ChebNet: Efficient and Stable Constructions of Deep Neural Networks with Rectified Power Units using Chebyshev Approximation

Shanshan Tang\textsuperscript{b,a,1}, Bo Li\textsuperscript{b,a}, Haijun Yu\textsuperscript{a,b,}\textsuperscript{*}

\textsuperscript{a}NCMIS & LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Beijing 100190, China
\textsuperscript{b}School of Mathematical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China

Abstract

In a recent paper\cite{Li03}, we show that deep neural networks with rectified power units (RePU) can give better approximation for sufficient smooth functions than those with rectified linear units by stably converting polynomial approximation given in power series into deep neural networks with optimal complexity and no approximation error. However, in practice, power series are not easy to compute. In this paper, we propose a new and more stable way to construct deep RePU neural networks using Chebyshev polynomial approximations. By using a hierarchical structure of Chebyshev polynomial approximation in frequency domain, we build efficient and stable deep neural network constructions. In theory, ChebNets and the deep RePU nets based on Power series have the same upper error bounds for general function approximations. But, numerically, ChebNets are much more stable. The constructed ChebNets can be further trained and obtain much better results than those obtained by training deep RePU nets constructed basing on power series.

Keywords: Deep neural networks, rectified power units, Chebyshev polynomial, ChebNet, stability

1. Introduction

Deep neural networks (DNNs), which compose multi-layers of affine transforms and nonlinear activations, is getting more and more popular as a universal modeling tool since the seminal works by Hinton et al.\cite{Hinton06} and Bengio et al.\cite{Bengio09}. DNNs have greatly boosted the developments in different areas including image classification, speech recognition, computational chemistry, numerical solutions of high-dimensional partial differential equations and other scientific problems, see e.g.\cite{Hinton06, Bengio09, Goodfellow15, Krizhevsky12, Szegedy15, Yosinski15} and the references therein.

The basic fact behinds the success of DNNs is that DNNs are universal approximators. It is well-known that neural networks with only one hidden layer can approximate any $C^0$ or $L^1$ functions with any given error tolerance\cite{Hornik89, Hornik91}. In fact, for neural networks with only one-hidden layer of non-polynomial $C^\infty$ activation functions, Mhaskar proved that the upper error bound of approximating multidimensional functions is of spectral type: Error rate $\varepsilon = n^{-k/d}$ can be obtained theoretically for approximating functions in Sobolev space $W^k([-1,1]^d)$\cite{Mhaskar95}. Here $d$ is the number of dimensions, $n$ is the number of hidden nodes in the neural network. Due to the success of DNNs, people believe that deep neural networks have broader scopes of representation than shallow ones. Recently, several works have demonstrated or proved this in different settings, see e.g.\cite{Telgarsky15, Telgarsky16, Telgarsky18}. One of the commonly used activation functions with DNNs is the so-called rectified linear unit (ReLU)\cite{ReLU}, which is defined as $\sigma(x) = \max(0,x)$. Telgarsky\cite{Telgarsky15} gave a simple and elegant construction showing that for any $k$, there exist $k$-layer, $O(1)$ wide ReLU networks on one-dimensional data, which can express a sawtooth function on $[0,1]$ with $O(2^k)$ oscillations. Moreover, such a rapidly oscillating function cannot be approximation by poly($k$)-wide ReLU networks with $o(k/\log(k))$
depth. Following this approach, several other works proved that deep ReLU networks have better approximation power than shallow ReLU networks \[18, 19, 20, 21\]. In particular, for $C^\beta$-differentiable $d$-dimensional functions, Yarotsky \[20\] proved that the number of parameters needed to achieve an error tolerance of $\varepsilon$ is $\mathcal{O}(\varepsilon^{-\frac{2}{\beta}} \log \frac{1}{\varepsilon})$. Petersen and Voigtlaender \[21\] proved that for a class of $d$-dimensional piecewise $C^\beta$ continuous functions with the discontinuous interfaces being $C^\beta$ continuous also, one can construct a ReLU neural network with $\mathcal{O}(\sqrt{d} \log (2 + \beta))$ layers, $\mathcal{O}(\varepsilon^{-\frac{2(d-1)}{\beta}})$ nonzero weights to achieve $\varepsilon$-approximation. The complexity bound is sharp. The spectral convergence of using deep ReLU network approximating analytic functions was proved by E and Wang \[22\], and Opschoor, Schwab and Zech \[23\]. The significance of the above mentioned works is that by using a very simple rectified nonlinearity, DNNs can obtain high order approximation property. Shallow networks do not hold such a good property.

A key fact used in the error estimates of deep ReLU networks is that $x^2, xy$ can be approximated by a ReLU network with $\mathcal{O}(\log \frac{1}{\varepsilon})$ layers, which introduces a $\log \frac{1}{\varepsilon}$ factor or a big constant related to the smoothness of functions to be approximated. To remove the approximation error and the extra $\log \frac{1}{\varepsilon}$ factor in the size of neural networks, we recently proposed to use rectified power units (RePU) to construct exact neural network representations of polynomials with optimal size\[24\]. The RePU function is defined as

$$
\sigma_s(x) = \begin{cases} 
x^s, & x \geq 0, \\
0, & x < 0,
\end{cases}
$$

where $s$ is a non-negative integer. Note that, the RePU functions have been first used by Mhaskar \[25\] as activation functions to construct neural networks based on spline approximation. Using Mhaskar’s construction, a polynomial with degree $n$ will be converted into a RePU network of size $\mathcal{O}(n \log n)$ with depth $\mathcal{O}(\log n)$, where $d$ is the dimension of space. We gave in \[24\] a different, optimal and stable construction, which converts a polynomial of degree $n$ into a RePU network of size $\mathcal{O}(n)$ with depth $\mathcal{O}(\log n)$. The work \[24\] focus on network constructions using $\sigma_2$, the generalization to general $\sigma_s, s \geq 2$ is studied in \[26\]. We call the constructed deep RePU network PowerNet. Combining with classical polynomial approximation theory, our constructed RePU PowerNet can approximate smooth functions with spectral accuracy. Moreover, PowerNets fit the situations where derivatives of network are involved in the loss function.

However, there is one drawback in the first version of RePU PowerNet constructed in \[23\] and \[26\], where polynomials based on power series are used. To approximate a smooth function, there are two ways to calculate the power series representation of a polynomial approximation. The first one is to use Taylor expansion to approximate the power series, which might diverge if the radius of convergence of the Taylor series is not large enough, and the high order derivatives used in Taylor series are not easy to calculate. The second approach first approximate the function using some orthogonal polynomial projection or interpolation, then convert the orthogonal polynomial approximation into power series. But in this approach, the condition number of the transforms from orthogonal polynomial bases to monomial bases are known grows very fast (see e.g. \[27\]).

In this paper, we propose a new version of deep RePU networks to remove the drawback mentioned above. we accomplish this goal by constructing deep RePU networks based on Chebyshev polynomial approximation directly. Chebyshev method is one the most popular spectral methods in numerical partial differential equations (see e.g. \[28, 29, 30\]). It is known that Chebyshev approximation can be efficiently calculated by using fast Fourier transforms. By using a hierarchical structure of Chebyshev polynomial approximation in frequency domain, we are able to convert Chebyshev polynomial approximations into deep RePU networks with optimal size, we call resulting neural networks ChebNets. The ChebNets constructed have all the good theoretical approximation properties that PowerNets have: they have faster convergence in approximating sufficient smooth functions than deep ReLU networks; they fit in situations when derivatives involved in the loss function, for which deep ReLU networks are hard to use. Meanwhile, ChebNets are numerically more stable. Our numerical results show that the constructed ChebNets can be further trained to obtain much better results than those obtained by training deep RePU networks constructed basing on power series.

The remaining part of this paper is organized as follows. We first present the optimal deep RePU network constructions (ChebNets) to represent Chebyshev polynomial approximations exactly in Section 2. We then
Lemma 1. For Chebyshev polynomials of the first kind \( T_n(x) \), \( n \in \mathbb{N}_0 \), \( x \in [-1,1] \), the following relations hold:

\[
\int_{-1}^{1} T_n(x)T_m(x)\omega(x)dx = \frac{c_n\pi}{2}\delta_{nm}, \tag{2.7}
\]

\( T_0(x) = 1 \), \( T_1(x) = x \), \( T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) \), \( n \geq 1 \), \( T_{m+n}(x) = 2T_m(x)T_n(x) - T_{|m-n|}(x) \), \( T_{2n}(x) = 2T_n(x)^2 - 1 \) \(, \tag{2.8} \)

where \( m, n \in \mathbb{N}_0 \), \( \omega(x) = (1-x^2)^{-\frac{1}{2}} \), \( c_0 = 2 \), \( c_n = 1 \). \( \delta_{nm} \) is the kronecker delta, it is 1 if \( m = n \) and 0 otherwise.

Lemma 2 (Lemma 1 in \[24\]). For \( \forall x, y \in \mathbb{R} \), the following identities hold:

\[
x^2 = \beta_2^T \sigma_2(\omega_2x), \tag{2.10}
\]

\[
xy = \beta_1^T \sigma_2(\omega_1x + \gamma_1y), \tag{2.11}
\]

\[
x = \beta_2^T \sigma_2(\omega_1x + \gamma_1). \tag{2.12}
\]

where

\[
\beta_1 = \frac{1}{4}\begin{bmatrix} 1, 1, -1, -1 \end{bmatrix}^T, \quad \beta_2 = [1, 1]^T, \quad \omega_1 = [1, -1, 1, -1]^T, \quad \omega_2 = [1, -1]^T, \quad \gamma_1 = [1, -1, -1, 1]^T. \tag{2.13}
\]
Remark 1. The Chebyshev polynomial $T_0(x) = 1$ can be realized by a one layer neural network $((0,1))$ without activation functions. $T_1$ can be realized either by a one layer neural network $((1,0))$ without activation functions or by a neural networks with four $\sigma$ activation functions in one hidden layer, the latter approach together with the $\sigma_2$ network realization of $T_2$ is given as:

$$T_1(x) = \beta_1^T \sigma_2(\omega_1 x + \gamma_1) \quad \text{(2.14)}$$

$$T_2(x) = 2\beta_2^T \sigma_2(\omega_2 x) - 1. \quad \text{(2.15)}$$

2.1. ChebNets for univariate Chebyshev polynomial expansions

Theorem 1. For $n \geq 1$, assume $p(x) = \sum_{j=0}^n c_j T_j$, with $c_n \neq 0$, $x \in [-1,1]$, then there exists a $\sigma_2$ neural network with at most $\lfloor \log_2 n \rfloor + 1$ hidden layers to represent $p(x)$ exactly. The number of neurons and total non-zero weights are both $\mathcal{O}(n)$.

Proof. (1) For $n = 1$, by Lemma 2, we have

$$p(x) = c_0 + c_1 T_1(x) = c_0 + c_1 \beta_1^T \sigma_2(\omega_1 x + \gamma_1), \quad \text{(2.16)}$$

which shows $p(x)$ can be represented exactly by a $\sigma_2$ network with one hidden layer. Written in following notation,

$$p(x) = A_2 \sigma_2(A_1 x + b_1) + b_2, \quad \text{(2.17)}$$

we have

$$A_1 = \omega_1, \quad b_1 = \gamma_1$$

$$A_2 = c_1 \beta_1^T, \quad b_2 = c_0.$$

(2) For $n = 2$, by Eq. (2.14) and (2.15), we have

$$p(x) = c_0 + c_1 T_1(x) + c_2 T_2(x) = (c_0 - c_2) + c_1 \beta_1^T \sigma_2(\omega_1 x + \gamma_1) + 2c_2 \beta_2^T \sigma_2(\omega_2 x). \quad \text{(2.18)}$$

This is a $\sigma_3$ network with one hidden layer, written in the form $p(x) = A_2 \sigma_2(A_1 x + b_1) + b_2$, we have

$$A_1 = \begin{bmatrix} \omega_1 \\ \omega_2 \end{bmatrix}, \quad b_1 = \begin{bmatrix} \gamma_1 \\ 0 \end{bmatrix}, \quad A_2 = [c_1 \beta_1^T, 2c_2 \beta_2^T], \quad b_2 = c_0 - c_2.$$

(2) For $n = 3$, by Lemma 1, we have

$$p(x) = c_0 + c_1 T_1(x) + c_2 T_2(x) + c_3 T_3(x) \quad \text{(2.19)}$$

$$= c_0 + (c_1 - c_3)T_1(x) + T_2(x)(c_2 + 2c_3 T_1(x)), \quad \text{(2.20)}$$

showing that a network with two hidden layers can represent $p(x)$ exactly. Details are shown in the following.

Immediate variables of the first hidden layer is

$$\xi_1^{(1)} = c_0 + (c_1 - c_3)T_1 = c_0 + (c_1 - c_3) \beta_1^T \sigma_2(\omega_1 x + \gamma_1), \quad \text{(2.21)}$$

$$\xi_1^{(2)} = c_2 + 2c_3 T_1 = c_2 + 2c_3 \beta_1^T \sigma_2(\omega_1 x + \gamma_1), \quad \text{(2.22)}$$

$$\xi_1^{(3)} = T_2 = 2\beta_2^T \sigma_2(\omega_2 x) - 1, \quad \text{(2.23)}$$
then
\[
\mathbf{x}_1 = \begin{bmatrix}
\sigma_2(\omega_1 x + \gamma_1) \\
\sigma_2(\omega_2 x)
\end{bmatrix} = \sigma_2(A_1 x + b_1), \quad \text{where } A_1 = \begin{bmatrix}
\omega_1 \\
\omega_2
\end{bmatrix}, \quad b_1 = \begin{bmatrix}
\gamma_1 \\
0
\end{bmatrix},
\tag{2.24}
\]
and
\[
\begin{bmatrix}
\xi_1^{(1)} \\
\xi_1^{(2)} \\
\xi_1^{(3)}
\end{bmatrix} = A_{20} \mathbf{x}_1 + b_{20}, \quad \text{where } A_{20} = \begin{bmatrix}
(c_1 - c_3)\beta_1^T & 0 \\
2c_3\beta_1^T & 0 \\
0 & 2\beta_2^T
\end{bmatrix}, \quad b_{20} = \begin{bmatrix}
c_0 \\
c_2 \\
-1
\end{bmatrix}.
\]

Immediate variables of the second hidden layer is
\[
\xi_2^{(1)} = \xi_1^{(1)} + \xi_1^{(3)} = \beta_1^T \sigma_2(\omega_1 \xi_1^{(1)} + \gamma_1) + \beta_1^T \sigma_2(\omega_1 \xi_1^{(2)} + \gamma_1 \xi_1^{(3)}),
\tag{2.25}
\]

from which, we see the variable after the activations are
\[
\mathbf{x}_2 = \begin{bmatrix}
\sigma_2(\omega_1 \xi_1^{(1)} + \gamma_1) \\
\sigma_2(\omega_1 \xi_1^{(2)} + \gamma_1 \xi_1^{(3)})
\end{bmatrix} = \sigma_2(A_{21} \begin{bmatrix}
\xi_1^{(1)} \\
\xi_1^{(2)} \\
\xi_1^{(3)}
\end{bmatrix} + b_{21}), \quad \text{where } A_{21} = \begin{bmatrix}
\omega_1 & 0 & 0 \\
0 & \omega_1 & \gamma_1 \\
0 & 0 & \gamma_1
\end{bmatrix}, \quad b_{21} = \begin{bmatrix}
\gamma_1 \\
0
\end{bmatrix}
\]
and
\[
A_2 = A_{21} A_{20}, \quad b_2 = A_{21} b_{20} + b_{21}.
\tag{2.26}
\]

Noticing \(p(x) = \xi_2^{(1)}\), so output of the neural network representing \(p(x)\) is
\[
p(x) = A_3 \mathbf{x}_2 + b_2, \quad \text{where } A_3 = [\beta_1^T, \beta_1^T], \quad b_3 = 0.
\tag{2.27}
\]

(3) For \(n \geq 4\), let \(m = \lfloor \log_2 n \rfloor\), then we can extend \(p(x)\) as
\[
p(x) = \sum_{j=0}^{2^{m+1} - 1} c_j T_j,
\tag{2.28}
\]
where \(c_j = 0\) if \(n + 1 \leq j \leq 2^{m+1} - 1\). By Lemma 1, we can rewrite \(p(x)\) as
\[
p(x) = (c_0 + \sum_{j=1}^{2^{m}-1} c_j T_j) + c_{2^m} T_{2^m} + \sum_{j=2^m+1}^{2^{m+1}-1} c_j T_j
\]
\[
= (c_0 + \sum_{j=1}^{2^m-1} (c_j - c_{2^m+j}) T_j) + T_{2^m} (c_{2^m} + 2 \sum_{j=1}^{2^m-1} c_{2^m+j} T_j) := r(x) + q(x)T_{2^m},
\]
where both \(q(x)\) and \(r(x)\) are polynomials of degree at most \(2^m - 1\). If \(q(x), r(x), T_{2^m}\) are known, then by Lemma 2, \(p(x) = r(x) + q(x)T_{2^m}\) can be realized by a \(\sigma_2\) neural networks with one-hidden layer of \(8\) \(\sigma_s\) and 24 non-zero weights. If both \(r(x)\) and \(q(x)\) can realized in \(m\) hidden layers, with no more than \(c 2^{m-1} - 28\) nodes and non-zero weights, and \(T_{2^m}\) can be realized in \(m\) hidden layers, with 4\(m\) non-zero weights, which is true, then \(p(x)\) can be realized in \(m + 1\) hidden layers, with no more than \(c 2^{m} - 28\) nodes and non-zero weights. Here \(c\) is a general constant that doesn’t depend on \(m\). By induction, for any \(n \geq 4\) the Chebyshev expansion Eq. \((2.28)\) can be realized in \(\lfloor \log_2 n \rfloor + 1\) hidden layers, with no more than \(O(n)\) neurons and total non-zero weights.
\[\square\]
Now we work out the detailed ChebNet construction described in Theorem 1.
For \( p(x) = \sum_{j=0}^{n} c_j T_j \), \( n \geq 3 \), \( m = \lfloor \log_2 n \rfloor \), using Eq. (2.9), we have
\[
\begin{align*}
p(x) &= (c_0 + \sum_{j=1}^{2^{m-1}-1} (c_j - c_{2^{m+1-j}})T_j) + T_{2^m}(c_{2^m} + 2 \sum_{j=1}^{2^{m-1}} c_{2^m+j}T_j) \\
&=: \sum_{j=0}^{2^{m-1}} \bar{c}_j \tilde{T}_j + T_{2^m} \left( \sum_{j=0}^{2^{m-1}} \bar{c}_{2^m+j} \tilde{T}_j \right) \\
&=: \sum_{j=0}^{n} \bar{c}_j \tilde{T}_j,
\end{align*}
\]
where \( \tilde{T}_{2^m+l} = T_{2^m+l} \) for \( l = 0, \ldots, 2^m - 1 \). The definition of \( \tilde{T}_k \) can be extended to all \( k \in \mathbb{N}_0 \) as
\[
\tilde{T}_n = T_n, \text{ for } n = 0, 1, 2; \quad \tilde{T}_n = T_{2^m-2^n}, \text{ for } n \geq 3, \quad m = \lfloor \log_2 n \rfloor.
\]
It is easy to see the transform between \( \{c_j\} \) and \( \{\bar{c}_j\} \) is a linear transform. We denote it by
\[
\begin{bmatrix}
\bar{c}_0 \\
\vdots \\
\bar{c}_n
\end{bmatrix} = S_n
\begin{bmatrix}
c_0 \\
\vdots \\
c_n
\end{bmatrix}.
\]
The \((n+1) \times (n+1)\) transform matrix \( S_n, n = 1, 3, 7, \ldots, 2^{m+1} - 1 \) can be calculated using following recursive formula
\[
S_{2^j+1-1} = \begin{bmatrix}
I_{2^j+1} & \tilde{\delta}^{(j-1)} \\
0_{(2^j-1) \times (2^j-1)} & 2I_{2^j-1}
\end{bmatrix}
\begin{bmatrix}
S_{2^j-1} & 0 \\
0 & S_{2^j-1}
\end{bmatrix}, \quad j \geq 1,
\]
with \( S_1 = I_2 \). Here \( I_k \) stands for \( k \times k \) identity matrix, \( \tilde{\delta}^{(r)} = [\delta^{(2^{j+1})}_{2^j+1}, \delta^{(2^{j+1})}_{2^j+1}, \ldots, \delta^{(2^{j+1})}_{2^j+1}] \), \( \delta^{(k)} = [0, \ldots, 0, -1, 0, \ldots, 0]^T \in \mathbb{R}^{k \times 1} \), \( k \leq s \in \mathbb{N} \).

After transform from Chebyshev basis expansion \( p(x) = \sum_{j=0}^{n} c_j T_j \) to hierarchical Chebyshev basis expansion \( p(x) = \sum_{j=0}^{n} \bar{c}_j \tilde{T}_j \), \( p(x) \) can be realized exactly using algorithms almost identical to the ones building PowerNets proposed in [24, 26], the only difference is we need to replace the \( \sigma_2 \) network implementation of \( x^{2^n} = (x^{2^{n-1}})^2 \) in the first version of PowerNet with \( T_{2^m} = 2T_{2^{m-2}} - 1 \).

### 2.2. ChebNets for multivariate Chebyshev polynomial expansions

The construction describe in last subsection, can be extended to multivariate cases.

#### 2.2.1. Multivariate polynomials in tensor product and hyper-triangular space

We first present the results of representing multivariate polynomials with fixed total degree.

**Theorem 2.** If \( p(x) \) is a multivariate polynomial with total degree on \([-1, 1]^d \), then there exists a \( \sigma_2 \) neural network with \( d|\log_2 n| + d \) hidden layers and no more than \( \mathcal{O}(C_d^{n+d}) \) activation functions and non-zero weights to approximate \( p(x) \) exactly.

**Proof.** We first consider 2-d case. Assume \( p(x, y) = \sum_{i+j=0}^{n} c_{ij} T_i(x)T_j(y), n \geq 3. \) Let \( m = \lfloor \log_2 n \rfloor \). Since the transform from \( \{c_j\}_{j=0}^{n} \) to \( \{\bar{c}_j\}_{j=1}^{n} \) using \( S_{2^{m+1}-1} \) with zero paddings for \( c_j, j = n + 1, \ldots, 2^{m+1} - 1 \)
terms will not lead to nonzero values of $\tilde{c}_j$, $j = n + 1, \ldots, 2^{m+1} - 1$, the 2-d polynomial can be transformed into form $p(x, y) = \sum_{i+j=0}^{n} \tilde{c}_{ij} \hat{T}_i(x)\hat{T}_j(y)$, from which we have

$$p(x, y) = \sum_{i=0}^{n} \sum_{j=0}^{n-i} \tilde{c}_{ij} \hat{T}_i(y)\hat{T}_j(x) =: \sum_{i=0}^{n} B_i(y)\hat{T}_i(x), \quad \text{where} \quad B_i(y) = \sum_{j=0}^{n-i} \tilde{c}_{ij} \hat{T}_j(y), \quad i = 0, \ldots, n. \quad (2.35)$$

That is, we regard $p(x, y)$ as a hierarchical Chebyshev polynomial expansion about variable $x$, which takes $B_i(y), i = 0, \ldots, n$ as coefficients. It takes 3 steps to construct a RePU network representing $p(x, y)$ exactly:

1) For any $B_i(y), i = 0, \ldots, n$, Theorem 1 can be used to construct a $\sigma_2$ neural network to express $B_i(y)$ exactly. In other words, there exists a $\sigma_2$ network $\Phi_1$ taking $y, x$ as input, $B_i(y), i = 0, \ldots, n - 1$, and $x$ as output. According to Theorem 1 depth of $\Phi_1$ is $\lceil \log_2 n \rceil + 1$, number of activation functions and non-zero weights are both $\sum_{k=0}^{n-1} O(k) = O(\frac{1}{2}n^2)$. Since, the subnet built for $B_i(y)$ according to Theorem 1 have different depths, we need to keep a record of $x$ at each layers by using (2.12). The cost for this purpose is $4[\log_2 n]$, which is negligible comparing to $O(\frac{1}{2}n^2)$.

2) Taking $[B_0(y), \ldots, B_{n-1}(y), x]^T$ as input and combining the constructive process of Theorem 1 a neural $\sigma_2$ network $\Phi_2$ with $p(x, y)$ as output can be constructed. It is easy to see depth of $\Phi_2$ is $[\log_2 n] + 1$, number of nodes and non-zero weights are both $O(n)$.

3) The concatenation of $\Phi_1$ and $\Phi_2$ is $\Phi$, which takes $y, x$ as input, outputs $p(x, y)$. The details about concatenating two neural networks can be found in [21] or [24]. The depth of $\Phi$ is $2([\log_2 n] + 1)$, number of non-zero weights and nodes are $O(\frac{1}{2}n^2)$.

The $d > 2$ cases can be proved using mathematical induction. For the case $n \geq 2$, one can build neural networks with only one hidden layer (see, e.g. [25]). Note that the constant behind the big $O$ can be made independent of dimension $d$. The theorem is proved.

Using similar approach, we can construct optimal ChebNet for polynomials in tensor product space $Q_N^d(I_1 \times \cdots \times I_d) := P_N(I_1) \otimes \cdots \otimes P_N(I_d)$.

**Theorem 3.** Polynomials from a tensor product space $Q_N^d(I_1 \times \cdots \times I_d)$ can be realized without error with a deep $\sigma_2$ neural network, in which the depth is $d[\log_2 N] + d$, the numbers of activation functions and non-zero weights are no more than $O(N^d)$.

*2.2.2. Multivariate polynomials in sparse downward closed polynomial spaces*

For high dimensional problems, it is obvious that the degree of freedoms increases exponentially as dimension $d$ increase if tensor-product or similar grids are used, which is known as curse of dimensionality. Fortunately, a lot of applications high-dimensional problems have low intrinsic dimension (see e.g. [31], [32]). A particular example is the class of high-dimensional smooth functions with bounded mixed derivatives, for which sparse grid (or hyperbolic cross) approximation is a very popular approximation tool (see e.g. [33], [34]). In the past few decades, sparse grid method and hyperbolic cross approximations have found many applications, such as general function approximation [35] [36], [37], [38], solving partial differential equations (PDE) [39] [40] [41], [42], [43], [44], computational chemistry [45] [46] [47], uncertainty quantification [48] [49] [50], etc.

The sparse grid finite element approximation was first used by Montanelli and Du [51] to construct a new upper error bound for deep ReLU network approximations in high dimensions. In our recent work [24], optimal deep RePU networks based on sparse grid and hyperbolic cross spectral approximations are constructed, which give better approximation bounds for sufficient smooth functions.

Now, we describe how to construct Deep RePU networks based on high dimensional sparse Chebyshev polynomial approximations without transform into power series form as done in [24]. Both hyperbolic cross set and sparse grids belong to a more general set: downward closed set(see e.g. [52], [24]), which is defined below. So we only present the result for downward closed polynomial spaces here.
Definition 1. A linear polynomial space $P_C$ is said to be downward closed, if it satisfies the following:

- if $d$-dimensional polynomial $p(x) \in P_C$, then $\partial_x^k p(x) \in P_C$ for any $k \in \mathbb{N}_0^d$,
- there exists a set of bases that is composed of monomials only.

Now we give a conclusion on approximating Chebyshev polynomial expansions in downward closed polynomial space $P_C$.

Theorem 4. Let $p(x)$ be a polynomial in downward closed polynomial space $P_C$. Let $n$ be the dimension of $P_C$, $d$ be the dimension of $x$. Then there exists a $\sigma_2$ neural network with no more than $\sum_{i=1}^d \lfloor \log_2 N_i \rfloor + d$ hidden layers, $O(n)$ activation functions and non-zero weights, can represent $p$ exactly, where $N_i$ is the maximum polynomial degree in $x_i$ for functions in $P_C$.

Proof. The proof is similar to Theorem 2. One key fact is the transforms from expansions using standard Chebyshev polynomials $T_k \in P_C$ as bases to expansions using hierarchical Chebyshev polynomials $\hat{T}_k$ as bases do not add nonzero coefficients for the bases $\hat{T}_k \notin P_C$. After rewrite $p(x) \in P_C$ into linear combinations of $\hat{T}_k$ basis, one construct corresponding deep RePU networks by dimension induction similar as in Theorem 2 or procedure described in Theorem 4.1 of [24].

Remark 2. The structures of deep RePU networks constructed by using hierarchical Chebyshev polynomial expansion (i.e. ChebNet) and those constructed by using power series expansions (first version of PowerNet) are very similar. There is one small difference. In ChebNet, to calculate $T_{2^{m+1}}$ from $T_{2^m}$, a constant shift vector 1 is added comparing to calculating $x^{2^{m+1}}$ from $x^{2^m}$ in PowerNet. So the depth and network complexity of ChebNet and PowerNet are exactly the same. The approximation property are also mathematical identical, which are given in [24].

Remark 3. Since hyperbolic cross and sparse grid polynomial spaces are special cases of downward closed polynomial spaces, the Theorem 4 can be directly applied to sparse grid and hyperbolic cross polynomial spaces.

3. Approximating general smooth functions

It is well known that polynomial approximation converge very fast for approximating smooth functions. The ChebNets constructed in last section can be used to approximate general smooth functions. These are three steps in using ChebNets for approximating general smooth functions

1. Construct the Chebyshev polynomial approximation for given smooth function. This can be done using fast Fourier transform. For low dimensional problem, e.g. for $d < 4$, one may use tensor-product grids. For high dimensional problem, one may use sparse grids or other downward closed sparse polynomial approximations. The fast Chebyshev transform on sparse grids is constructed in [41]. For problems in unbounded high dimensional domain, one can use mapped Chebyshev method, fast convergence [38] and fast Chebyshev transform [42] are also available.

2. Construct the corresponding ChebNets for the polynomial approximation obtained from the first step using constructions described in Section 2.

3. Train the constructed ChebNets using more data to improve the approximation accuracy.

There are several remarks on the approximation properties of the ChebNet for general smooth functions.

Remark 4. Without training, the approximation properties of ChebNets and the first version PowerNets are mathematical identical. Those approximation properties are given in [24]. However, the coefficients obtained are different. So numerically, they might have different behaviors.

Remark 5. To calculate best $L^2$ approximations in low dimensions, one may use Legendre polynomial approximation. To construct ChebNets, one can first calculate the Legendre approximations by Legendre spectral transform, then transform Legendre basis representation into Chebyshev basis representation, from which the ChebNets can be constructed using the approach described above.
Remark 6. For high dimensional problems, we use sparse grid Chebyshev approximations to build ChebNets. It is known that sparse grid is not isotropic, i.e., using different coordinates may have different convergence properties. Another issue is that the complexity of sparse grids still weak-exponentially depends on dimension $d$. To overcome these two issues, we add one extra full connected RePU subnet to accomplish dimension reduction and coordinates transform before feeding the data into ChebNets. The networks can be trained separately or collectively.

4. Preliminary numerical experiments

In this section, we show the performance of ChebNets in approximating a given smooth function, and compare the results with the first version PowerNets. In this paper we focus on the performance differences between ChebNets and PowerNets, so we only use 1-dimensional examples, more results for approximating high-dimensional problems will be reported separately.

4.1. Numerical results

We test two smooth functions defined as follows. We use truncated $N$ item Legendre and Chebyshev polynomial approximations for PowerNet and ChebNet, respectively. For PowerNet, we transform the Legendre approximation to power series representation before using the construction method proposed in [53]. The training data are 200 uniform points come from the interval $[-1,1]$. All the experiments are executed on Tensorflow with RMSPropOptimizer, where $\gamma = 0.99, \eta = 0.00001$, the loss function during training is the average of $l_2$ norm squared.

(1) Gauss function:

$$f(x) = \exp(-x^2), \; x \in [-1,1].$$ (4.1)

We take $N = 15$ here and show the training performances in Figure 1. The result of PowerNet is on the left sub-figure and the result of ChebNet is on the right side. The horizontal axis represents the iteration number, and the vertical axis is the error on training set. We see the initial errors are almost the same. After training, the error of ChebNet on the right side decreases more than 6 times, while the error of PowerNet decreases only a very small percentage.

(2) Cauchy function:

$$f(x) = \begin{cases} \exp(-\frac{1}{x^2}), & x \neq 0, \\ 0, & x = 0. \end{cases}$$ (4.2)

This function is smooth but not analytic. We take $N = 11$ and the results are shown in Figure 2. Similar to Gauss function, the error of ChebNet reduced much more than PowerNet after training. Notice that the precision is not high by taking $N = 11$, so we hope to achieve high-accuracy and compare the corresponding results for $N = 30$. However, PowerNet blows up after the 1st iteration of training for $N = 30$, on the other hand side, the ChebNet can still be trained and obtains better accuracy.

4.2. Explanations of the numerical experiments

We give some explanations on the numerical results here. To approximate a function $f(x)$, we do in PowerNet as follows:

$$f(x) \approx f_N = \sum_{j=0}^{N} c_j L_j(x) = \sum_{j=0}^{N} \tilde{c}_j x^j$$ (4.3)
where $\tilde{c}_j$ are calculated using a linear transform

$$
\begin{bmatrix}
\tilde{c}_0 \\
\tilde{c}_1 \\
\vdots \\
\tilde{c}_N
\end{bmatrix}
= A_N 
\begin{bmatrix}
c_0 \\
c_1 \\
\vdots \\
c_N
\end{bmatrix} \tag{4.4}
$$

Correspondingly, the following formula are used in constructing ChebNet:

$$
f(x) \approx f_N = \sum_{j=0}^{N} b_j T_j(x) = \sum_{j=0}^{N} \tilde{b}_j \tilde{T}_j, \tag{4.5}
$$

where $b_j$ and $\tilde{b}_j$ satisfy:

$$
\begin{bmatrix}
\tilde{b}_0 \\
\tilde{b}_1 \\
\vdots \\
\tilde{b}_N
\end{bmatrix}
= S_N 
\begin{bmatrix}
b_0 \\
b_1 \\
\vdots \\
b_N
\end{bmatrix} \tag{4.6}
$$

Now we plot $c_j, \tilde{c}_j, b_j, \tilde{b}_j, \ j = 0, \ldots, N$ in Figure 3-6 for approximating Gauss function using 15 terms and for approximating Cauchy function with 30 terms. From these figures, we see the differences between $b_j$ and $\tilde{b}_j$ are very small, but the differences between $c_j$ and $\tilde{c}_j$ are very large, when $N$ is large. Especially, in
Figure 3: The coefficients of Legendre expansion: \( c_j, j = 0, \ldots, N \) (Left) and power series expansion: \( \tilde{c}_j, j = 0, \ldots, N \) (Right) for Gauss function with \( N = 15 \).

Figure 4: The coefficients of Chebyshev expansion: \( b_j, j = 0, \ldots, N \) (Left) and coefficients of hierarchical Chebyshev expansion: \( \tilde{b}_j, j = 0, \ldots, N \) (Right) for Gauss function with \( N = 15 \).

Figure 5: The coefficients of Legendre expansion: \( c_j, j = 0, \ldots, N \) (Left) and coefficients of power series expansion: \( \tilde{c}_j, j = 0, \ldots, N \) (Right) for Cauchy function with \( N = 30 \).
approximating Cauchy function with $N = 30$ using power series expansion, we have some coefficients almost as large as $4 \times 10^5$, see Figure 5. The big coefficients make the resulting PowerNet hard to train.

To explain why big coefficients happens, we calculate the condition numbers of $A_N$ and $S_N$, denoted by $\kappa(A_N)$ and $\kappa(S_N)$, and the results are showed in Table 1. We see from the table that the condition number of $\kappa(A_N)$ increases very fast, but the condition number of $\kappa(S_N)$ does not increase as $N$ increases. The large condition number of $A_N$ indicates that transform from Legendre expansion to power series is not a good approach, which may introduce large numerical truncation error due to the large condition number.

| $N$  | 10     | 20     | 30     | 40     |
|------|--------|--------|--------|--------|
| $\kappa(A_p)$  | 874.99 | 4.1E6  | 2.2E10 | 1.3E14 |
| $\kappa(L_p)$  | 2.618  | 2.618  | 2.618  | 2.618  |

Table 1: The condition number of $A_N$, $L_N$.

5. Summary

In this paper, we improve the RePU network construction based on polynomial approximation we proposed early in [24], by constructing deep RePU networks directly from Chebyshev polynomial approximation. By removing the procedure of transform a polynomial into power series, we eliminate the potential numerical instability in the first version of deep RePU network constructions. Due to the availability of fast Chebyshev transforms, the proposed new approach, which we call ChebNets can be efficiently applied to a large class of smooth functions than the first version of PowerNet. Considering other good properties that RePU networks have: 1) obtain high order convergence with less layers than ReLU networks; 2) fit in the situation where derivatives are involved in the loss function, e.g. the deep Ritz method [51]; we expect that deep RePU networks and ChebNets be more efficient in applications where high dimensional functions to be approximated are smooth.

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