Ladder Polynomial Neural Networks

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Abstract

Polynomial functions have plenty of useful analytical properties, but they are rarely used as learning models because their function class is considered to be restricted. This work shows that when trained properly polynomial functions can be strong learning models. Particularly this work constructs polynomial feedforward neural networks using the product activation, a new activation function constructed from multiplications. The new neural network is a polynomial function and provides accurate control of its polynomial order. It can be trained by standard training techniques such as batch normalization and dropout. This new feedforward network covers several previous polynomial models as special cases. Compared with common feedforward neural networks, the polynomial feedforward network has closed-form calculations of a few interesting quantities, which are very useful in Bayesian learning. In a series of regression and classification tasks in the empirical study, the proposed model outperforms previous polynomial models.

1. Introduction

Well studied by mathematicians, polynomial functions have many favorable theoretical properties. Polynomial models also bridge the analysis of general neural networks to the properties of polynomial functions [Livni et al., 2014]. For example, polynomial models can approximate other feedforward neural networks, and they are polynomial-time learnable.

One method of constructing polynomial models is to use the quadratic function as activations in a feedforward network (FF-QUAD). However, it has a clear drawback: an FF-QUAD cannot have an arbitrary polynomial order, as its order grow exponentially with its number of layers. As a result, a deep FF-QUAD is hard train, and its performance is not stable.

Polynomial learning models can also be devised by representing polynomial coefficients with some type of decomposition. We simply call these models as decomposition models. One approach is to define a polynomial kernel over input features and network parameters [Blondel et al., 2016b; 2017]. Another approach is to use a tensor-train decomposition as the coefficients of a polynomial model [Chen et al., 2018]. These models do not have a layer structure, so they often need specialized training methods. Furthermore, it is very hard to compare these models with neural networks, so some of their good properties are not well understood.

In this work, we propose a new method of constructing polynomial learning models in the form of feedforward networks. One key component of a feedforward network is the activation function. We devise the product activation, which creates nonlinearity by multiplying a hidden layer to a linear transform of the. Then we construct a Ladder Polynomial Neural Network (LPNN) with product activations. The LPNN has a layer structure by construction, but it is also a decomposition model at the same time. Therefore, it enjoys benefits from both sides. As a feedforward neural network, it can be trained by standard deep learning techniques such as batch normalization [Ioffe & Szegedy, 2015] and dropout [Srivastava et al., 2014]. Its polynomial order, which is the number of hidden layers plus 1, can be exactly controlled. As a decomposition model, LPNN also covers two previous models as special cases. When network weights are stochastic, the moments of a LPNN’s outputs can be computed in closed-form. This property is very useful in Bayesian learning.

The empirical study shows that the LPNN outperforms previous polynomial models in a list of classification and regression tasks. The investigation also indicates the necessity of dropout and batch normalization in training. In the setting of Bayesian learning, we show that Gaussian distributions can well approximate a LPNN’s network output when the network is given a Gaussian prior.
2. Related Work

Feedforward network with quadratic activations. Livni et al. (2014) analyze FF-QUADs with quadratic activations and show several positive properties of polynomial neural networks. For example, they are as expressive as networks with threshold activations, and they are learnable in polynomial time. Kileel et al. (2019) analyze the algebraic structure of polynomial functions behind FF-QUAD. Du & Lee (2018) show that training a one-hidden-layer FF-QUAD is efficient when the model is overly parameterized. All these analyses depend on the special function form. There are also other special optimization methods (Lin et al., 2017; Soltani & Hegde, 2018; 2019) for training FF-QUADs with one hidden layer.

Decomposition models. Blondel et al. (2016b) construct polynomial models with polynomial kernels. They also show that factorization machines (Rendle, 2010) can be constructed in the same way with ANOVA kernels. Blondel et al. (2016a) propose high order factorization machines with high order ANOVA kernels. Blondel et al. (2017) extend factorization machines and polynomial networks to output multiple values. Chen et al. (2018) use tensor-train decomposition (Oseledets, 2011) to express the coefficients of a polynomial model. By design, the model is for small problems. The coefficients of the LPNN in this work also has a tensor-train (Oseledets, 2011).

3. The Polynomial Neural Network

We first define the general form of a feedforward neural network. Suppose the input to the neural network is a feature vector \( x \in \mathbb{R}^{d_0} \) and denote \( h^0 = x \). Suppose the network has \( L \) hidden layers, with each layer \( \ell \in \{1, \ldots, L\} \) takes the input \( h^{\ell-1} \) and has the output \( h^\ell \). Each layer is defined by

\[
\sigma^\ell(x) = \sigma(W^\ell h^{\ell-1}).
\]

(1)

Here \( W^\ell \) is the weight matrix for layer \( \ell \), and \( \sigma(x) \) is the activation function. For notational simplicity, we omit intercept vectors for now and will include them later.

We use a new activation, the **product activation** \( \sigma_p(x) \) in the neural network.

\[
\sigma_p(u; V, x) = u \odot (Vx).
\]

(2)

Here \( \odot \) is the element-wise product. The learnable parameter \( V \) is a matrix with size \( (d \times d_0) \) when \( u \) has \( d \) entries.

Since \( u = W^\ell h^{\ell-1} \) is a function of \( x \), the activation is nonlinear in \( u \). Particularly, if \( u \) is a polynomial function of \( x \), then \( \sigma^\ell_p(u; V, x) \) is also a polynomial function of \( x \) with the polynomial order increased by 1. Note that the product activation is not a function of \( u \) because different \( x \) values may give the same \( u \) value but different responses from \( \sigma_p(u; V, x) \).

The product activation is inspired by self-attention (Vaswani et al., 2017), in which the multiplication (of hidden vectors and attention weights) is an important way of processing information. The product activation keeps the multiplication operation and removes all non-linear operations.

Then we use product activations in a feedforward structure to construct a LPNN. We use a different matrix \( V^\ell \) for the product activation in each layer \( \ell \). Suppose \( H_L \) is the output of the neural network, the function of the LPNN is formally defined as \( \text{lpnn}(x; \theta) = h^L \).

\[
h^0 = x, 
\]

\[
h^\ell = W^\ell h^{\ell-1} \odot (V^\ell x), \quad \ell = 1, 2, \ldots, L.
\]

(4)

Here \( \odot \) denotes element-wise multiplication. Let \( \theta = (W^1, \ldots, W^L, V^1, \ldots, V^L) \) denote all network parameters. The first hidden layer \( h^1 \) is a second-order polynomial of the input, and each activation increase the order by 1, so the hidden layer \( h^\ell \) is an order \( (\ell + 1) \) polynomial.

We further re-write the function with simple additions and multiplications. The \( i \)-th entry of \( h^\ell \) is

\[
h^\ell_i = (W_i^\ell h^\ell) (V_i^\ell x).
\]

(5)

Here \( W_i^\ell \) and \( V_i^\ell \) are the \( i \)-th rows of \( W \) and \( V \) respectively, so both \( (W_i^\ell h^\ell) \) and \( (V_i^\ell x) \) are scalars.

After expanding all product activations and taking out all summations, the \( i_L \)-th entry of the network function \( \text{lpnn}(x; \theta) \) is

\[
h^L_{i_L} = \sum_{i_{L-1}=1}^{d_{L-1}} \cdots \sum_{i_1=1}^{d_1} \left( \prod_{\ell=2}^{L} W_{i_\ell, i_{\ell-1}} \right) (W_{i_1}^1 x) \prod_{\ell=1}^{L} V_{i_\ell}^\ell x. \]

(6)

This equation further show that the polynomial order of the network is \( L + 1 \).

To include terms with different orders, we need to include intercept vectors. Suppose each layer has an intercept vector \( b^\ell \), then the layer is defined by

\[
h^\ell = \sigma_p(W^\ell h^{\ell-1} + b^\ell; V^\ell, x).
\]

(7)

We can re-write the input, hidden vectors, and weight matrices in the following form,

\[
W^\ell = \begin{bmatrix} W^\ell & b^\ell \\ 0 & 1 \end{bmatrix}, \quad h^\ell = \begin{bmatrix} h \\ 1 \end{bmatrix},
\]

(8)

\[
V^\ell = \begin{bmatrix} V^\ell & 0 \\ 0 & 1 \end{bmatrix}, \quad x = \begin{bmatrix} x \\ 1 \end{bmatrix},
\]

(9)
then we still have the previous form, \( h^\ell = \sigma_p(W^\ell h^{\ell-1}; V^\ell, \mathbf{x}) \), and then all previous derivations still apply. For notational simplicity, the following analysis continues to use notations without the intercept term.

The LPNN shares the same principle as the ResNet [He et al., 2016]: a deeper network should not have larger training error than a shallower one. Similar to skip connections, which allows a deep ResNet to implement a shallower one, a special parameter setting of \( \theta \) also reduces a LPNN to a shallower one. Setting \( W^\ell = 0 \) and \( b^\ell = 1 \) in (8) will reduce the LPNN to \( L - \ell \) layers.

## 4. Analysis

In this section, we first connect LPNN with a few previous decomposition models, highlighting a few properties of LPNN as a polynomial function. Then we emphasize that LPNN can be trained with batch normalization and dropout. Finally we analyze LPNN from the perspective of neural networks and show its properties in Bayesian learning.

### 4.1. Relation with decomposition models

By making comparison between a LPNN and previous polynomial models, we understand their respective weakness and strength.

**Relation with polynomial kernels.** We first show that the polynomial networks constructed from polynomial kernel functions by [Blondel et al., 2016b] are special cases of the LPNN model. The following theorem formalize the relationship, and its proof is in the supplement.

**Theorem 4.1.** The learning models in the form of \( y(\mathbf{x}) = \sum_{k=1}^{K} \pi_k (\lambda + \mathbf{p}_k^T \mathbf{x})^m \) [Blondel et al., 2016b] can be written as a LPNN function.

Compared with a LPNN, a model constructed from polynomial kernels has a limited capacity. When it is written in the form of a LPNN, a kernel is used across all hidden layers, so it form is rather restricted. The model with multiple kernels has multiple hidden units, but there is no information exchange between hidden units from different kernels.

**Relation with factorization machines.** By the following theorem, second-order factorization machines [Rendle, 2010] are special cases of LPNNs. The proof is in the supplement.

**Theorem 4.2.** The second-order factorization machines taking the form \( y(\mathbf{x}) = w_0 + \mathbf{w}_1^T \mathbf{x} + \sum_{i=1}^{d_0} \sum_{j=i+1}^{d_0} \mathbf{v}_j^T \mathbf{v}_i \mathbf{x}_i \mathbf{x}_j \) [Rendle, 2010] can be written as a LPNN function.

Factorization machines exclude monomials that contain variables having exponents more than 1, e.g. \( x_i^2 \) in the example above, so it is hard to write high-order factorization machines into the LPNN form. However, it is easy to construct a LPNN to match all its non-zero coefficients. In this sense, factorization machines have less model capacity than LPNN.

**Relation with tensor-train models.** The coefficients of LPNN has a tensor-train decomposition [Oseledets, 2011], so it is a special case of the tensor-train model [Chen et al., 2018].

**Theorem 4.3.** The coefficients of LPNN’s network function has a tensor-train decompositon.

**Proof.** Write \( W^1_{i_1} \mathbf{x} = \sum_{i_0=1}^{d_0} W^1_{i_1,i_0} W^0_{i_0} \mathbf{x}_{i_0} \) with \( W^0 \) being an identity matrix. Then (6) can be written as

\[
\begin{align*}
h^\ell_{i_L} &= \frac{d_L-1}{i_L-1} \ldots \frac{d_1}{i_1-1} \sum_{i_0=1}^{d_0} \left[ (W^0_{i_0} \mathbf{x}) \prod_{\ell=1}^{L} W^\ell_{i_\ell,i_{\ell-1}} V^\ell_{i_\ell} \mathbf{x}_{i_\ell} \right].
\end{align*}
\]

Let \( G^\ell(i_\ell, n_\ell, i_{\ell-1}) = W^\ell_{i_\ell,i_{\ell-1}} V^\ell_{i_\ell} \mathbf{x}_{i_\ell} \) be a three-way tensor for \( \ell = 1, \ldots, L - 1 \). Let \( G^L \) be a three-way tensor with size 1 in the first dimension, and \( G^L(1, n_L, i_{\ell-1}) = W^L_{i_L,i_{\ell-1}} V^L_{i_L} \mathbf{x}_{i_L} \). Let \( G^0 \) be a three-way tensor with size 1 in the last dimension, and \( G^0(:, :, 1) = \mathbf{1} \). Then \( h^\ell_{i_L} = \prod_{\ell=0}^{L}(G^\ell \times_2 \mathbf{x}) \). Here \( \times_2 \) is the 2-mode product of a three-way tensor and a vector; the product represents matrix multiplications. By Lemma 1 in [Chen et al., 2018], the coefficients of \( h^\ell_{i_L} \) is the tensor-train decomposition expressed by \( G^0, \ldots, G^L \).

We can analyze the complexity of a LPNN and a tensor-train model. In the decomposition above, each three-way tensor \( G^\ell \) with \( \ell \geq 1 \) is constructed from two matrices. A LPNN layer has about \( (d_\ell \times d_\ell - 1 + d_\ell \times d_0) \) parameters, which is at the same level as a feedforward layer. However, we use general three-way tensors in a tensor-train model, then there will be \( d_\ell \times d_0 \times d_{\ell-1} \) parameters in each “layer” and excessively many parameters in the entire model. Then it is unnecessary to use a dense \( G^\ell \)'s as in a general tensor-train model.

### 4.2. Special properties

As a polynomial function, a LPNN has the following two interesting properties.

**Multilinear in parameters** The network function \( \text{lpnn}(\mathbf{x}; \theta) \) is multilinear in model parameters \( \theta = \{W^1, \ldots, W^L, V^1, \ldots, V^L\} \). We see so by examining the network function in (6); if we focus on one matrix (a \( W^\ell \) or a \( V^\ell \)) and hold all other parameters fixed, then the network output is linear in this matrix. Furthermore, if we optimize the network against a convex loss function \( \text{loss}(h^\ell; y) \), then the loss is multiconvex in \( \theta \).
This property means that the change of a single $W^\ell$ linearly change the network output. Therefore, the optimization of network output poses straightforward gradient directions to network weights in $\theta$. There are no issues of gradient explosion. Compared with a LPNN, the effect of network weights in a normal feedforward network are transformed through the network’s hidden layers, so the gradient can be skewed when it is back-propagated through layers.

**The network function along a gradient.** The network function along a gradient direction is a univariate polynomial function. We can write the polynomial into its canonical form.

We compute the polynomial coefficients recursively. Let’s restrict $x$ to a line $x = tg + x_0$, with $t$ being a scalar variable, $x_0 \in \mathbb{R}^{d_0}$ being a point, and $g \in \mathbb{R}^{d_0}$ being a direction. Then $\text{lpnn}(x; \theta)$ is a polynomial function of $t$ with order $L + 1$.

We view each $h^\ell$ as a function of $t$ and use an operation $\alpha(h^\ell)$ to extract polynomial coefficients of $h^\ell$. Note that each entry of $h^\ell$ is an $(\ell + 1)$-order polynomial and has $\ell + 2$ coefficients, so $\alpha(h^\ell)$ is a matrix of size $d_\ell \times (\ell + 2)$. Also note that $\alpha(\cdot)$ is a linear operation.

We have $\alpha(h^0) = \alpha(x) = [g, x_0]$. Then we calculate $\alpha(h^\ell)$ recursively. Substitue the line expression into (3).

$$h^\ell = \text{diag}(V^\ell g)W^\ell h^{\ell-1} + \text{diag}(V^\ell x_0)W^\ell h^{\ell-1}.$$  

The function $\alpha(\cdot)$ is a linear operation. If $f$ is a vector-valued polynomial function of $t$, and $W$ is a constant matrix with proper sizes, then $\alpha(Wf) = W\alpha(f)$. We also have $\alpha(tf) = [\alpha(f), 0]$, with $0$ being zero vector with the same length as $f$. The relation is true because $tf$ raises the coefficients of $f$ one order higher.

By using these properties of $\alpha(\cdot)$, we have the recursive formula for computing $\alpha(h^\ell)$.

$$\alpha(h^\ell) = [\text{diag}(V^\ell g)W^\ell \alpha(h^{\ell-1}), 0] + [0, \text{diag}(V^\ell g)W^\ell \alpha(h^{\ell-1})]. \quad (10)$$

If we want compute only the coefficients of lower-order monomials, then we only need to store the right-most few columns of $\alpha(h^\ell)$. We omit the details here.

This property is useful in adversarial learning. The generation of adversarial samples often relies on the optimization of a perturbation of an instance $x$. If we know a perturbation direction, then finding the optimal perturbation along the direction is equivalent to finding the minimum of a univariate polynomial function, which can be solved efficiently.

### 4.3. Training with batch normalization and dropout

As a layer network, a LPNN is trained with standard techniques including stochastic optimization, batch normalization (BN), and dropout, which have been proved to be effective in practice. We can apply batch normalization and dropout to a LPNN without any modification. Here we put the BN layer after the activation per some practitioners’ advice.

Let’s consider one hidden layer and omit layer indices for notational simplicity. Let $h_k$ be the hidden layer of an instance $k$ in a batch, then the batch-normalized hidden layer $\tilde{h}_k$ is computed by

$$\tilde{h}_k = \gamma(h_k - \mu)/(\sigma + \epsilon) + \beta. \quad (11)$$

Here the division / is an element-wise operation, $\epsilon$ is a small positive number, and $(\gamma, \beta)$ are learnable parameters. The two vectors, $\mu$ and $\sigma$, are computed from the batch during training and are constants during testing.

Note that the trained LPNN model with constant BN parameters is still a polynomial function because the BN operation in $[\text{11}]$ is a linear operation. The model in training is not a polynomial function since $\sigma$ is computed from the batch that includes $h_k$. Here we want to integrate BN parameters into network weights so that previous derivations still apply.

Now we merge a BN layer into its previous LPNN layer. Let $W'$ and $V'$ denote weight matrices in the previous layer, then the equivalent LPNN layer is given by setting $W$ and $b$ in [7] as follows.

$$W = W' \text{diag}((\gamma/\sigma + \epsilon)), \quad b = -W' \text{diag}(\gamma\mu/(\sigma + \epsilon) + \beta) \quad (13)$$

In this result, we can see that BN changes the norm of weight matrices. Based on the study by Santurkar et al. [2018], BN can simply shrink the norms of weight matrices to avoid having steep slopes in the function surface.

**Dropout** can be directly applied to LPNN. In the training phase, using dropout is equivalent to removing some entries in summations of [6] and rescaling the summation. In the testing phase, dropout have no effect, and the trained model is just as the definition above.

### 4.4. Moments of network outputs in Bayesian learning

The LPNN is convenient for Bayesian learning attribute to the multilinear property. One important problem in Bayesian learning is to compute the distribution of network predictions when the network parameters are from
We first check the uniqueness of the product activation. In this experiment, we check how well a two-layer feedforward neural network can fit the multiplication function. If they cannot easily fit such a function, then it means common activations are unlikely to imitate a product activation. We randomly generate two features \((x_1, x_2)\) from the range \([-1, 1] \times [-1, 1]\) and then define the multiplication \(y_p = 4x_1 x_2\) to represent a product activation. With the constant, the average of the absolute value of \(y_p\) is 1.

We use a feedforward network with the tanh activation, \(y_f = w^\top \tanh(\mathbf{W}[x_1, x_2]^\top + b_1) + b_2\), to fit the multiplication \(y_p\). Here the number of rows in \(\mathbf{W}\) is the number of hidden units in this one-layer neural network. We train the neural network for 200 epochs and record the RMSE. We run the experiment for 10 times and take the average and variance of 10 RMSE values.

The results are tabulated in the first row of Table 1. It is actually hard for the feedforward neural network to fit the product operation. The feedforward neural network needs to use 4 hidden units to get satisfying results. As a reference, it is much easier for the same network to fit a ReLU activation. The ReLU activation is incorporated into a function \(y_f = \text{relu}(0.5x_1 + 1.5x_2)/C\), with \(C\) normalizing \(y_f\) to have an average absolute value of 1. The feedforward network has much smaller error when fitting the function \(y_f\) (see RMSEs in the second row of Table 1). When the product activation is an effective way to combine two features through multiplication, it is not easy for other activations like tanh to approximate the same operation. This result indicates that some information processing by product activations are actually hard for common activations.

We then examine the product activation function \(h = \sigma_p(u; \mathbf{V}, \mathbf{x})\) in a trained model. We set up a LPNN with three hidden layers and then train it on the mnist dataset. The training finishes after 20 epochs when the network has a validation accuracy of 0.984. Then we check the input \(u\) and the response \(h\) of the activation functions at three different layers. We plot the response \(h_i\) against the corresponding \(u_i\) for each hidden unit to generate a subplot. We randomly select 400 instances and plot each \((h_i, u_i)\) pair. We plot four hidden units at each of all three hidden layers and then train it on the mnist dataset. We plot four hidden units at each of all three hidden layers and then train it on the mnist dataset. We plot the response \(h_i\) against the corresponding \(u_i\) for each hidden unit to generate a subplot. We randomly select 400 instances and plot each \((h_i, u_i)\) pair. We plot four hidden units at each of all three hidden layers and then train it on the mnist dataset.
5.2. Regression and Classification

In this section, we evaluate the LPNN on several regression and classification tasks. The LPNN is compared against feedforward network and three polynomial learning models. All models are summarized below.

**Feedforward network (FF-RELU):** feedforward networks uses ReLU functions as activations. We add $l_2$ norm regularization to the model. The regularization weight is chosen from $\{1e-6, 1e-5, 1e-4, 5e-4\}$. When dropout is applied, the dropout rate is chosen from $\{0, 0.05, 0.1, 0.2, 0.4\}$.

**Polynomial Neural Network (FF-QUAD):** the model is the same as the FF-RELU except its activations are the quadratic function. It has the same hyperparameters as FF-RELU, and it is trained in the same way as FF-RELU.

**Factorization Machine (FM):** we use the implementation from the sklearn package [Niculae Accessed in 2019]. The order of FM in this implementation can be 2 or 3. It add several ANOVA kernel functions (called factors) to increase model complexity. The model is also regularized by $l_2$ norm. The hyperparameters of FM include the order, the number of factors, and the weight of regularization. The number of factors is chosen from from $\{2, 4, 8, 16\}$, and the regularization weight is chose from the same range as FF-RELU. This implementation of FF-RELU does not have multiple outputs, so we have used one-vs-rest for multiclass classification problems.

**Polynomial Kernel (PK):** PK uses polynomial kernels. Other than that, PK is similar to FM. We can specify the order of the underlying polynomial function of PK. The hyperparameters of PK are the same as FM. The implementation is also from the sklearn package.

**LPNN:** the model is the same as the FF-RELU except its activations are product activations. Its hyperparameters are the same as FF-RELU, and it is trained in the same way as FF-RELU.

We test these models on five regression datasets (wine-quality, power-plant, kin8nm, boston-housing, and concrete-strength) and six classification datasets (mnist, fashion-mnist, skin, sensIT, letter, covtype-b, and covtype). The mnist and fasion-mnist datasets come with the Keras package, the skin, sensIT, and covtype-b datasets are from the libSVM website, and all other datasets are from the UCI

| methods               | wine red | power plant | kin8nm | boston housing | concrete |
|-----------------------|----------|-------------|--------|----------------|----------|
| FF-RELU               | 0.60 ± 0.04 | 4.02 ± 0.18 | 0.100 ± 0.002 | 2.82 ± 0.76 | 5.10 ± 0.49 |
| FM                    | **0.73 ± 0.09** | 4.43 ± 0.15 | 0.155 ± 0.004 | 4.80 ± 1.14 | 8.52 ± 0.59 |
| PK                    | 4.39 ± 5.50 | **4.14 ± 0.14** | 0.100 ± 0.005 | 41.9 ± 77.2 | 7.95 ± 2.42 |
| FF-QUAD               | 5.49 ± 16.5 | 5.83 ± 1.39 | **0.102 ± 0.007** | **4.59 ± 2.74** | 5.58 ± 0.48 |
| LPNN                  | **0.82 ± 0.18** | **4.24 ± 0.18** | **0.099 ± 0.006** | **4.05 ± 2.13** | **5.20 ± 0.62** |

Figure 1: Product activations of LPNN on the mnist dataset. The model has three hidden layers. From each layer, activations of four hidden units are plot here in the same color.

Table 2: RMSE of different models on regression tasks
Regression. We first apply the model to five regression tasks. We use the same data splits by Gal (Accessed in 2019). Each dataset has 20 random splits. On each split, we run model selection through five-fold cross validation, re-train the model, and then test the model on the test set. The results are averaged over the 20 splits. For FF-RELU, FF-QUAD, and LPNN, we set three hidden layers and 50 hidden units in each hidden layer. We apply dropout and batch normalization to all the three models. We set the polynomial order to be 4 for the PK model to match the order of LPNN. All other hyperparameters of a model are also selected together with architectures.

The error rates of different models are reported in Table 3. We omit standard deviations in the table to save space. Polynomial models are compared with paired $t$-tests. The performance of the best polynomial model is bolded. We also compare LPNN against FF-RELU: if LPNN is significantly better than FF-RELU, we underline the LPNN’s performance. The performance of LPNN is better other polynomial models in general. LPNN is comparable to FF-RELU on classification tasks. We speculate the reason is that an LPNN only needs to decide discrete labels from its outputs in classification tasks while it needs to fit the exact value in regression tasks. LPNN may not be flexible enough for fitting continuous values compared to feedforward networks.

In a summary, the LPNN narrows the performance gap between polynomial models and the well-studied feedforward neural networks, making the polynomial more practical in typical learning tasks.

5.3. The effect of batch normalization and dropout

In this subsection, we investigate the effects of batch normalization and dropout on LPNN. We use $L \in \{1, 2, 3, 5, 10\}$. For each depth, we try four combinations: using/not using batch normalization and/or dropout. We select other hyperparameters through model selection. We run the experiment

Table 3: Error rates of different models on classification tasks

| methods | mnist | fashion-mnist | skin | sensIT | letter | covtype-b | covtype |
|---------|-------|---------------|------|--------|--------|-----------|---------|
| FF-RELU | 0.0185 | 0.108         | 0.0313 | 0.176  | 0.096  | 0.113     | 0.146   |
| FM      | 0.0573 | 0.167         | 0.0439 | 0.260  | 0.546  | 0.208     | 0.575   |
| PK      | 0.0506 | 0.168         | 0.0039 | 0.225  | 0.248  | 0.191     | 0.494   |
| FF-QUAD | 0.0503 | 0.127         | 0.0018 | 0.199  | 0.104  | 0.097     | 0.103   |
| LPNN    | 0.0171 | 0.117         | 0.0017 | 0.175  | 0.0729 | 0.117     | 0.140   |

Table 4: Effect of batch normalization and dropout

| $L$ | 1   | 2   | 3   | 5   | 10  |
|-----|-----|-----|-----|-----|-----|
| Neither | $7.76 \pm 0.53$ | $6.30 \pm 0.96$ | $6.89 \pm 2.06$ | $7.86 \pm 3.10$ | $7.49 \pm 2.77$ |
| Only dropout | $7.78 \pm 0.54$ | $5.98 \pm 0.57$ | $5.12 \pm 0.58$ | $4.92 \pm 0.78$ | $4.71 \pm 0.90$ |
| Only BN | $7.82 \pm 0.55$ | $6.26 \pm 0.87$ | $5.82 \pm 1.13$ | $5.46 \pm 1.83$ | $4.97 \pm 0.97$ |
| BN and dropout | $7.77 \pm 0.53$ | $6.05 \pm 0.50$ | $5.20 \pm 0.62$ | $4.72 \pm 0.66$ | $4.58 \pm 0.74$ |

We shrink the number of hidden units from the bottom to the top. The number of hidden units is computed by $\alpha(d_{out} - d_{in}) + d_{out}$ so that the number of hidden units in a middle layer is between the input dimension and the output dimension. The shrinking factor $\alpha$ is chose from $\{0.3, 0.5, 0.7, 0.8\}$. We also select the order for PK from $\{2, 3, 5\}$ to match the order of LPNN. All other hyperparameters of a model are also selected together with architectures.

Classification. We then test these models on seven classification tasks. For each dataset, we set 30% as the test set, except for mnist and fashion-mnist datasets, which come with test sets. We do model selection for both architecture and hyperparameters on 20% of the training set. For neural networks, the number of hidden layers is chosen from $\{1, 2, 4\}$. We shrink the number of hidden units from the bottom to the top. The number of hidden units is computed by $\alpha(d_{out} - d_{in}) + d_{out}$ so that the number of hidden units in a middle layer is between the input dimension and the output dimension. The shrinking factor $\alpha$ is chose from $\{0.3, 0.5, 0.7, 0.8\}$. We also select the order for PK from $\{2, 3, 5\}$ to match the order of LPNN. All other hyperparameters of a model are also selected together with architectures.

The error rates of different models are reported in Table 3. We omit standard deviations in the table to save space. Polynomial models are compared with paired $t$-tests. The performance of the best polynomial model is bolded. We also compare LPNN against FF-RELU: if LPNN is significantly better than FF-RELU, we underline the LPNN’s performance. The performance of LPNN is better other polynomial models in general. LPNN is comparable to FF-RELU on classification tasks. We speculate the reason is that an LPNN only needs to decide discrete labels from its outputs in classification tasks while it needs to fit the exact value in regression tasks. LPNN may not be flexible enough for fitting continuous values compared to feedforward networks.

In a summary, the LPNN narrows the performance gap between polynomial models and the well-studied feedforward neural networks, making the polynomial more practical in typical learning tasks.

5.3. The effect of batch normalization and dropout

In this subsection, we investigate the effects of batch normalization and dropout on LPNN. We use $L \in \{1, 2, 3, 5, 10\}$. For each depth, we try four combinations: using/not using batch normalization and/or dropout. We select other hyperparameters through model selection. We run the experiment...
on a regression task (concrete-strength) and a classification task (mnist).

The results are shown in Table 4 and 5. For each depth $L$, the four combinations are compared with paired $t$-tests, and the best performance(s) across four combinations are bolded. From this result, we see that both batch normalization and dropout are needed to train a good LPNN model when the model is deep. On the mnist dataset, the LPNN without batch normalization has very bad performance when $L = 5$. Its performance drops sharply after a few epochs. This observation indicates that the LPNN without batch normalization is very unstable due to some bad optimization directions.

We also have the following observations in training: batch normalization in training tends to increase the depth of the model; and dropout tends to decrease the scale of weight matrices. These observations are consistent with previous observations in the literature.

5.4. Network outputs with stochastic network weights

In this experiment we check the network output $h^L$ when the network parameters in $\theta$ are from a Gaussian prior. We use a LPNN with $L = 5$ layers. The mean of the prior is given by network weights of a trained LPNN. The variance of the prior is set to $\sigma^2 I$. Then we sample 10,000 samples from the Gaussian prior as network weights to compute samples of $h^L$. Here $h^L$ has only one entry, so we can plot its samples into a histogram. At the same time, we compute the moments of the distribution of $h^L$ and get a Gaussian approximation. Figure 2 shows the histograms and the corresponding approximate Gaussian distributions for $\sigma^2 = 0.05$ (left) and $\sigma^2 = 0.1$ (right). From this result, we see that the Gaussian approximation is very accurate.

6. Conclusion

In this paper, we propose the product activation and use it to construct the LPNN, a new type of polynomial neural networks. As a neural network, a LPNN can be trained with modern training techniques, such as dropout and batch normalization. As a decomposition model, it connects other decomposition models with neural networks. Now we have a new approach to convert other decomposition models to neural networks that have a similar structure as a LPNN.

The network function of LPNN is multilinear in its parameters. With this property, we can efficiently calculate moments of the network’s outputs when the network is given a prior. The moments allow us to approximate the distribution of the network outputs, then we will be able to approximately maximize the likelihood of the data without using complex inference algorithms.

With its unique theoretical properties and competitive performances in practice, the LPNN a valuable learning model.

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References

Blondel, M., Fujino, A., Ueda, N., and Ishihata, M. Higher-order factorization machines. In Advances in Neural Information Processing Systems, pp. 3351–3359, 2016a.

Blondel, M., Ishihata, M., Fujino, A., and Ueda, N. Polynomial networks and factorization machines: New insights and efficient training algorithms. In International Conference on Machine Learning, pp. 850–858, 2016b.

Blondel, M., Niculae, V., Otsuka, T., and Ueda, N. Multi-output polynomial networks and factorization machines. In Advances in Neural Information Processing Systems, pp. 3349–3359, 2017.

Blundell, C., Cornebise, J., Kavukcuoglu, K., and Wierstra, D. Weight uncertainty in neural networks. arXiv preprint arXiv:1505.05424, 2015.

Chen, Z., Batselier, K., Suykens, J. A. K., and Wong, N. Parallelized tensor train learning of polynomial classifiers. IEEE Transactions on Neural Networks and Learning Systems, 29(10):4621–4632, Oct 2018.

Du, S. S. and Lee, J. D. On the power of over-parametrization in neural networks with quadratic activation. In International Conference on Machine Learning, pp. 1328–1337, 2018.

Gal, Y. https://github.com/yaringal/Dropout

UncertaintyExps, Accessed in 2019.
He, K., Zhang, X., Ren, S., and Sun, J. Deep residual learning for image recognition. In Proceedings of the IEEE conference on computer vision and pattern recognition, pp. 770–778, 2016.

Ioffe, S. and Szegedy, C. Batch normalization: Accelerating deep network training by reducing internal covariate shift. arXiv preprint arXiv:1502.03167, 2015.

Kileel, J., Trager, M., and Bruna, J. On the expressive power of deep polynomial neural networks. arXiv preprint arXiv:1905.12207, 2019.

Lin, M., Qiu, S., Hong, B., and Ye, J. The second order linear model. arXiv preprint arXiv:1703.00598, 2017.

Livni, R., Shalev-Shwartz, S., and Shamir, O. On the computational efficiency of training neural networks. In Advances in neural information processing systems, pp. 855–863, 2014.

Niculae, V. https://github.com/scikit-learn-contrib/polylearn, Accessed in 2019.

Oseledets, I. V. Tensor-train decomposition. SIAM Journal on Scientific Computing, 33(5):2295–2317, 2011.

Rendle, S. Factorization machines. In 2010 IEEE International Conference on Data Mining, pp. 995–1000. IEEE, 2010.

Santurkar, S., Tsipras, D., Ilyas, A., and Madry, A. How does batch normalization help optimization? In Advances in Neural Information Processing Systems, pp. 2483–2493, 2018.

Soltani, M. and Hegde, C. Towards provable learning of polynomial neural networks using low-rank matrix estimation. In International Conference on Artificial Intelligence and Statistics, pp. 1417–1426, 2018.

Soltani, M. and Hegde, C. Fast and provable algorithms for learning two-layer polynomial neural networks. IEEE Transactions on Signal Processing, 67(13):3361–3371, 2019.

Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., and Salakhutdinov, R. Dropout: a simple way to prevent neural networks from overfitting. The journal of machine learning research, 15(1):1929–1958, 2014.

Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., Kaiser, L. u., and Polosukhin, I. Attention is all you need. In Guyon, I., Luxburg, U. V., Bengio, S., Wallach, H., Fergus, R., Vishwanathan, S., and Garnett, R. (eds.), Advances in Neural Information Processing Systems 30, pp. 5998–6008. 2017.