Depth Separation for Neural Networks

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Abstract

Let \( f : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R} \) be a function of the form \( f(x, x') = g(\langle x, x' \rangle) \) for \( g : [-1, 1] \to \mathbb{R} \). We give a simple proof that shows that poly-size depth two neural networks with (exponentially) bounded weights cannot approximate \( f \) whenever \( g \) cannot be approximated by a low degree polynomial. Moreover, for many \( g \)'s, such as \( g(x) = \sin(\pi d^3 x) \), the number of neurons must be \( 2^{\Omega(d \log(d))} \). Furthermore, the result holds w.r.t. the uniform distribution on \( \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \). As many functions of the above form can be well approximated by poly-size depth three networks with poly-bounded weights, this establishes a separation between depth two and depth three networks w.r.t. the uniform distribution on \( \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \).

Keywords: Neural Networks, Depth Separation, Uniform Distribution

1. Introduction and main result

Many aspects of the expressive power of neural networks has been studied over the years. In particular, separation for deep networks (Telgarsky, 2016; Safran and Shamir, 2016), expressive power of depth two networks (Cybenko, 1989; Hornik et al., 1989; Funahashi, 1989; Barron, 1994), and more (Delalleau and Bengio, 2011; Cohen et al., 2016). We focus on the basic setting of depth 2 versus depth 3 networks. We ask what functions are expressible (or well approximated) by poly-sized depth-3 networks, but cannot be approximated by an exponential size depth-2 network.

Two recent papers (Martens et al., 2013; Eldan and Shamir, 2016) addressed this issue. Both papers presented a specific function \( f : \mathbb{R}^d \to \mathbb{R} \) and a distribution \( D \) on \( \mathbb{R}^d \) such that \( f \) can be approximated w.r.t. \( D \) by a poly\((d)\)-size depth 3 network, but not by a poly\((d)\)-size depth 2 network. In Martens et al. (2013) this was shown for \( f \) being the inner product mod 2 and \( D \) being the uniform distribution on \( \{0, 1\}^d \times \{0, 1\}^d \). In Eldan and Shamir (2016) it was shown for a different (radial) function and some (unbounded) distribution.

We extend the above results and prove a similar result for an explicit and rich family of functions, and w.r.t. the uniform distribution on \( \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \). In addition, our lower bound on the number of required neurons is stronger: while previous papers showed that the number of neurons has to be exponential in \( d \), we show exponential dependency on \( d \log(d) \). Last, our proof is short, direct and is based only on basic Harmonic analysis over the sphere. In contrast, Eldan and Shamir (2016)'s proof is rather lengthy and requires advanced technical tools such as tempered distributions, while Martens et al. (2013) relied on the discrepancy of the inner product function mod 2. On the other hand, Eldan and Shamir (2016) do not put any restriction on the magnitude of the weights, while we and Martens et al. (2013) do require a mild (exponential) bound.

Let us fix an activation function \( \sigma : \mathbb{R} \to \mathbb{R} \). For \( x \in \mathbb{R}^n \) we denote \( \sigma(x) = (\sigma(x_1), \ldots, \sigma(x_n)) \). We say that \( F : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R} \) can be implemented by a depth-2 \( \sigma \)-network of width \( r \) and...
weights bounded by \( B \) if

\[
F(x, x') = w_2^T \sigma(W_1 x + W'_1 x' + b_1) + b_2 ,
\]

where \( W_1, W'_1 \in [-B, B]^{r \times d}, w_2 \in [-B, B]^r, b_1 \in [-B, B]^r \) and \( b_2 \in [-B, B] \). Similarly, \( F : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R} \) can be implemented by a depth-3 \( \sigma \)-network of width \( r \) and weights bounded by \( B \) if

\[
F(x, x') = w_3^T \sigma(W_2 \sigma(W_1 x + W'_1 x' + b_1) + b_2) + b_3
\]

for \( W_1, W'_1 \in [-B, B]^{r \times d}, W_2 \in [-B, B]^{r \times r}, w_3 \in [-B, B]^r, b_1, b_2 \in [-B, B]^r \) and \( b_3 \in [-B, B] \). Denote

\[
N_{d,n} = \left( \frac{d + n - 1}{d - 1} \right) - \left( \frac{d + n - 3}{d - 1} \right) = \frac{2n + d - 2(n + d - 3)!}{n!(d - 2)!}.
\]

Let \( \mu_d \) be the probability measure on \([-1, 1]\) given by \( d\mu_d(x) = \frac{\Gamma\left(\frac{d}{2}\right)}{\sqrt{\pi} \Gamma\left(\frac{d+1}{2}\right)} (1-x^2)^{\frac{d-3}{2}} dx \) and define

\[
A_{n,d}(f) = \min_{p \text{ is degree } n-1 \text{ polynomial}} \|f - p\|_{L^2(\mu_d)}
\]

Our main theorem shows that if \( A_{n,d}(f) \) is large then \( (x, x') \mapsto f(\langle x, x' \rangle) \) cannot be approximated by a small depth-2 network.

**Theorem 1 (main)** Let \( N : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R} \) be any function implemented by a depth-2 \( \sigma \)-network of width \( r \), with weights bounded by \( B \). Let \( f : [-1, 1] \to \mathbb{R} \) and define \( F : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R} \) by \( F(x, x') = f(\langle x, x' \rangle) \). Then, for all \( n \),

\[
\|N - F\|_{L^2(\mathbb{S}^{d-1} \times \mathbb{S}^{d-1})} \geq A_{n,d}(f) \left( A_{n,d}(f) - \frac{2rB \max_{\|x\| \leq \sqrt{4d}B + B} |\sigma(x)| + 2B}{\sqrt{N_{d,n}}} \right)
\]

**Example 1** Let us consider the case that \( \sigma(x) = \max(0, x) \) is the ReLU function, \( f(x) = \sin(\pi^d x) \), \( n = d^2 \) and \( B = 2^d \). In this case, lemma 4 implies that \( A_{n,d}(f) \geq \frac{1}{5\pi} \). Hence, to have \( \frac{1}{50\pi d^2} \)-approximation of \( F \), the number of hidden neurons has to be at least,

\[
\frac{\sqrt{N_{d,d}}}{20\pi 2^d (1 + \sqrt{4d}) + 2d^2} = 2^\Omega(d \log(d))
\]

On the other hand, corollary 6 implies that \( F \) can be \( \epsilon \)-approximated by a ReLU network of depth 3, width \( \frac{16\pi d^2}{\epsilon^2} \) and weights bounded by \( 2\pi d^2 \).

**2. Proofs**

Throughout, we fix a dimension \( d \). All functions \( f : \mathbb{S}^{d-1} \to \mathbb{R} \) and \( f : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R} \) will be assumed to be square integrable w.r.t. the uniform measure. Likewise, functions \( f : [-1, 1] \to \mathbb{R} \) and \( f : [-1, 1] \times [-1, 1] \to \mathbb{R} \) will be assumed to be square integrable w.r.t. \( \mu_d \) or \( \mu_d \times \mu_d \). Norms and inner products of such functions are of the corresponding \( L^2 \) spaces. We will use the fact that \( \mu_d \) is the probability measure on \([-1, 1]\) that is obtained by pushing forward the uniform measure on \( \mathbb{S}^{d-1} \) via the function \( x \mapsto x_1 \). We denote by \( \mathcal{P}_n : L^2(\mu_d) \to L^2(\mu_d) \) the projection on the complement of the space of degree \( \leq n - 1 \) polynomials. Note that \( A_{n,d}(f) = \|\mathcal{P}_n f\|_{L^2(\mu_d)} \).
2.1. Some Harmonic Analysis on the Sphere

The $d$ dimensional Legendre polynomials are the sequence of polynomials over $[-1, 1]$ defined by the recursion formula

$$P_n(x) = \frac{2n+d-4}{n+d-3}xP_{n-1}(x) - \frac{n-1}{n+d-3}P_{n-2}(x)$$

$$P_0 = 1, \quad P_1(x) = x$$

We also define $h_n : S^{d-1} \times S^{d-1} \rightarrow \mathbb{R}$ by $h_n(x, x') = \sqrt{N_{d,n}P_n(\langle x, x' \rangle)}$, and for $x \in S^{d-1}$ we denote $L_n^x(x') = h_n(x, x')$. We will make use of the following properties of the Legendre polynomials.

**Proposition 2** (e.g. Atkinson and Han (2012) chapters 1 and 2)

1. For every $d \geq 2$, the sequence $\{ \sqrt{N_{d,n}}P_n \}$ is orthonormal basis of the Hilbert space $L^2(\mu_d)$.
2. For every $n$, $\|P_n\|_\infty = 1$ and $P_n(1) = 1$.
3. $\langle L_n^x, L_j^{x'} \rangle = P_1(\langle x, x' \rangle)\delta_{ij}$.

2.2. Main Result

We say that $f : S^{d-1} \times S^{d-1} \rightarrow \mathbb{R}$ is an inner product function if it has the form $f(x, x') = \phi(\langle x, x' \rangle)$ for some function $\phi : [-1, 1] \rightarrow \mathbb{R}$. Let $\mathcal{H}_d \subset L^2(S^{d-1} \times S^{d-1})$ be the space of inner product functions. We note that

$$\|f\|^2 = \mathbb{E}_{x,x'} \phi^2(\langle x, x' \rangle) = \mathbb{E}_{x} \|\phi\|^2 = \|\phi\|^2$$

Hence, the correspondence $\phi \leftrightarrow f$ defines an isomorphism of Hilbert spaces between $L^2(\mu_d)$ and $\mathcal{H}_d$. In particular, the orthonormal basis $\{ \sqrt{N_{d,n}}P_n \}_{n=0}^\infty$ is mapped to $\{h_n\}_{n=0}^\infty$. Likewise,

$$P_n \left( \sum_{i=0}^\infty \alpha_i h_i \right) = \sum_{i=0}^\infty \alpha_i h_i$$

Let $v, v' \in S^{d-1}$. We say that $f : S^{d-1} \times S^{d-1} \rightarrow \mathbb{R}$ is $(v, v')$-separable if it has the form $f(x, x') = \psi(\langle v, x \rangle, \langle v', x' \rangle)$ for some $\psi : [-1, 1]^2 \rightarrow \mathbb{R}$. We note that each neuron implements a separable function. Let $\mathcal{H}_{v,v'} \subset L^2(S^{d-1} \times S^{d-1})$ be the space of $(v, v')$-separable functions. We note that

$$\|f\|^2 = \mathbb{E}_{x,x'} \psi^2(\langle v, x \rangle, \langle v', x' \rangle) = \|\psi\|^2$$

Hence, the correspondence $\psi \leftrightarrow f$ defines an isomorphism of Hilbert spaces between $L^2(\mu_d \times \mu_d)$ and $\mathcal{H}_{v,v'}$. In particular, the orthonormal basis $\{ \sqrt{N_{d,n}}P_n \otimes \sqrt{N_{d,m}}P_m \}_{n,m=0}^\infty$ is mapped to $\{ L_n^x \otimes L_n^{x'} \}_{n,m=0}^\infty$.

The following theorem implies theorem 1, as under the conditions of theorem 1, any hidden neuron implements a separable function with norm at most $B \max |x| \leq \sqrt{4d}B + B |\sigma(x)|$, and the bias term is a separable function with norm at most $B$. 

DEPTH SEPARATION FOR NEURAL NETWORKS

3
Theorem 3 Let \( f : S^{d-1} \times S^{d-1} \to \mathbb{R} \) be an inner product function and let \( g_1, \ldots, g_r : S^{d-1} \times S^{d-1} \to \mathbb{R} \) be separable functions. Then

\[
\left\| f - \sum_{i=1}^r g_i \right\|^2 \geq \|P_n f\| \left( \|P_n f\| - \frac{2 \sum_{i=1}^r \|g_i\|}{\sqrt{N_{d,n}}} \right)
\]

(1)

Proof We note that

\[
\mathbb{E}_{x, x'} h_n(x, x') L_i^y(x) L_j^y(x') = \mathbb{E}_{x, x'} L_i^y(x) \mathbb{E}_{x, x'} h_n(x, x') L_j^y(x') = \delta_{i,j} \mathbb{E}_{x, x'} L_i^y(x) P_n(\langle x, v' \rangle)
\]

(2)

\[
= \frac{\delta_{i,j}}{\sqrt{N_{d,n}}} \mathbb{E}_{x, x'} L_i^y(x) L_n^y(x)
\]

Suppose now that \( f = \sum_{i=n}^{\infty} \alpha_i h_i \) and suppose that \( g = \sum_{j=1}^r g_j \) where each \( g_j \) depends only on \( \langle v_j, x \rangle, \langle v_j', x' \rangle \) for some \( v_j, v_j' \in S^{d-1} \). Write \( g_j(x, x') = \sum_{k,l=0}^{\infty} \beta_{k,l} L_k^y(x) L_l^y(x') \). By equation (2), \( L_k^y(x) L_l^y(x') \) is orthogonal to \( f \) whever \( k \neq l \). Hence, if we replace each \( g_j \) with \( \sum_{k=0}^{\infty} \beta_{k,k} L_k^y(x) L_k^y(x') \), the l.h.s. of (1) does not increase. Likewise, the r.h.s. does not decrease. Hence, we can assume w.l.o.g. that each \( g_j \) is of the form \( g_j(x, x') = \sum_{i=0}^{\infty} \beta_i^j L_i^y(x) L_i^y(x') \).

Now, using (2) again, we have that

\[
\|f - g\|^2 = \sum_{i=0}^{\infty} \left\| \alpha_i h_i - \sum_{j=1}^r \beta_i^j L_i^y \otimes L_j^y \right\|^2 \geq \sum_{i=n}^{\infty} \left\| \alpha_i h_i - \sum_{j=1}^r \beta_i^j L_i^y \otimes L_j^y \right\|^2 \\
\geq \sum_{i=n}^{\infty} \alpha_i^2 - 2 \sum_{i=n}^{\infty} \sum_{j=1}^r \langle \alpha_i h_i, \beta_i^j L_i^y \otimes L_j^y \rangle \\
= \|P_n f\|^2 - 2 \sum_{i=n}^{\infty} \sum_{j=1}^r \frac{\beta_i^j \alpha_i P_1(\langle v_j, v_j' \rangle)}{\sqrt{N_{d,k}}} \\
\geq \|P_n f\|^2 - 2 \sum_{j=1}^r \sum_{i=n}^{\infty} \frac{\beta_j^i \|\alpha_i\|}{\sqrt{N_{d,n}}} \\
\geq \|P_n f\|^2 - 2 \sum_{j=1}^r \sum_{i=n}^{\infty} \frac{1}{\sqrt{N_{d,n}}} \sqrt{\sum_{i=n}^{\infty} |\alpha_i|^2} \\
\geq \|P_n f\|^2 - \frac{2 \sum_{j=1}^r \|g_j\|}{\sqrt{N_{d,n}}}
\]
2.3. Approximating the cosine function

**Lemma 4** Define \( g_{d,m}(x) = \sin\left(\pi \sqrt{dxm}\right) \). Then, for any \( d \geq d_0 \), for a universal constant \( d_0 > 0 \), and for any degree \( k \) polynomial \( p \) we have

\[
\int_{-1}^{1} (g_{d,m}(x) - p(x))^2 d\mu_d(x) \geq \frac{m - k}{4\pi m}
\]

**Proof** We have that (e.g. Atkinson and Han (2012)) \( d\mu_d(x) = \frac{\Gamma(\frac{d}{2})}{\sqrt{\pi^d (2^d)}} (1 - x^2)^{\frac{d-3}{2}} dx \). Likewise, for large enough \( d \) and \( |x| < \frac{1}{\sqrt{d}} \) we have \( 1 - x^2 \geq e^{-2x^2} \geq e^{-\frac{d}{\pi}} \) and hence \( (1 - x^2)^{\frac{d-3}{2}} \geq e^{-\frac{d-3}{d}} \geq e^{-1} \). Likewise, since \( \frac{\Gamma(\frac{d}{2})}{\Gamma(\frac{d+1}{2})} \sim \sqrt{\frac{d}{2}} \), we have that for large enough \( d \) and \( |x| \leq \frac{1}{\sqrt{d}} \), \( d\mu_d(x) \geq \frac{\sqrt{d}}{2\pi} \). Hence, for \( f \geq 0 \) we have

\[
\int_{-1}^{1} f(x) d\mu_d(x) \geq \frac{\sqrt{d}}{2\pi} \int_{-\frac{1}{\sqrt{d}}}^{\frac{1}{\sqrt{d}}} f(x) dx = \frac{1}{2\pi} \int_{-1}^{1} f \left( \frac{t}{\sqrt{d}} \right) dt
\]

Applying this equation for \( f = g_{d,m} - p \) we get that

\[
\int_{-1}^{1} (g_{d,m}(x) - p(x))^2 d\mu_d(x) \geq \frac{1}{2\pi} \int_{-1}^{1} (\sin(\pi mx) - q(x))^2 dx
\]

Where \( q(x) := p \left( \frac{x}{\sqrt{d}} \right) \). Now, in the \( 2m \) segments \( I_i = \left(-1 + \frac{i-1}{m}, -1 + \frac{i}{m}\right), \; i \in [2m] \) we have at least \( m - k \) segments on which \( x \mapsto \sin(\pi mx) \) and \( q \) do not change signs and have opposite signs. On each of these intervals we have \( \int_{I_i} (\sin(\pi mx) - q(x))^2 dx \geq \frac{1}{2m} \sin^2(\pi mx) dx = \frac{1}{2m} \).

\(\square\)

**Lemma 5** (e.g. Eldan and Shamir (2016)) Let \( \sigma(x) = \max(x, 0) \) be the ReLU activation, \( f : [-R, R] \to \mathbb{R} \) an \( L \)-Lipschitz function, and \( \epsilon > 0 \). There is a function

\[
g(x) = f(0) + \sum_{i=1}^{m} \alpha_i \sigma (\gamma_i x - \beta_i)
\]

for which \( \|g - f\|_{\infty} \leq \epsilon \). Furthermore, \( m \leq \frac{2RL}{\epsilon}, \; |\beta_i| \leq R, \; |\alpha_i| \leq 2L, \; \gamma_i \in \{-1, 1\}, \) and \( g \) is \( L \)-Lipschitz on all \( \mathbb{R} \).

**Corollary 6** Let \( f : [-1, 1] \to [-1, 1] \) be an \( L \)-Lipschitz function and let \( \epsilon > 0 \). Define \( F : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to [-1, 1] \) by \( F(\mathbf{x}, \mathbf{x}') = f(\langle \mathbf{x}, \mathbf{x}' \rangle) \). There is a function \( G : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to [-1, 1] \) that satisfies \( \|F - G\|_{\infty} \leq \epsilon \) and furthermore \( G \) can be implemented by a depth-3 ReLU network of width \( \frac{16dL}{\epsilon} \) and weights bounded by \( \max(4, 2L) \).

**Proof** By Lemma 5 there is a depth-2 network \( \mathcal{N}_{\text{square}} \) that calculates \( \frac{x^2}{2} \) in \([-2, 2]\), with an error of \( \frac{1}{2dL} \) and has width at most \( \frac{16dL}{\epsilon} \) and hidden layer weights bounded by 2, and prediction layer
weights bounded by 4. For each $i \in [d]$ we can compose the linear function $(x, x') \mapsto x_i + x'_i$ with $N_{\text{square}}$ to get a depth-2 network $N_i$ that calculates $(x_i + x'_i)^2$ with an error of $\frac{\epsilon}{2dL}$ and has the same width and weight bound as $N_{\text{square}}$. Summing the networks $N_i$ and subtracting 1 results with a depth-2 network $N_{\text{inner}}$ that calculates $\langle x, x' \rangle$ with an error of $\frac{\epsilon}{L}$ and has width $\frac{16d^2L}{\epsilon}$ and hidden layer weights bounded by 2, and prediction layer weights bounded by 4.

Now, again by lemma 5 there is a depth-2 network $N_f$ that calculates $f$ in $[-1, 1]$, with an error of $\frac{\epsilon}{2}$, has width at most $\frac{2L}{\epsilon}$, hidden layer weights bounded by 1 and prediction layer weights bounded by $2L$, and is $L$-Lipschitz. Finally, consider the depth-3 network $N_F$ that is the composition of $N_{\text{inner}}$ and $N_f$. $N_F$ has width at most $\frac{16d^2L}{\epsilon}$ weight bound of $\max(4, 2L)$, and it satisfies

$$|N_F(x, x') - F(x, x')| = |N_f(N_{\text{inner}}(x, x')) - f(\langle x, x' \rangle)|$$

$$\leq |N_f(N_{\text{inner}}(x, x')) - N_f(\langle x, x' \rangle)| + |N_f(\langle x, x' \rangle) - f(\langle x, x' \rangle)|$$

$$\leq L|N_{\text{inner}}(x, x') - \langle x, x' \rangle| + \frac{\epsilon}{2}$$

$$\leq \frac{L}{2L} + \frac{\epsilon}{2} = \epsilon$$

□

References


