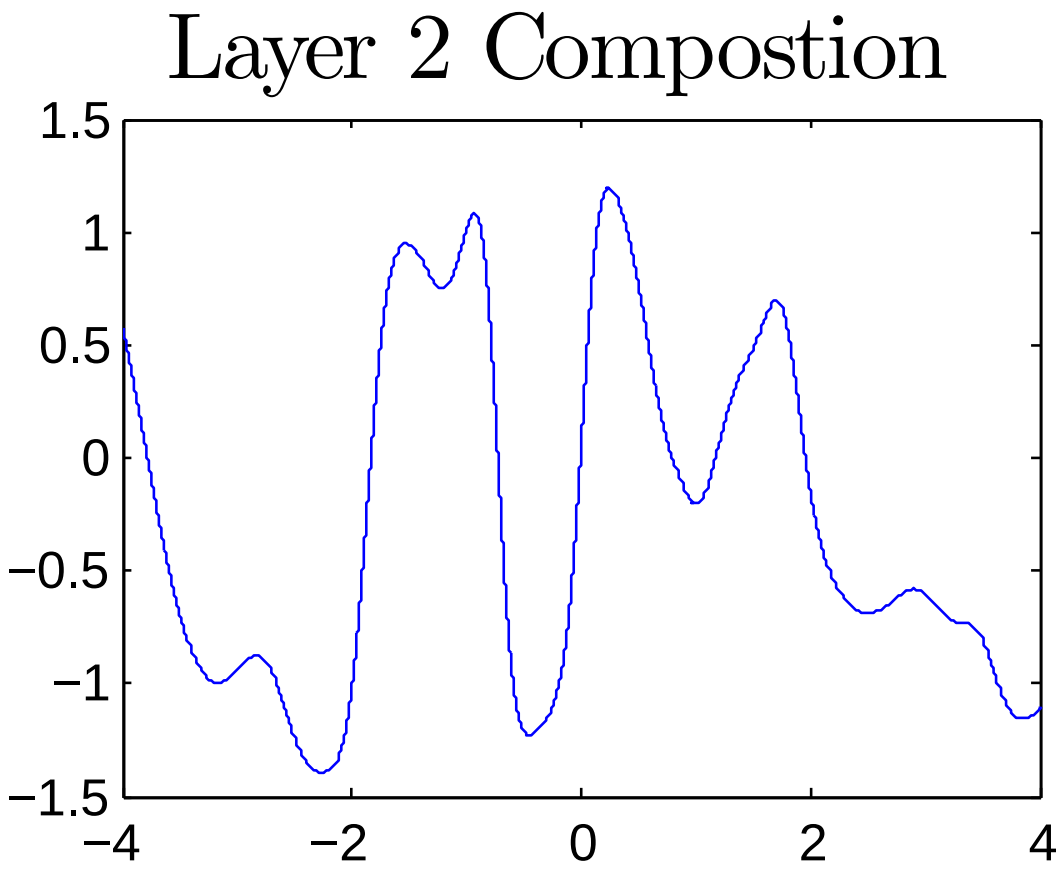

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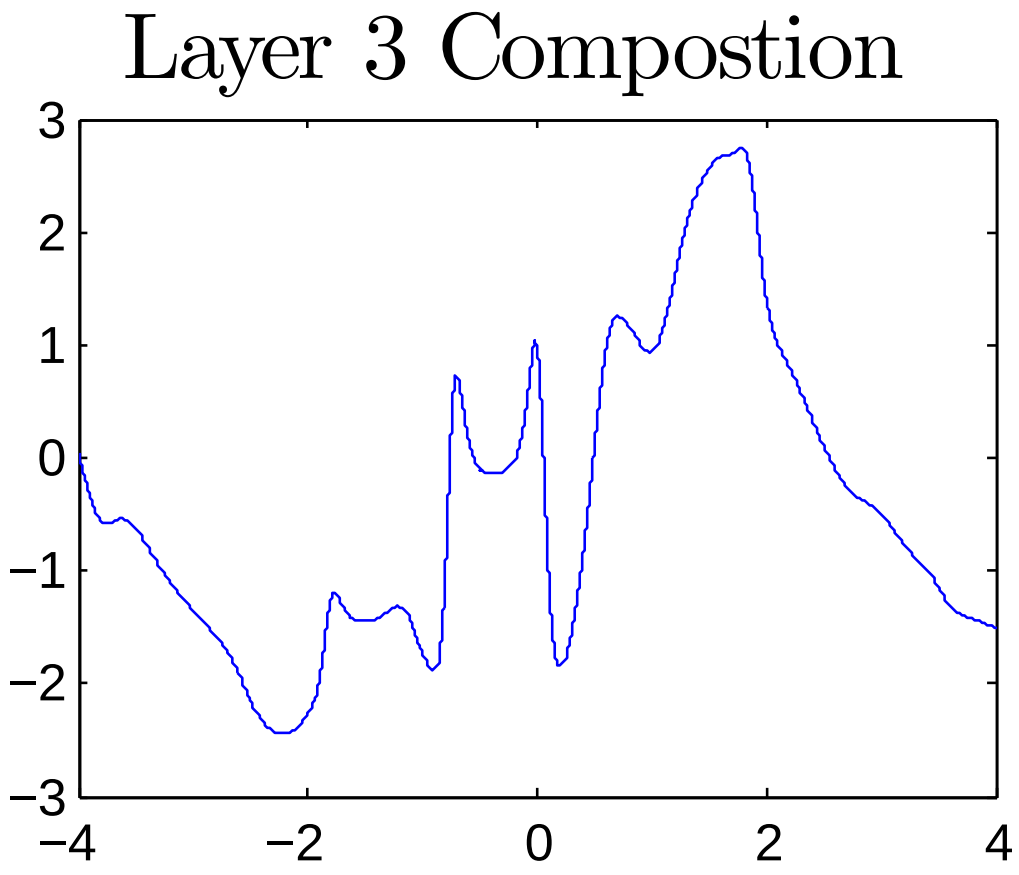

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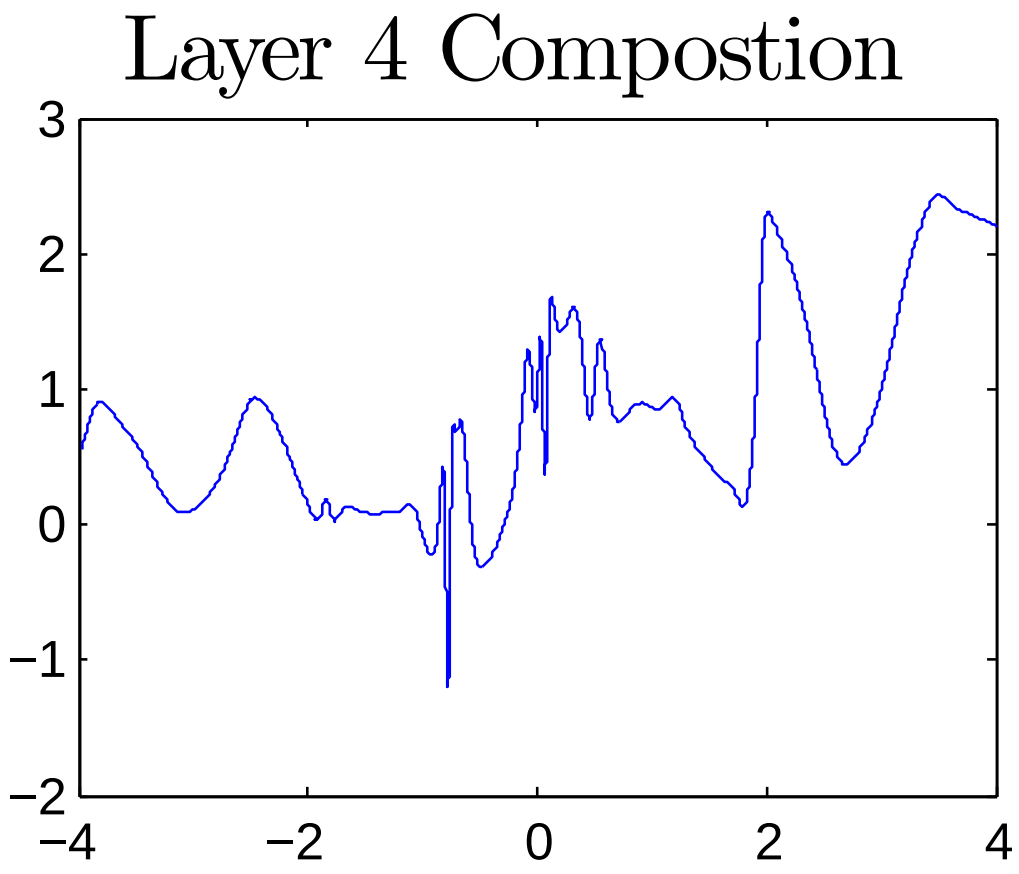

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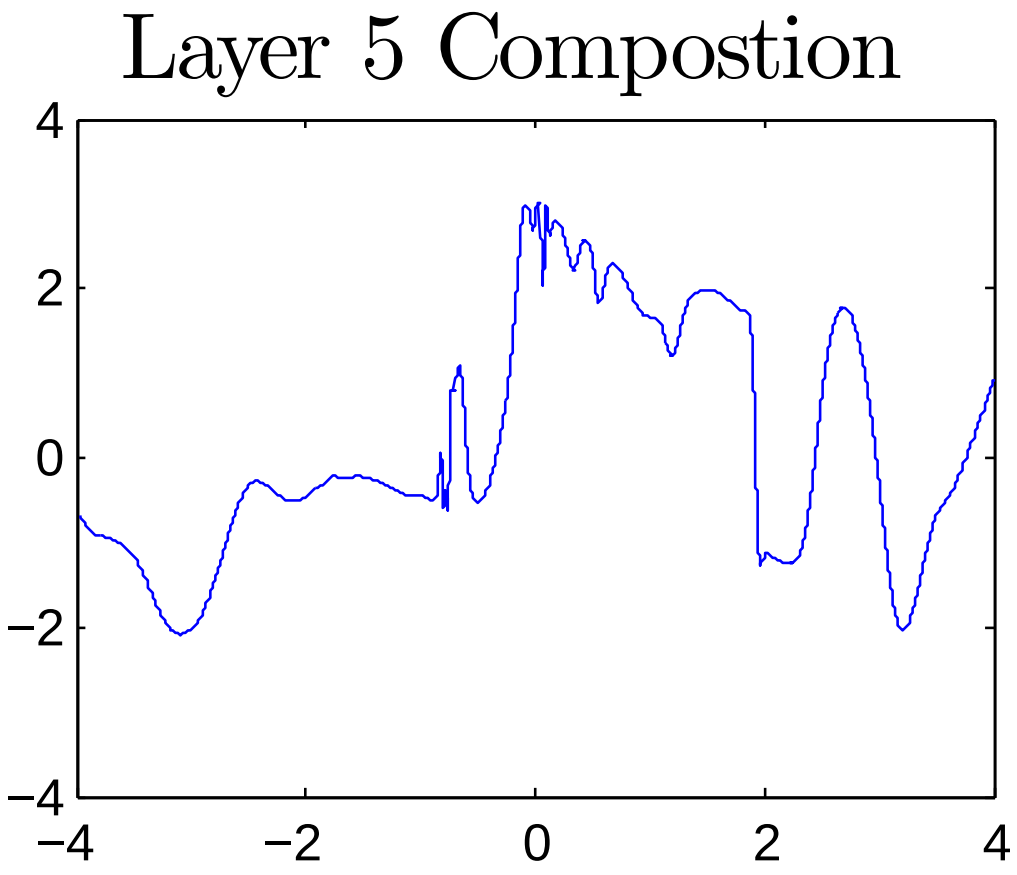

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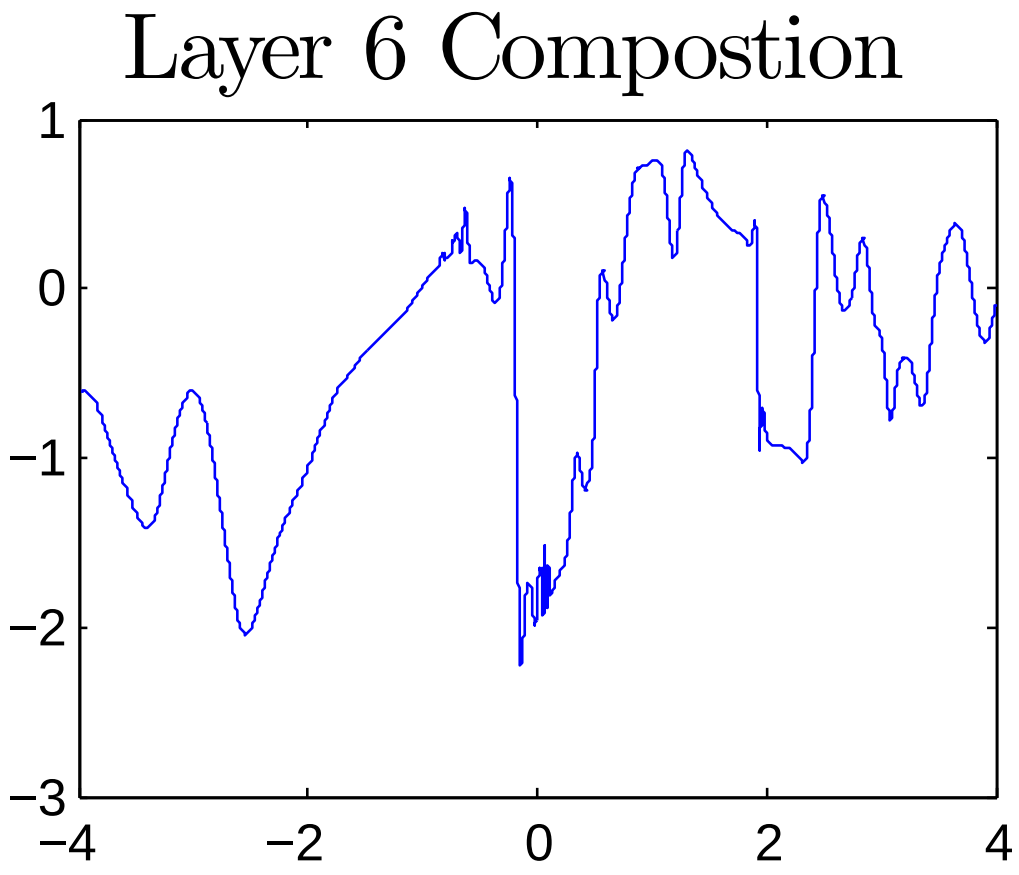

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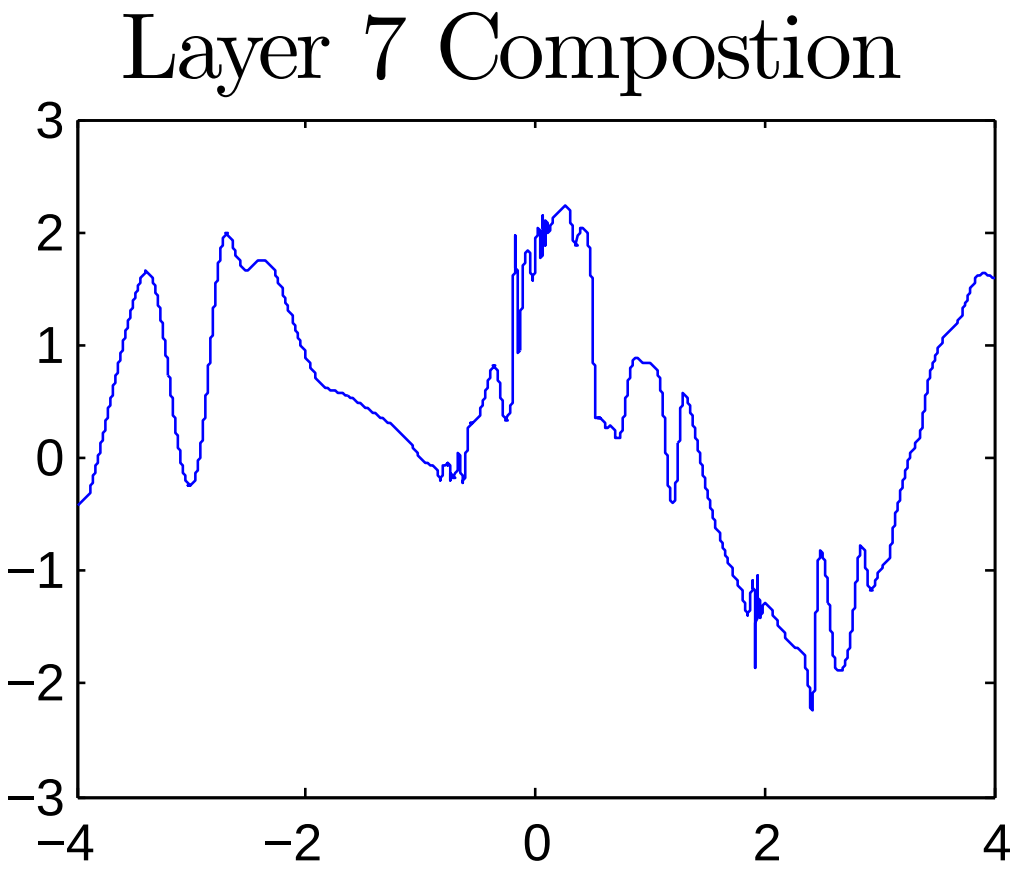

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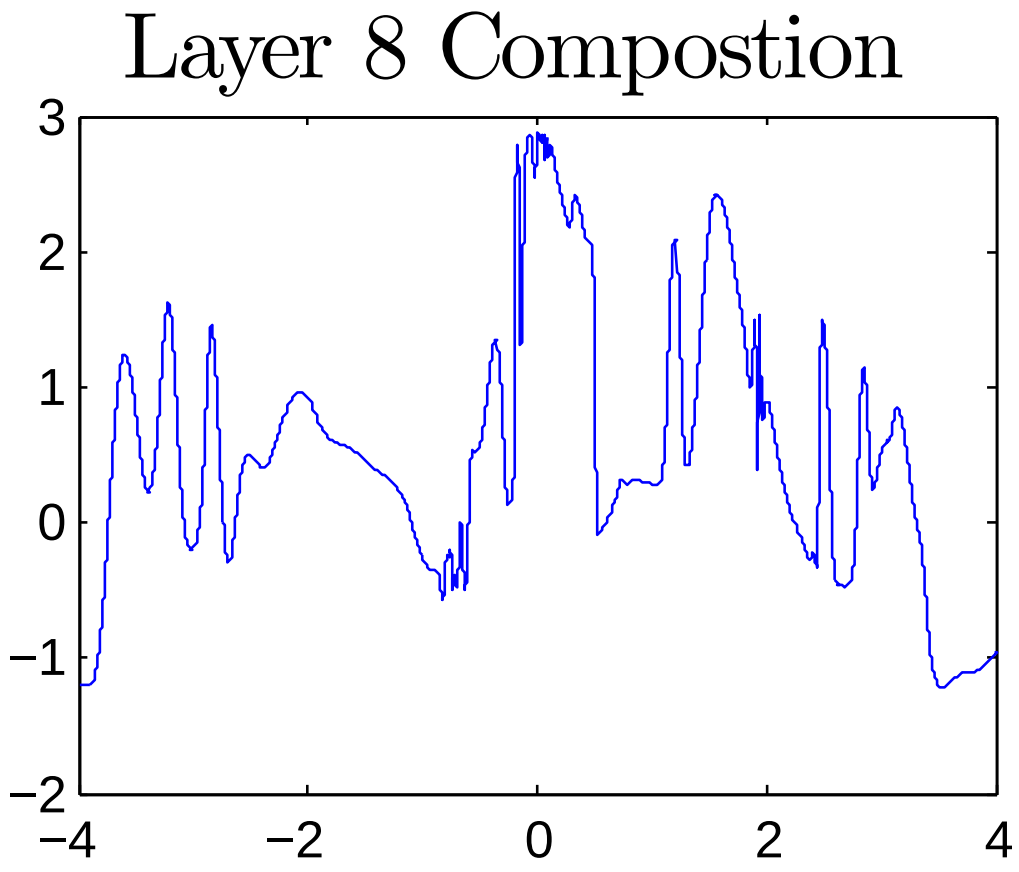

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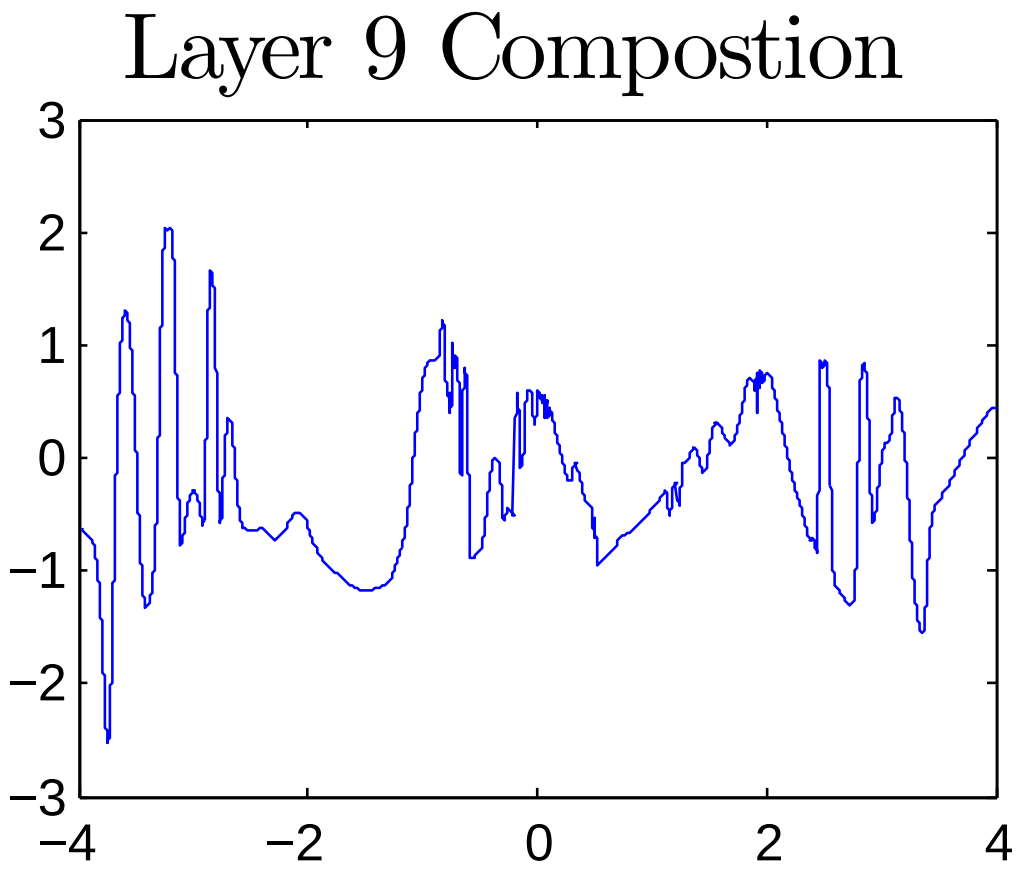

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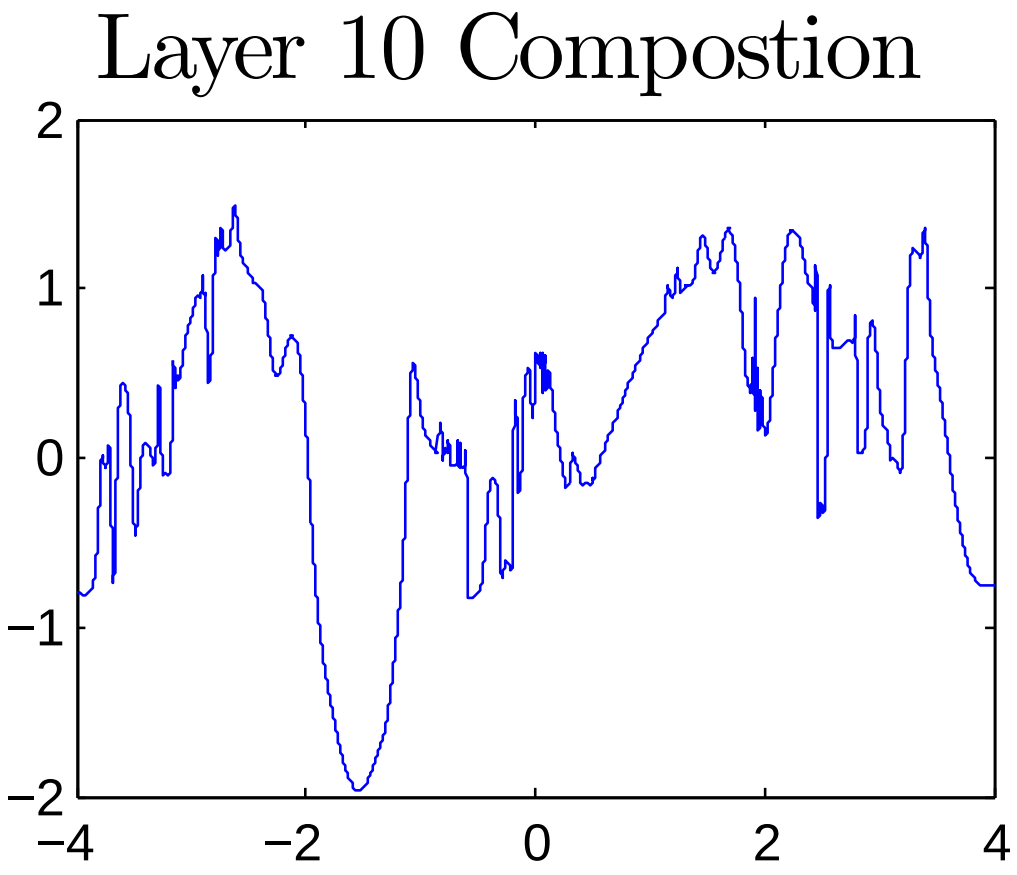
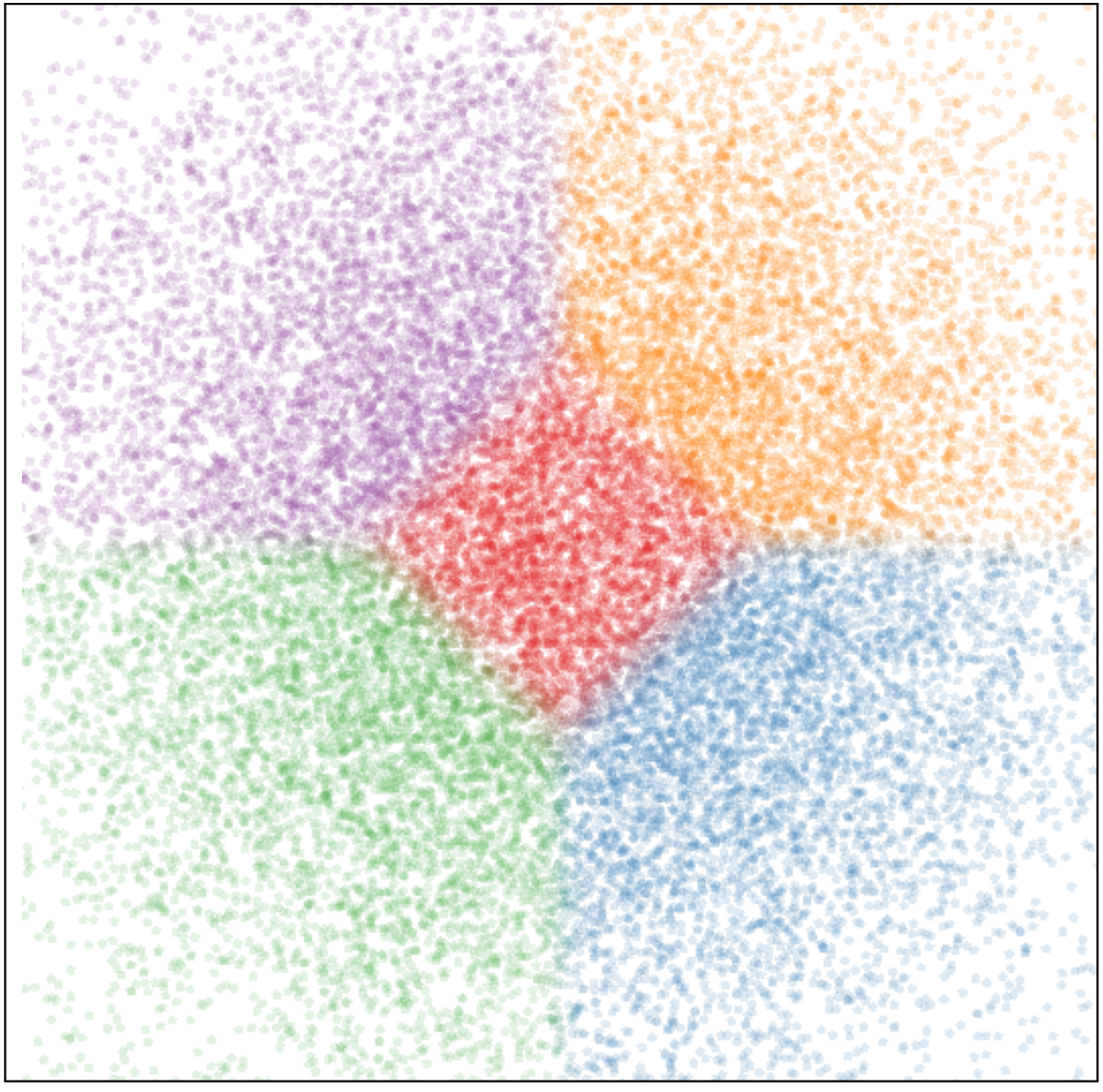


Deep Gaussian Processes

- input-connected 2D to 2D warpings of a Gaussian density:



Deep Gaussian Processes

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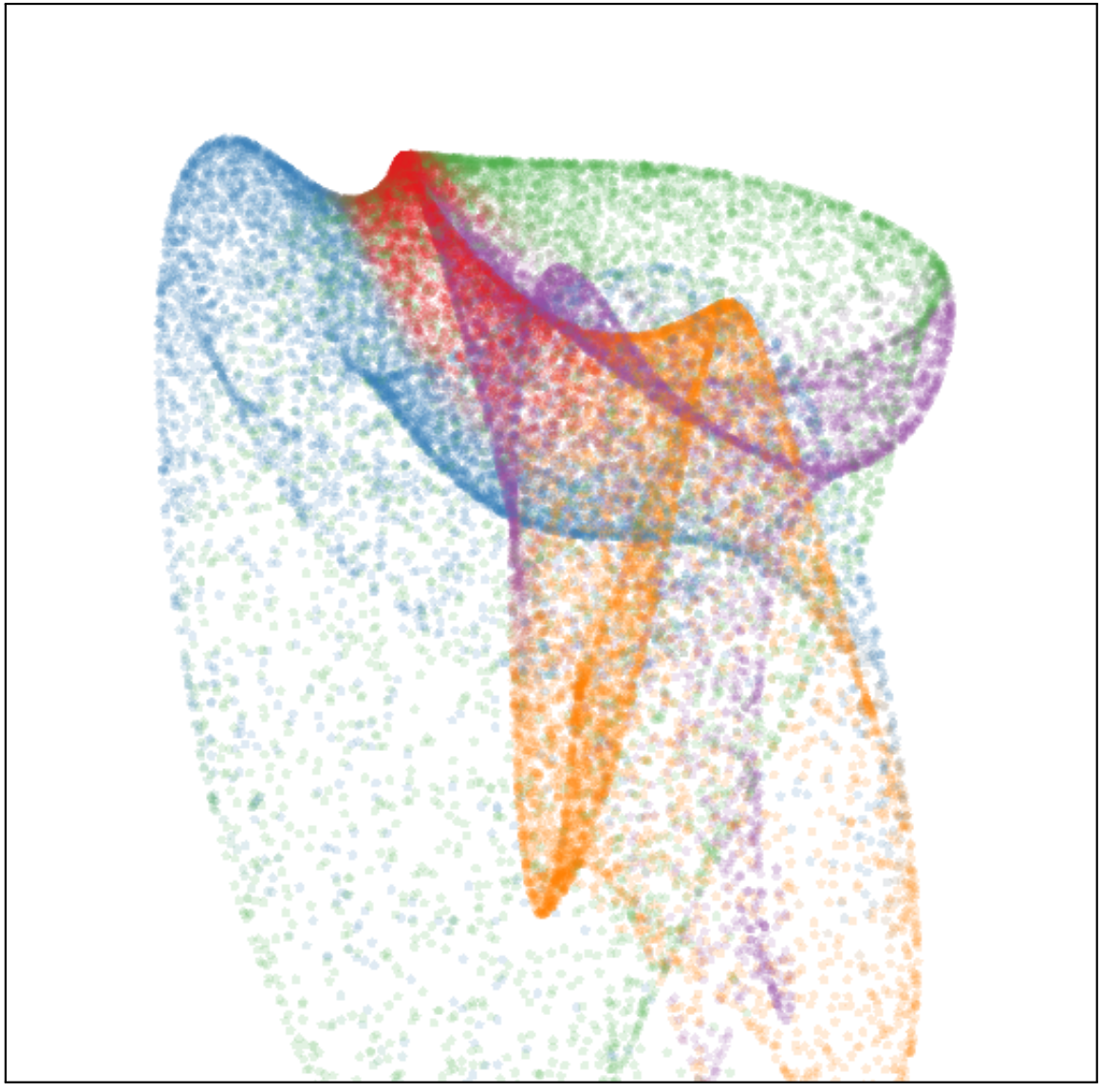

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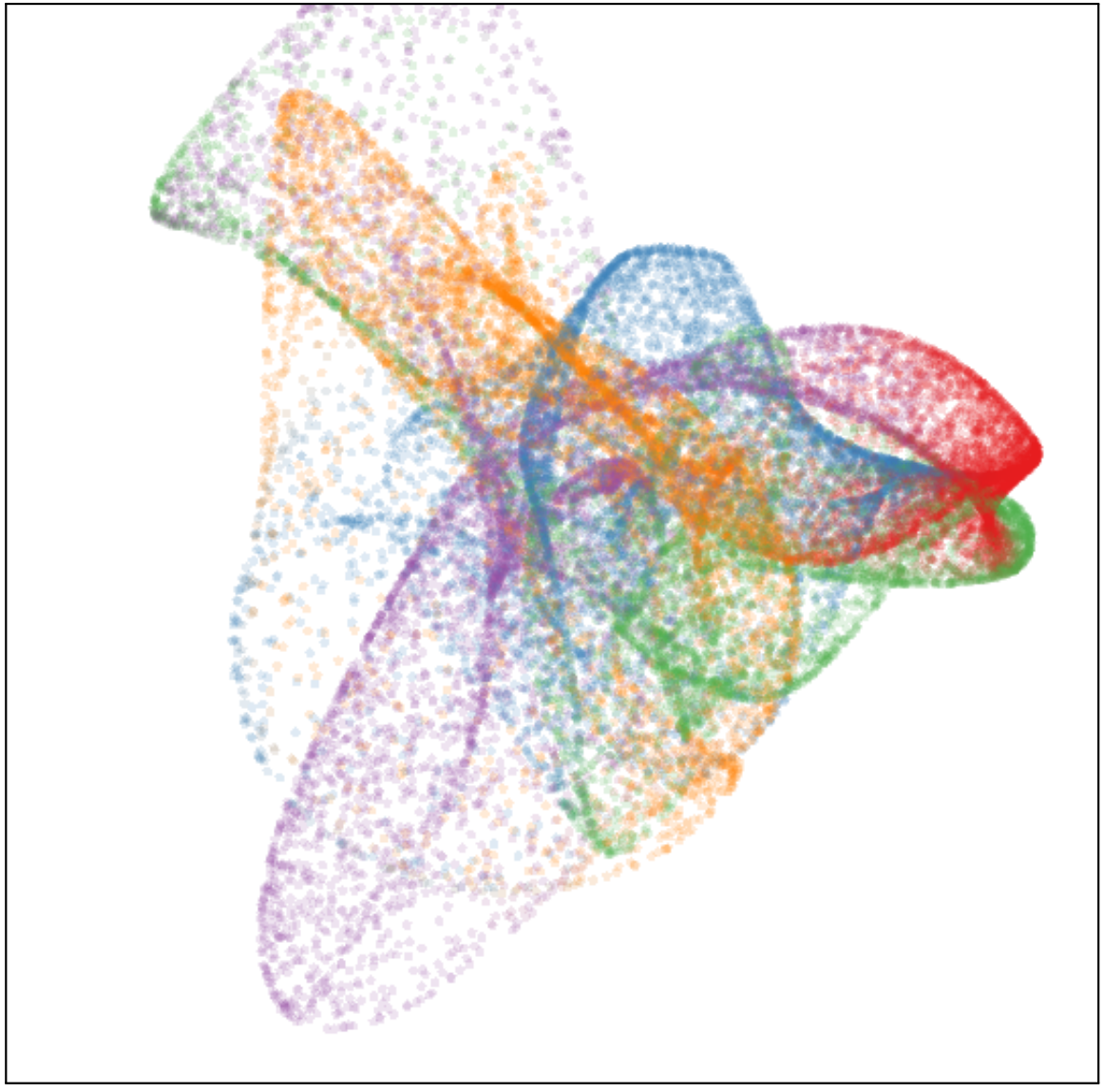

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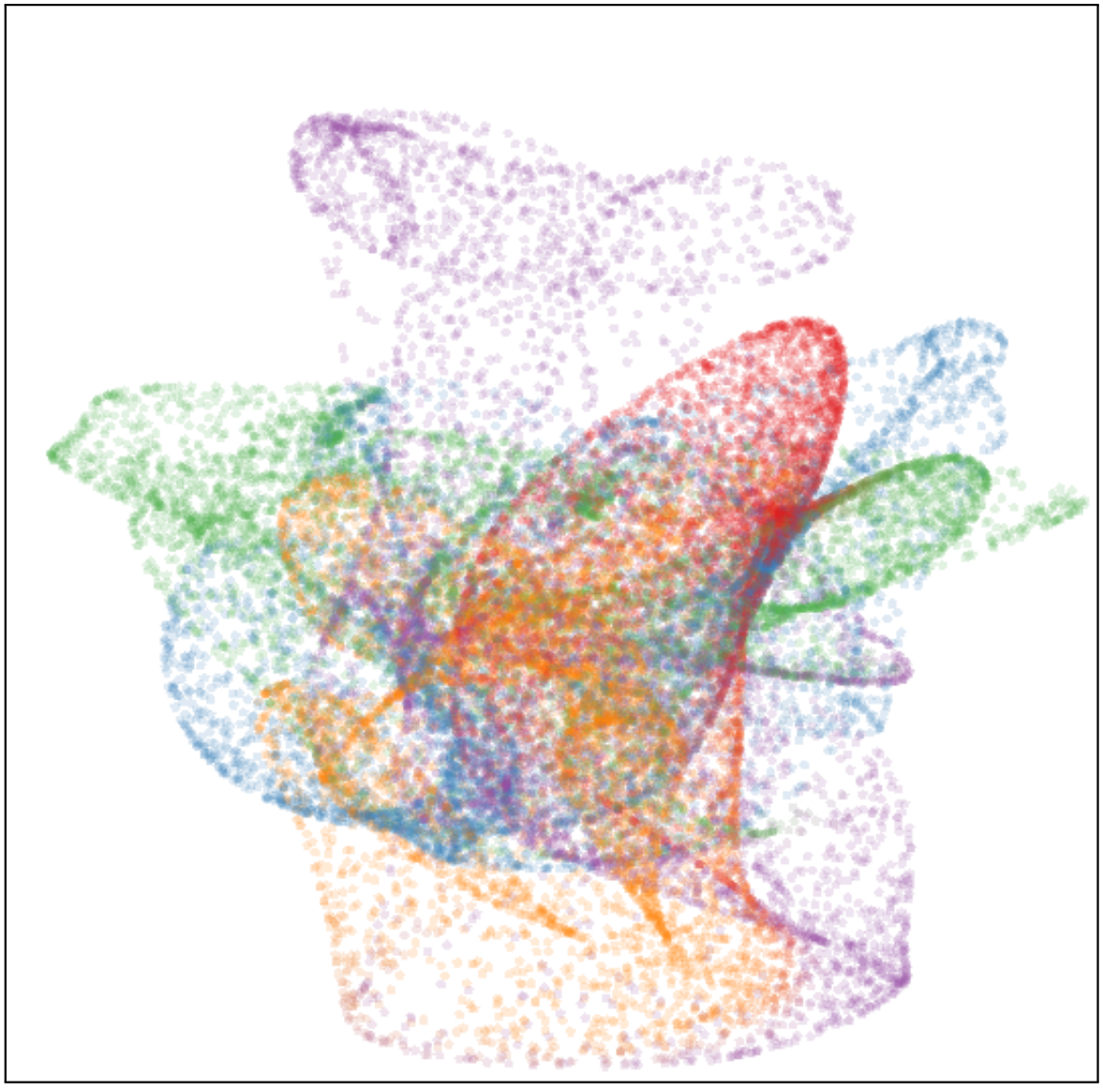

Deep Gaussian Processes

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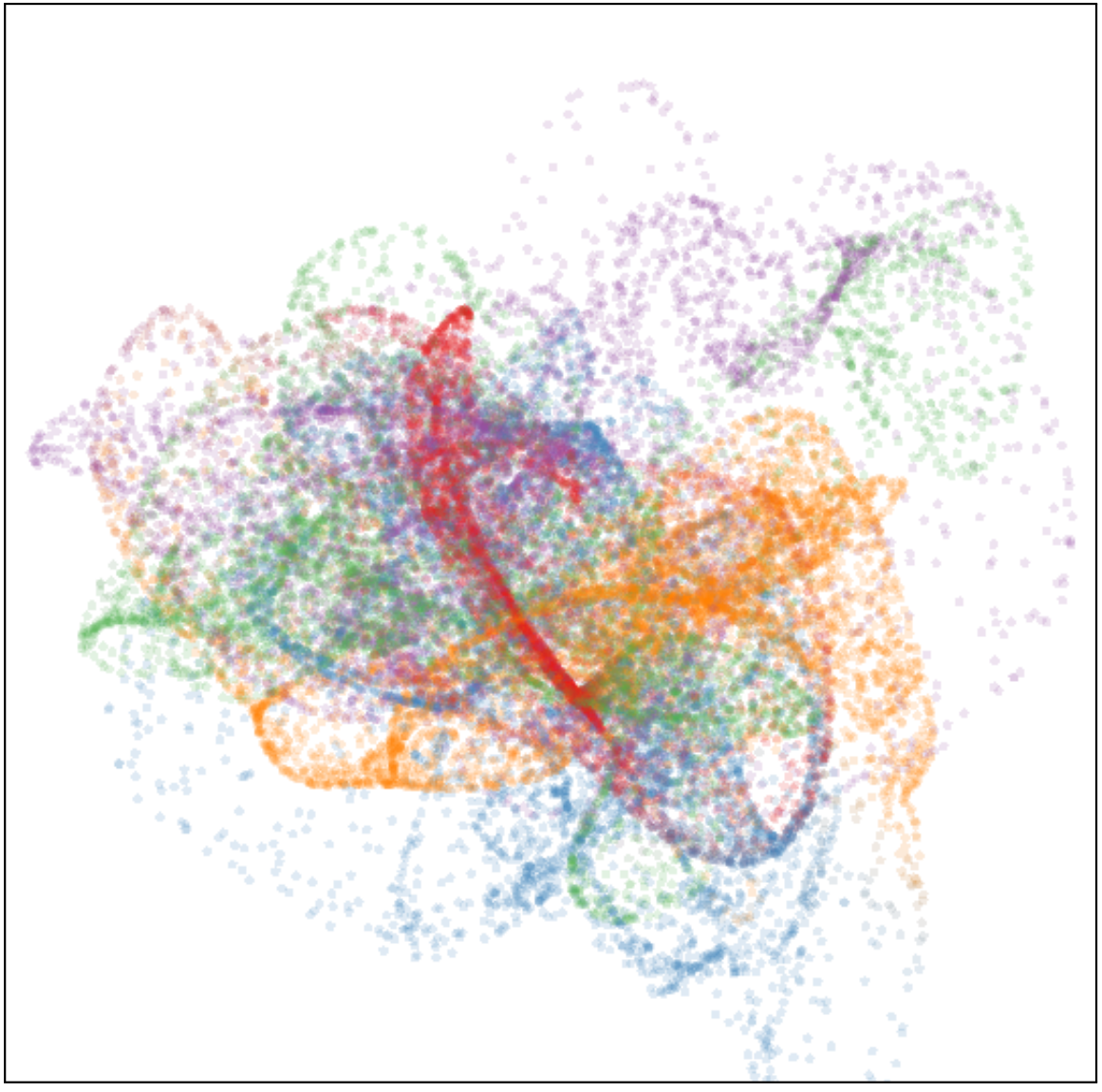
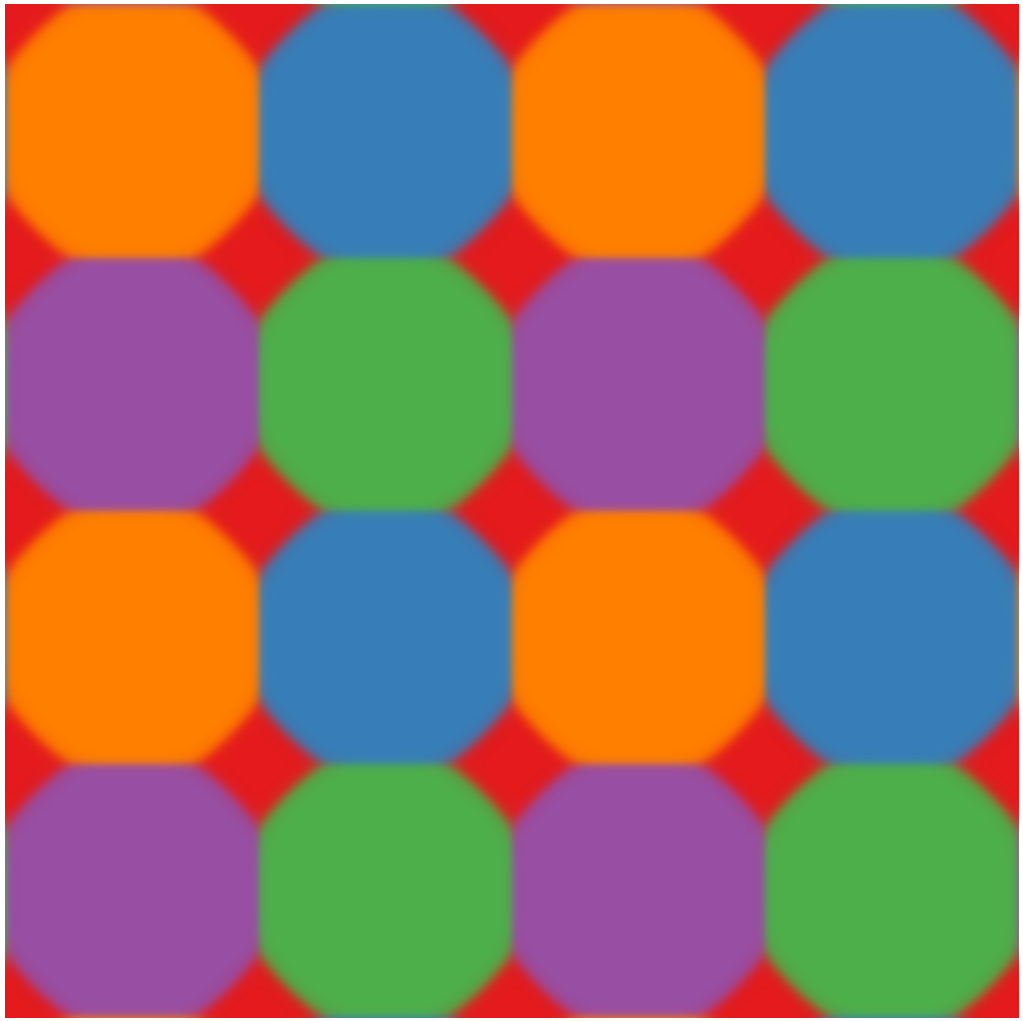


Deep Gaussian Processes

- input-connected 2D to 2D warpings of a Gaussian density:

Deep Gaussian Processes

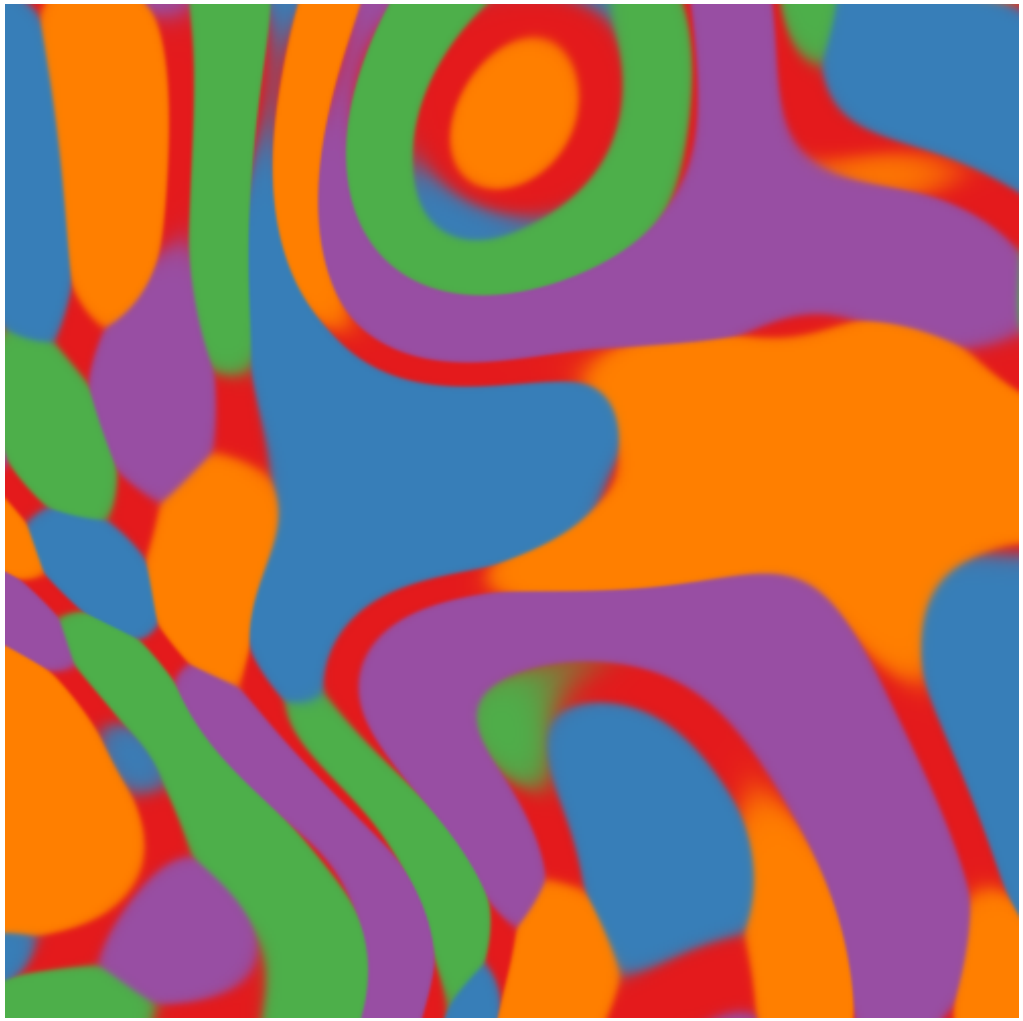
- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)



No warping

Deep Gaussian Processes

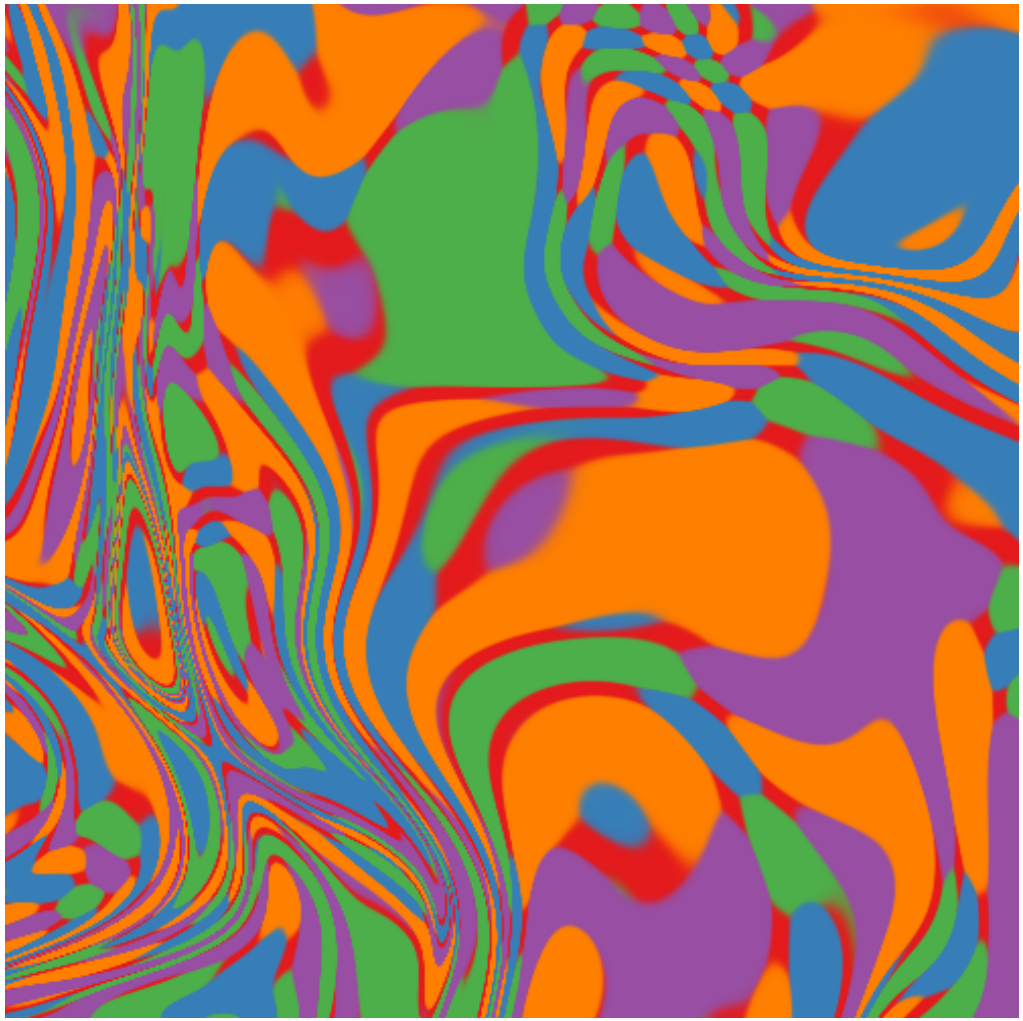
- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)



Two Layers

Deep Gaussian Processes

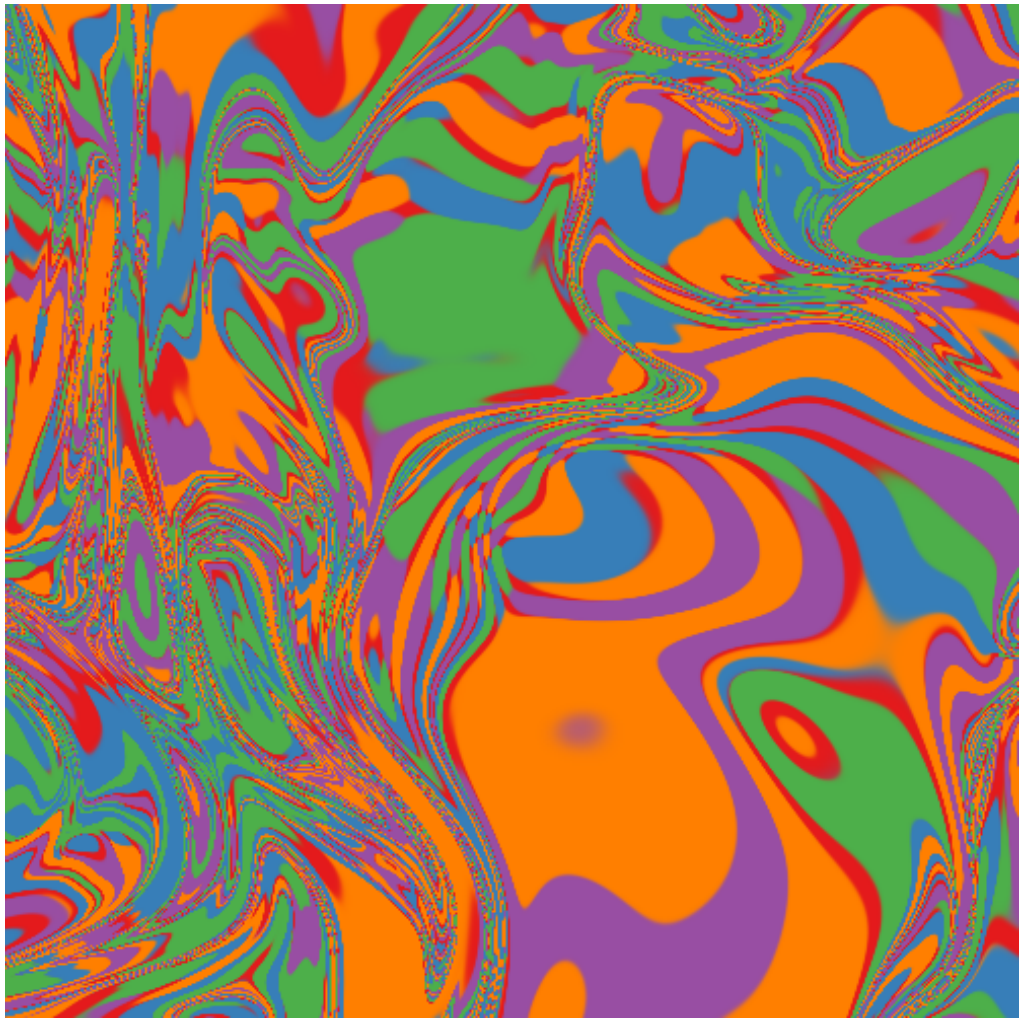
- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)



Ten Layers

Deep Gaussian Processes

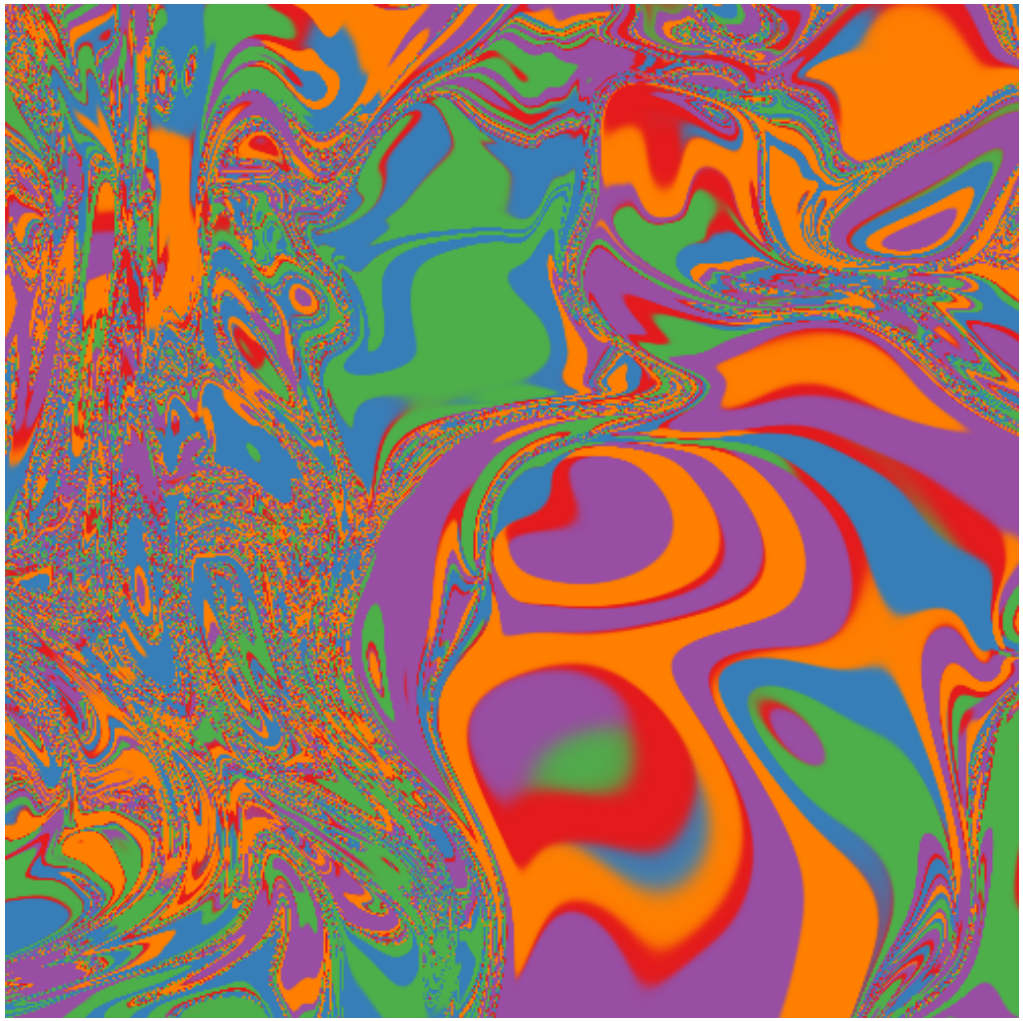
- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)



Twenty Layers

Deep Gaussian Processes

- Showing the x that gave rise to a particular y
- (i.e. decision boundaries)

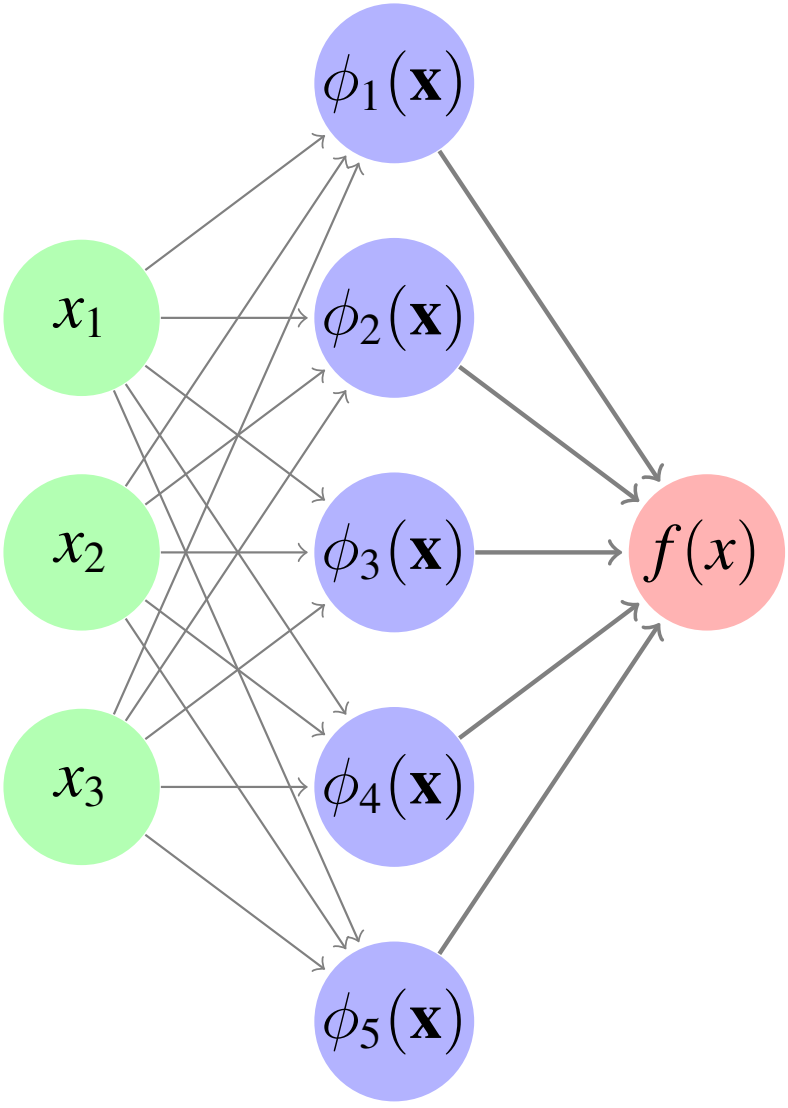


Forty Layers

DROPOUT

- Dropout is a method for regularizing neural networks.
- Recipe:
  1. randomly set half of feature activations to zero
  2. Double the remaining features activations
  3. Average over all possible ways of dropping out
- Gives robustness, since neurons can't depend on one another.
- What do we get when we do dropout in GPs?

Dropout on Feature Activations



Original formulation:

$$f(\mathbf{x}) = \frac{1}{K} \sum_{i=1}^{K} \alpha_i \phi_i(\mathbf{x})$$

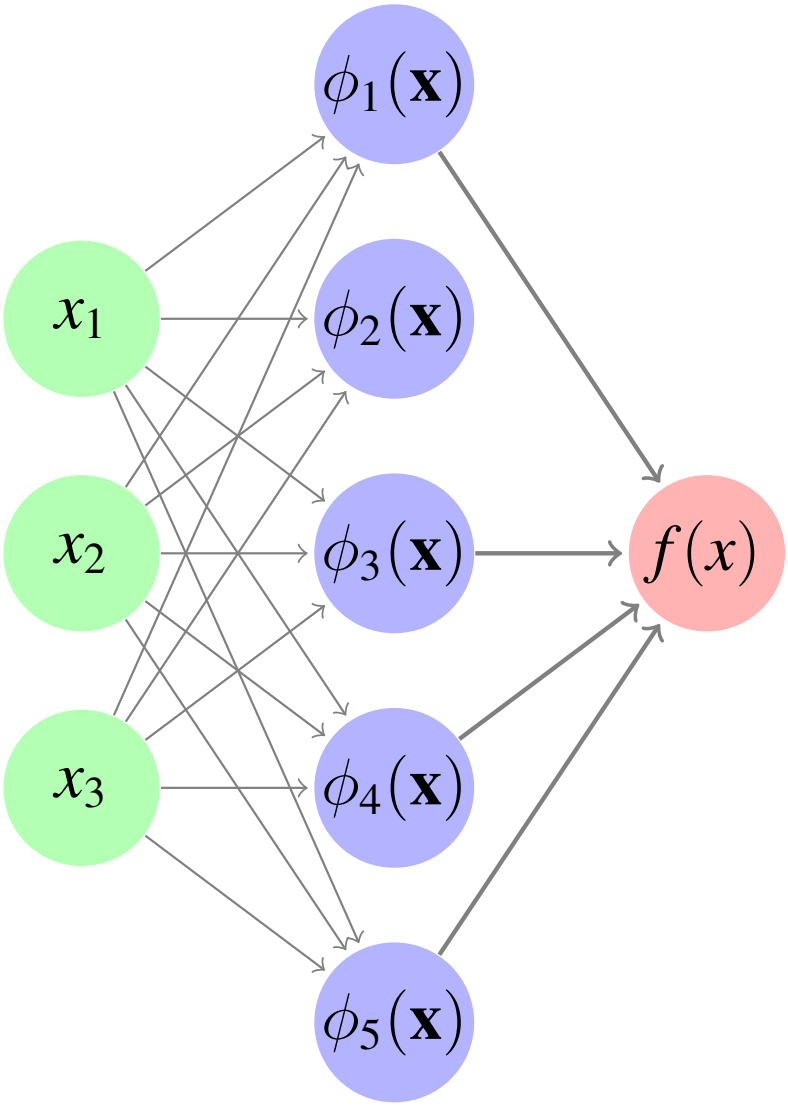
with any weight distribution,

$$\mathbb{E}\left[\alpha_i\right] = 0, \quad \mathbb{V}\left[\alpha_i\right] = \sigma^2$$

by CLT, gives a GP as $K \to \infty$

$$\operatorname{cov}\begin{bmatrix} f(\mathbf{x}) \\ f(\mathbf{x}') \end{bmatrix} \to \frac{\sigma^2}{K} \sum_{i=1}^{K} \phi_i(\mathbf{x}) \phi_i(\mathbf{x}')$$

Dropout on Feature Activations



Remove units with probability ½:

$$f(\mathbf{x}) = \frac{1}{K}\sum_{i=1}^{K} r_i \alpha_i \phi_i(\mathbf{x}) \quad r_i \overset{\text{iid}}{\sim} \text{Ber}(1/2)$$

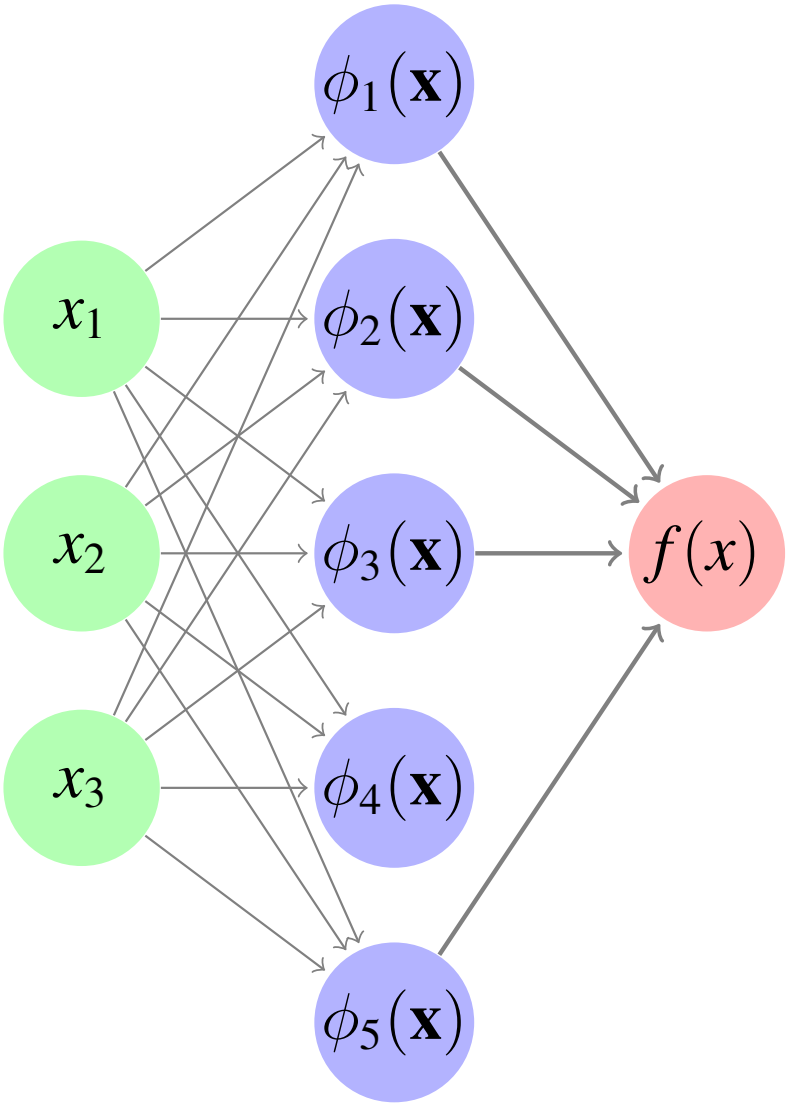
with any weight distribution,

$$\mathbb{E}\left[r_i \alpha_i\right] = 0, \quad \mathbb{V}\left[r_i \alpha_i\right] = \frac{1}{4}\sigma^2$$

by CLT, gives a GP as $K \to \infty$

$$\text{cov}\begin{bmatrix} f(\mathbf{x}) \\ f(\mathbf{x}') \end{bmatrix} \to \frac{1}{4}\frac{\sigma^2}{K}\sum_{i=1}^{K} \phi_i(\mathbf{x})\phi_i(\mathbf{x}')$$

Dropout on Feature Activations



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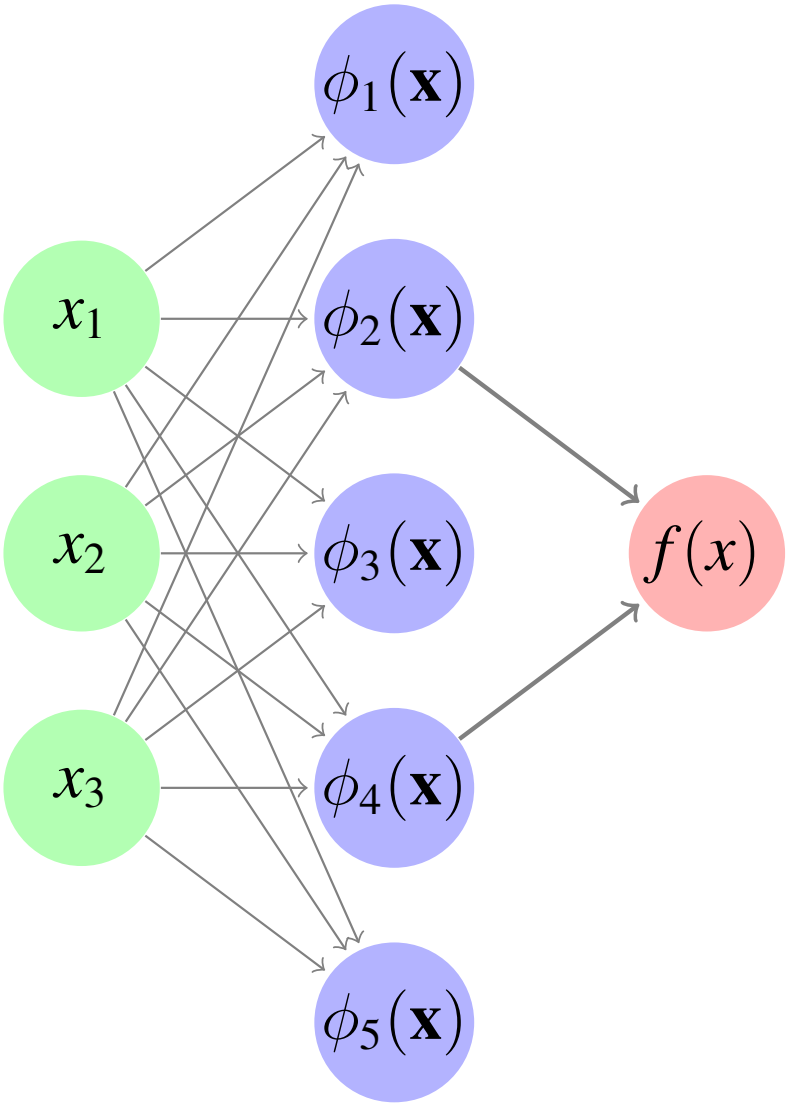

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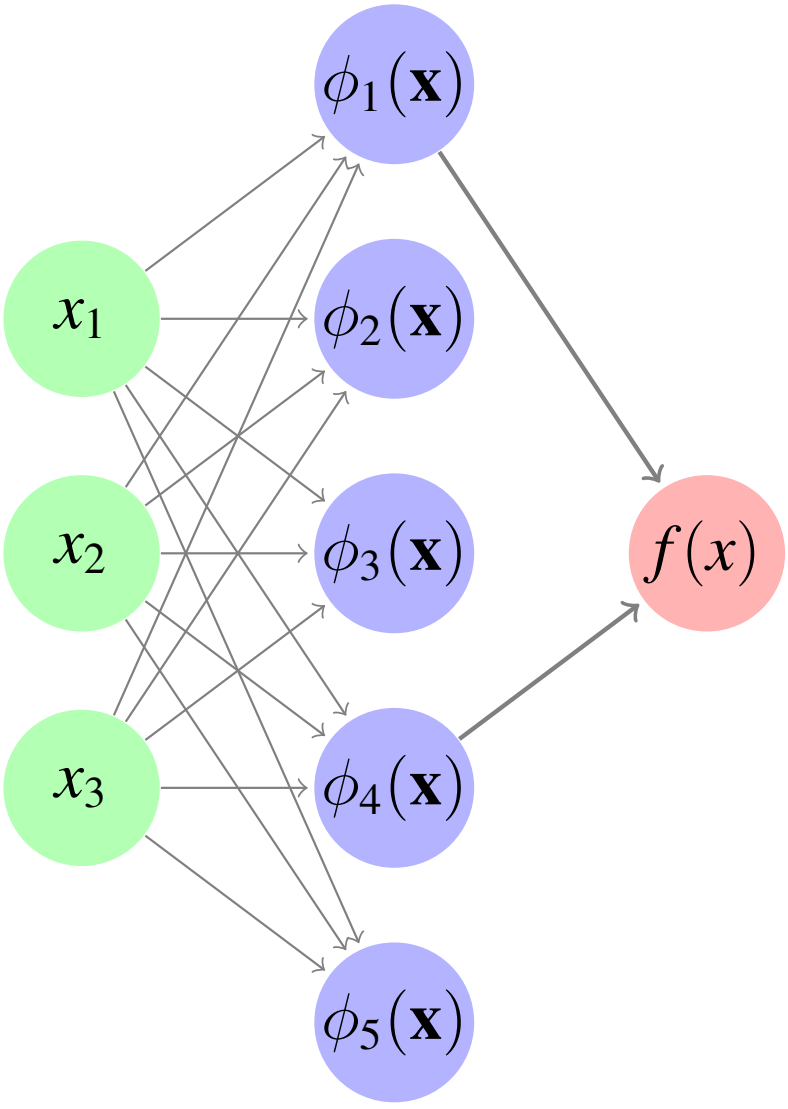

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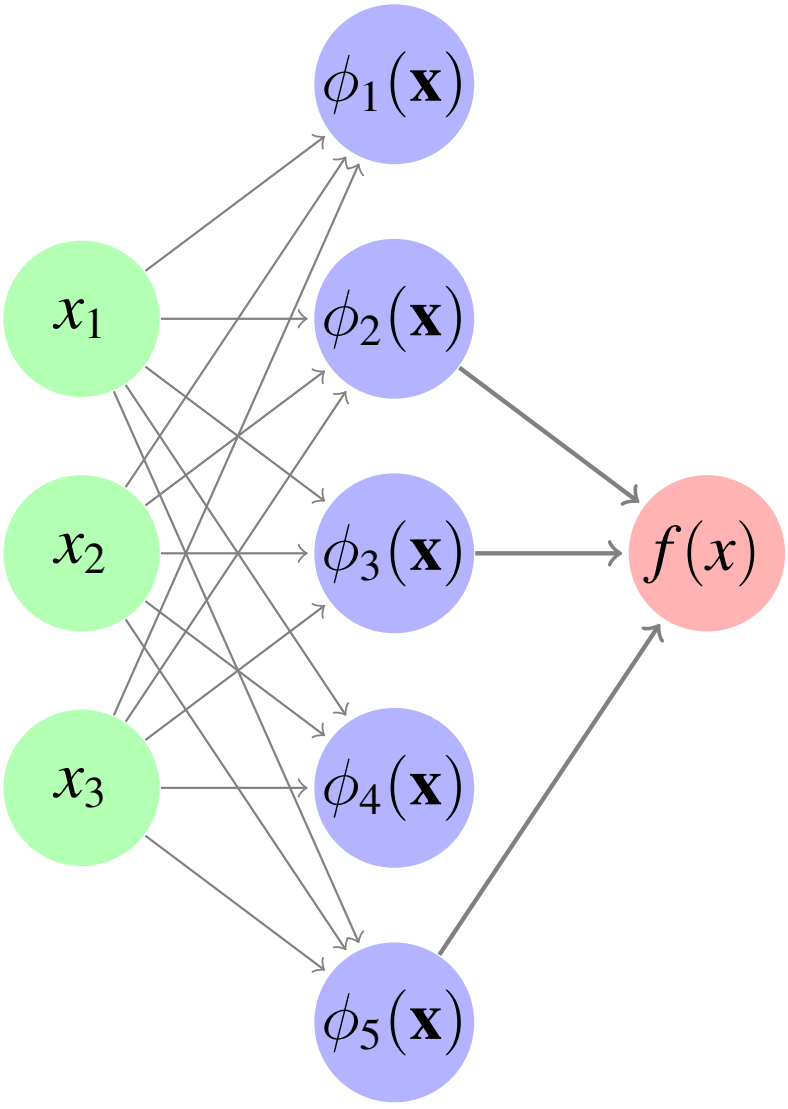
Dropout on Feature Activations



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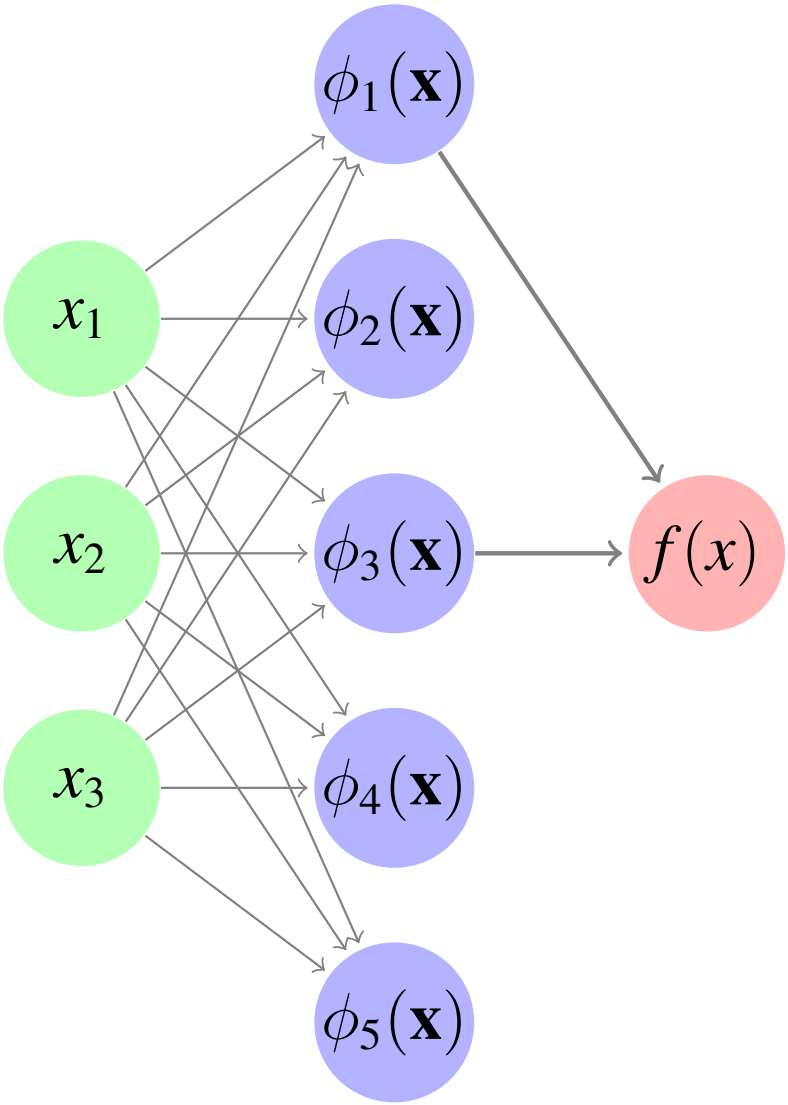

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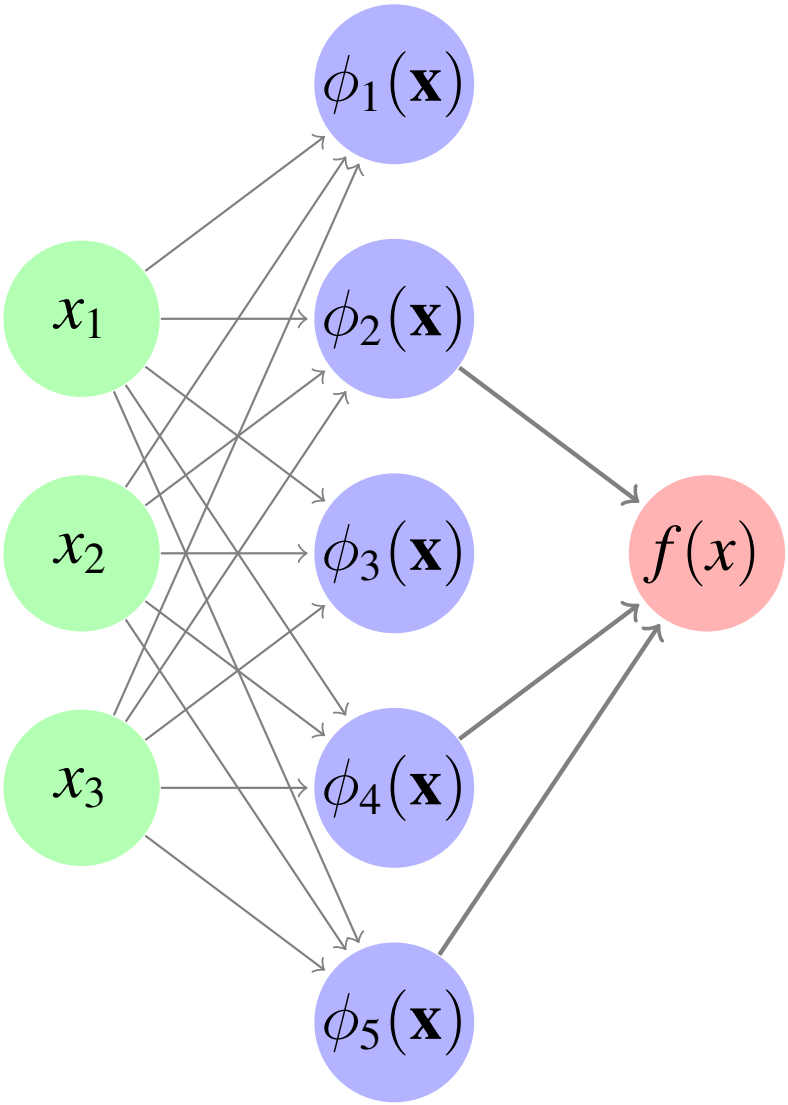

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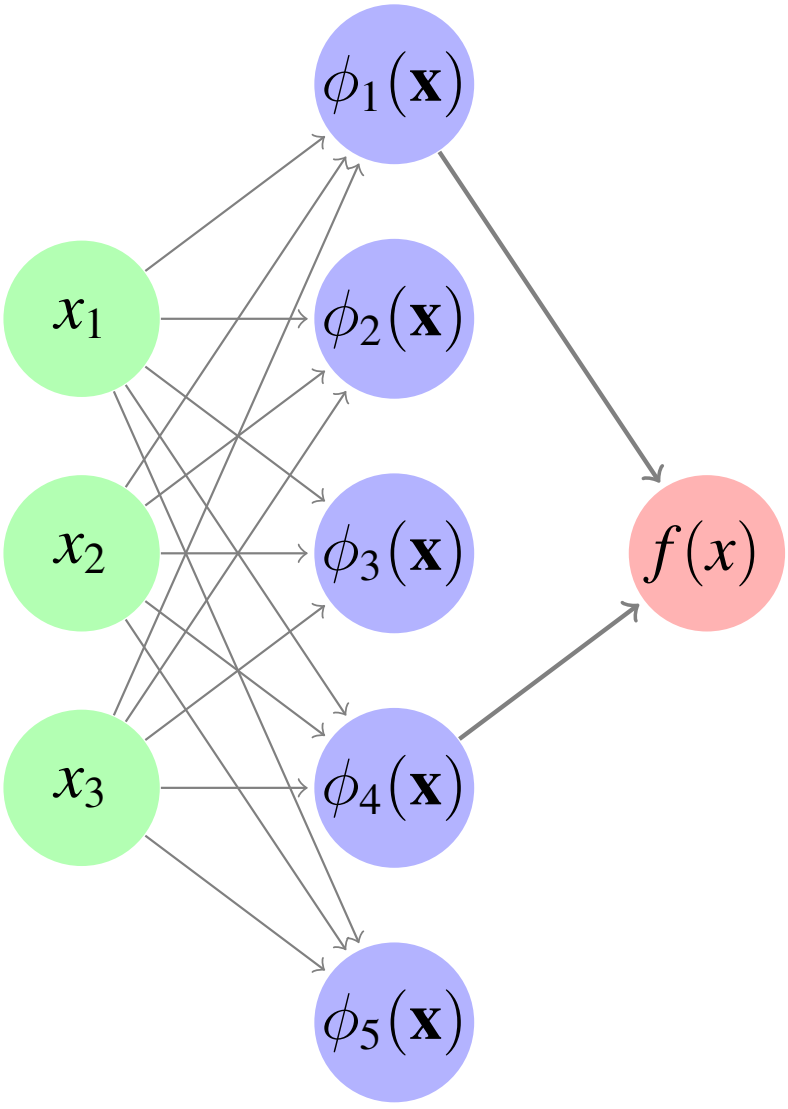

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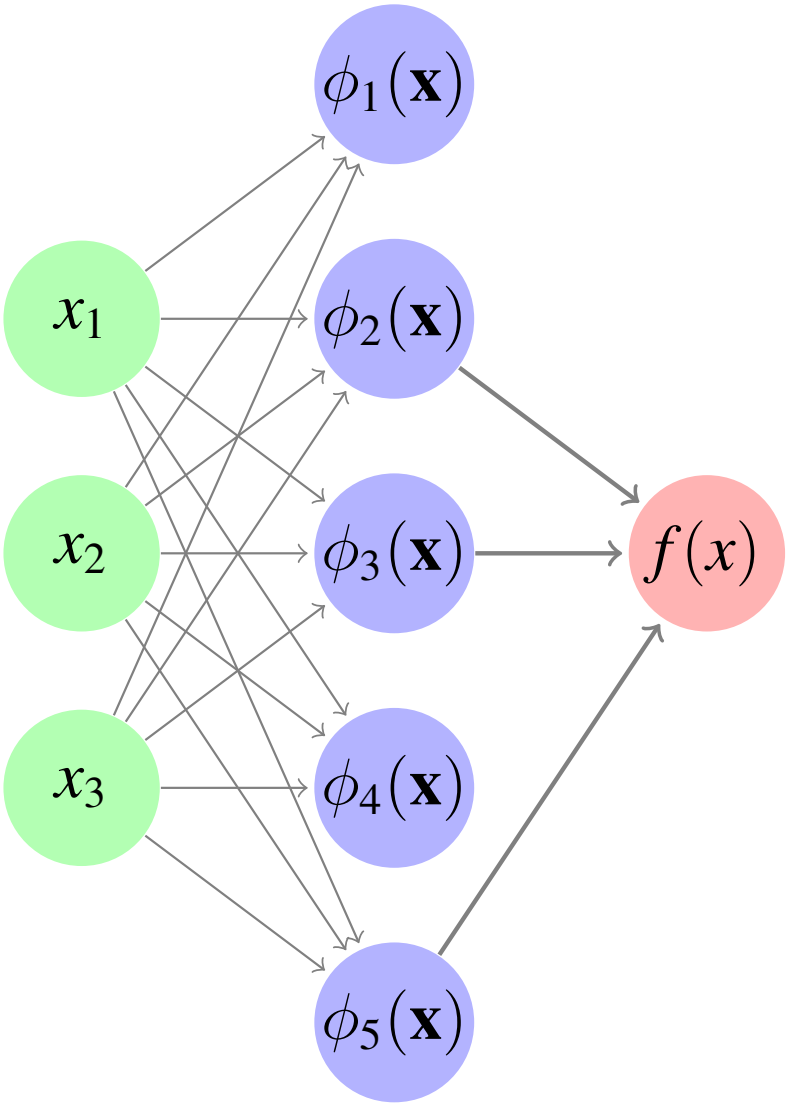

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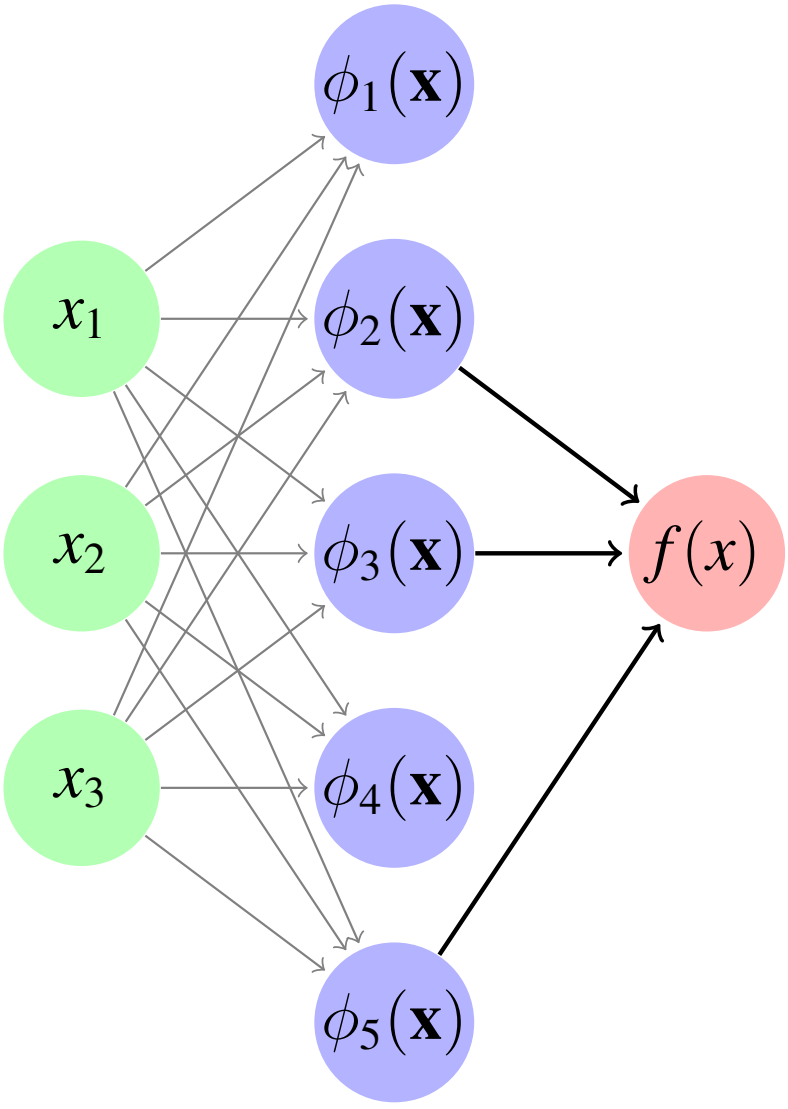
by CLT, gives a GP as $K \to \infty$

$$\text{cov}\begin{bmatrix} f(\mathbf{x}) \\ f(\mathbf{x}') \end{bmatrix} \to \frac{1}{4}\frac{\sigma^2}{K}\sum_{i=1}^{K} \phi_i(\mathbf{x})\phi_i(\mathbf{x}')$$

Dropout on Feature Activations



Double output variance:

$$f(\mathbf{x}) = \frac{2}{K} \sum_{i=1}^{K} r_i \alpha_i \phi_i(\mathbf{x}) \quad r_i \overset{\text{iid}}{\sim} \text{Ber}(1/2)$$

with any weight distribution,

$$\mathbb{E}\left[2 r_i \alpha_i\right] = 0, \quad \mathbb{V}\left[2 r_i \alpha_i\right] = \frac{4}{4}\sigma^2$$

by CLT, gives a GP as $K \to \infty$

$$\text{cov}\begin{bmatrix} f(\mathbf{x}) \\ f(\mathbf{x}') \end{bmatrix} \to \frac{4}{4}\frac{\sigma^2}{K} \sum_{i=1}^{K} \phi_i(\mathbf{x})\phi_i(\mathbf{x}')$$

Dropout on Feature Activations

- Dropout on feature activations gives same GP
  - Averaging the same model doesn't do anything
- GPs were doing dropout all along? ☺
- GPs strange because any one feature doesn't matter.
- Is there a better way to drop out features that would lead to robustness?

Dropout on Inputs

- Let $k(\mathbf{x}, \mathbf{x}') = \prod_{d=1}^{D} k_d(\mathbf{x}_d, \mathbf{x}'_d)$
- Exact averaging over all dropouts is a mixture of GPs:

$$p(f(\mathbf{x})) = \frac{1}{2^D} \sum_{\mathbf{r} \in \{0,1\}^D} \text{GP}\left(0, \prod_{d=1}^{D} k_d(\mathbf{x}_d, \mathbf{x}'_d)^{r_d}\right)$$

- Probably a nice model, but presumably intractable.
- In neural net literature, exponentially-many dropout models are averaged over in tractable ways.
- For instance, dropout mixture has same covariance as

$$f(\mathbf{x}) \sim \text{GP}\left(0, \frac{1}{2^D} \sum_{\mathbf{r} \in \{0,1\}^D} \prod_{d=1}^{D} k_d(\mathbf{x}_d, \mathbf{x}'_d)^{r_d}\right)$$

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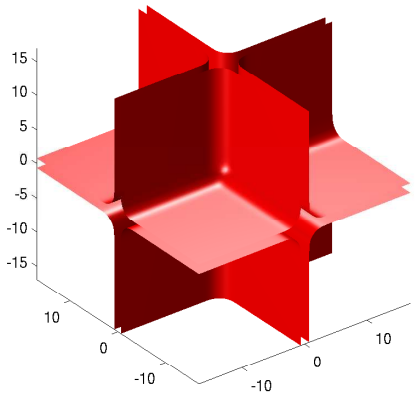
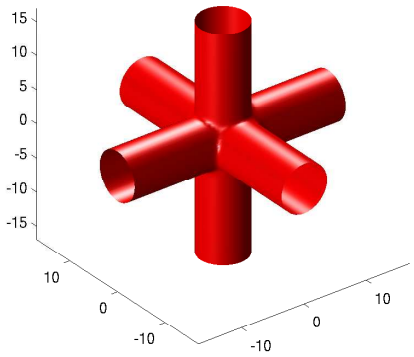
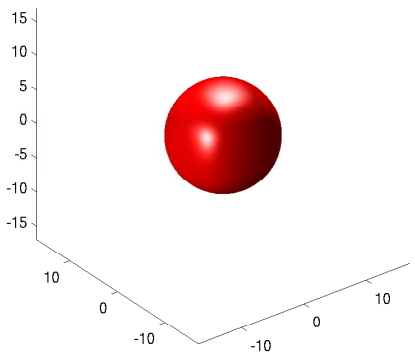
- That's exactly additive GPs! Kernel isocontours look like:



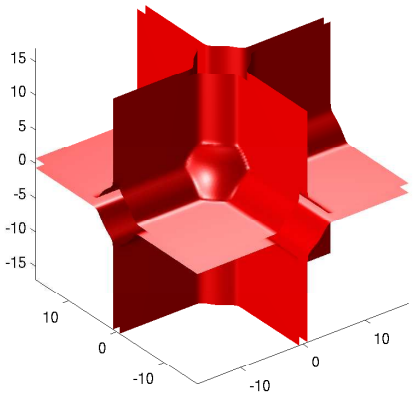
$k_1 + k_2 + k_3$



$k_1k_2 + k_2k_3 + k_1k_3$



$k_1k_2k_3$



all terms

- Can compute all 2^D terms in $\mathcal{O}(D^2)$
- lots of functions, each only depends on some of the inputs

SUMMARY

- At least two different ways to make GPs deep:
  - composing kernels (inference easy, have to specify kernel)
  - composing GPs (inference is hard, but can learn structure)
- Kernel learning is a form of representation learning

- Building priors over functions can shed light on architectures choices or initialization strategies in a data-independent way.
- What sorts of structures do we want to be able to learn?

- We can bring tricks from the neural net literature back to GPs. (still need to try translation-invariant image kernels!)

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Thanks!