Literature Review: Neural Network Gaussian Processes

1. Central Limit Theorem

The Central Limit Theorem states that for $\{X_1, \dots X_N\}$ i.i.d. random variables with $\mathbb{E}[X_n] = \mu$ and $\mathbb{V}[X_n] = \sigma^2 < \infty$ for all $n = 1 \dots N$, then as $N \to \infty$:

$$\sqrt{N}\left(\bar{X}_N - \mu\right) \xrightarrow{d} \mathcal{N}\left(0, \sigma^2\right) \tag{1}$$

where $\bar{X}_N = \frac{1}{N}\sum_{n=1}^{N} X_n$. In other words, the average across N random variables will approach a Gaussian distribution as N approaches infinity.

2. Single-layer Neural Network Proof [lee2018deep]

We will show that by assume i.i.d Gaussian distributions on the weights and biases of a neural network, we can show that the output of a single layer network is the sum of N i.i.d random variables, where N is the network width. Thus by the central limit theorem, the network output will be Gaussian distributed as the network width $N \to \infty$.

2.1 Single-layer Neural Networks

For an input vector $\mathbf{x}^{(in)} \in \mathbb{R}^D$, the m^{th} output of a single layer neural network can be expressed as:

$$y_m = f_m\left(\mathbf{x}^{(in)}\right) = f_m^{post}\left(\mathbf{g^{pre}}\left(\mathbf{x}^{(in)}\right)\right) = f_m^{post}\left(g_1^{pre}\left(\mathbf{x}^{(in)}\right), \dots, g_{N^{(h)}}^{pre}\left(\mathbf{x}^{(in)}\right)\right) \tag{2}$$

with f_m^{post} and g_n^{pre} are defined:

$$y_m = f_m^{post}\left(x_1^{(h)}, \dots, x_{N^{(h)}}^{(h)}\right) = b_m^{(h)} + \sum_{n=1}^{N^{(h)}} W_{m,n}^{(h)} x_n^{(h)} \tag{3}$$

$$x_n^{(h)} = g_n^{pre}\left(\mathbf{x}^{(in)}\right) = \phi\left(b_n^{(in)} + \sum_{d=1}^{D} W_{n,d}^{(in)} x_d^{(in)}\right) \tag{4}$$

where $N^{(h)}$ is the width of the single hidden layer and ϕ is some non-linear activation function.
[JW: ↓ Need to double check ↓]

2.2 Infinite-width Limit

By assuming $b_n^{(in)}$ and $W_{n,d}^{(in)}$ are i.i.d for all $n = 1, \dots, N^{(h)}$ and $d = 1, \dots D$, we can see from (**??**) that:

$$x_n^{(h)} \perp x_{n'}^{(h)}, \forall n \neq n' \text{ and } n, n' = 1, \dots, N^{(h)} \tag{5}$$

As a result from (**??**), f_m is a linear sum of $N^{(h)}$ i.i.d terms, $x_n^{(h)}$. In other words, y_m is a sum of i.i.d random variables which by the central limit theorem states that in the infinite limit as $N^{(h)} \to \infty$, y_m will approach a Gaussian distribution. Moreover, for K inputs $\{\mathbf{x}^1, \ldots, \mathbf{x}^K\}$, the corresponding output set $\{y_m^{(1)}, \ldots, y_m^{(K)}\}$ will follow a joint multivariate Gaussian distribution, meaning that the random function $f_m(\cdot)$ is exactly a Gaussian process.

If we choose $b_m^{(h)}$ and $W_{m,n}^{(h)}$ are i.i.d for all $n = 1, \ldots, N^{(h)}$ and $m = 1, \ldots M$ with zero mean, then the mean $\mu(\mathbf{x})$

[JW: ↑ Need to double check ↑]

3. Multi-layer Neural Network Proof [lee2018deep]

Building on the single layer case, we will show that the elements of the ℓ^{th} layer of a multi-layer neural network is the sum of $N_{\ell-1}$ i.i.d random variables from the $(\ell-1)^{th}$ layer and so in the infinite-width limit as $N_{\ell-1} \to \infty$, the elements of the ℓ^{th} layer will be Gaussian distributed. Thus, by successively taking the infinite-width limit for each $\ell = 1, ..., L$ hidden layer, it is shown that the output of a multi-layer neural network is also Gaussian distributed. [JW: ↓ Need to finish ↓]

3.1 Multi-layer Neural Networks

We can generalise single-layer neural network formulation:

$$y_m = f_m\left(\mathbf{x}^{(in)}\right) = f_m^L\left(\mathbf{g^L}\left(\cdots \mathbf{f^1}\left(\mathbf{g^1}\left(\mathbf{x}^{(in)}\right)\right)\cdots\right)\right) \tag{6}$$

with f_m^ℓ and g_n^ℓ are defined:

$$y_m = f_m^{post}\left(z_1^L, \ldots, z_{N(L)}^L\right) = b_m^L + \sum_{n=1}^{N(L)} W_{m,n_L}^L z_{n_L}^L \tag{7}$$

$$z_{n_\ell} = f_m^{post}\left(x_1^{(h)}, \ldots, x_{N^{(h)}}^{(h)}\right) = b_m^{(h)} + \sum_{n=1}^{N^{(h)}} W_{m,n}^{(h)} x_n^{(h)} \tag{8}$$

$$x_n^{(h)} = g_n^{pre}\left(\mathbf{x}^{(in)}\right) = \phi\left(b_n^{(in)} + \sum_{d=1}^{D} W_{n,d}^{(in)} x_d^{(in)}\right) \tag{9}$$

References