

1 **EFFECTIVE RANK AND THE STAIRCASE PHENOMENON: NEW
2 INSIGHTS INTO NEURAL NETWORK TRAINING DYNAMICS***

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4 **Abstract.** In recent years, deep learning, powered by neural networks, has achieved widespread
5 success in solving high-dimensional problems, particularly those with low-dimensional feature struc-
6 tures. This success stems from their ability to identify and learn low dimensional features tailored
7 to the problems. Understanding how neural networks extract low-dimensional features from high-
8 dimensional data remains a fundamental challenge in deep learning theory. In this work, we introduce
9 the concept of ‘effective rank’ to measure the linear independence of the basis functions represented
10 by the neurons in the final hidden layer. Through extensive numerical experiments, we have discov-
11 ered a notable phenomenon: the effective rank increases progressively during training, exhibiting a
12 staircase-like pattern, while the loss function concurrently decreases. We refer to this observation as
13 the ‘staircase phenomenon’. In addition, for deep neural networks, we rigorously provide a theoretical
14 explanation for this phenomenon by establishing the negative correlation between the loss function
15 and effective rank, demonstrating that the lower bound of the loss function decreases with increasing
16 effective rank. Therefore, to achieve a rapid descent of the loss function, it is critical to promote the
17 swift growth of effective rank. We also evaluate several advanced learning methodologies and find
18 that they can indeed accelerate the training process by quickly increasing the effective rank.

19 **Key words.** deep neural network, training dynamics, staircase phenomenon, effective rank.

20 **MSC codes.** 68Q32, 68T07

21 **1. Introduction.** Deep neural networks (DNNs) have exhibited remarkable per-
22 formance across a wide range of fields, including computer vision, natural language
23 processing, and computational physics, due to their extraordinary representation ca-
24 pabilities. However, the training process of DNNs remains highly complex and, in
25 many respects, poorly understood. Developing a comprehensive understanding of the
26 training mechanisms is critical for the design, optimization, and interpretability of
27 these models.

28 There are various approaches attempting to explain the mechanism of training
29 dynamics in neural networks. Visualization-based methods, such as those in [39, 21],
30 analyze the hierarchical formation of feature maps in convolutional networks and
31 investigate how network architecture influences the geometry of the loss landscape
32 during training. The impact of flat and sharp minima on generalization performance
33 has been extensively studied in [13, 5, 19], providing insights into the relationship
34 between the optimization landscape and generalization behavior. The neural tan-
35 gent kernel (NTK) theory provides a rigorous framework for analyzing the training
36 dynamics of wide neural networks in the infinite-width limit. Jacot et al. [18] intro-
37 duce the NTK to describe the training dynamics as a convergent kernel in function
38 space, offering valuable insights into how networks evolve during training. Extensions
39 of the NTK framework in [32, 1, 4] further examine the generalization behavior of
40 neural networks across various contexts. Another important perspective comes from
41 the frequency principle (or spectral bias), suggesting that neural networks tend to
42 learn low-frequency patterns during the early stages of training [34, 27, 36, 35]. This

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43 observation demonstrates that, when the training process of the neural network is
 44 projected into the spectral domain, the number of effective frequencies exhibits an
 45 increasing trend over time.

46 A multilayer perceptron (MLP) neural network can be constructed as

$$47 \quad (1.1) \quad \begin{cases} y_0 = x, \\ y_{k+1} = \sigma(W_k y_k + b_k), \quad k = 0, \dots, L-1, \\ y = \beta \cdot y_L, \end{cases} \quad \text{Diagram icon}$$

48 where $x \in \mathbb{R}^d$, $y_k \in \mathbb{R}^n$, and $W_0 \in \mathbb{R}^{n \times d}$, $W_k \in \mathbb{R}^{n \times n}$, $b_k, \beta \in \mathbb{R}^n$ are trainable parameters.
 49 Denoting $\theta = \{W_k, b_k\}_{k=0}^{L-1}$, the output of the neural network can alternatively
 50 be expressed in the form

$$51 \quad y(x; \theta) = \sum_{j=1}^n \beta_j \phi_j(x; \theta).$$

52 We decompose the neural network into two parts: the **neuron functions** $\{\phi_j\}_{j=1}^n$
 53 correspond to the **neurons in the last hidden layer**, and the coefficients $\{\beta_j\}_{j=1}^n$ are the
 54 weights in the output layer. This work focus on examining neural networks from the
 55 perspective of traditional computational mathematics. Specifically, when the output
 56 of a neural network is expressed as a linear combination of the neurons in the last
 57 hidden layer, these neurons can be interpreted as a set of basis functions. [11, 10]
 58 show that ReLU-activated deep neural networks can reproduce all linear finite element
 59 functions and [23, 24, 30] provide algorithms to combine classical finite element
 60 methods with neural networks. As discussed in [16, 26], randomly generated neuron
 61 functions in shallow neural networks also exhibit sufficient representation ability.
 62 A detailed analysis of the coefficient matrices associated with the random features,
 63 particularly in terms of the distribution of their singular values, has been provided
 64 in [3]. The decay rate of the eigenvalues of the Gram matrix of a two-layer neural
 65 network with ReLU activation under general initialization has been analyzed in [40].
 66 Its further numerical study suggests that smoother activation functions lead to faster
 67 spectral decay of the Gram matrix. These findings underscore the connection between
 68 traditional computational methods and deep learning frameworks, motivating
 69 a deeper mathematical exploration of neural network representations.

70 In this work, we focus on understanding how neuron functions evolve during the
 71 training dynamics of neural networks. Motivated by prior researches, we investigate
 72 the behavior of the singular values of the mass matrix associated with the neuron
 73 functions during the training process. To formalize the observations, we introduce
 74 the concept of **ϵ -rank** (effective rank) for a set of functions (see as Definition 2.5),
 75 which quantitatively represents the number of effective features in the network.

76 Our key finding in this paper is the identification of a novel phenomenon concerning
 77 the ϵ -rank of neuron functions, stated as follows:

78 **Staircase phenomenon:** *In training dynamics, the loss function often decreases
 79 rapidly along with a significant growth of ϵ -rank of neurons, and the evolution of the
 80 ϵ -rank over time resembles a staircase-like pattern.*

81 As shown in the Figure 1, this increase in ϵ -rank occurs in a stepwise fashion,
 82 closely resembling the structure of a staircase. Specifically, under standard parameter
 83 initialization, neuron functions initially exhibit low linear independence. Throughout
 84 the training process, variations in the loss function are closely linked to changes in the
 85 linear independence of these neuron functions. When the decline in the loss function

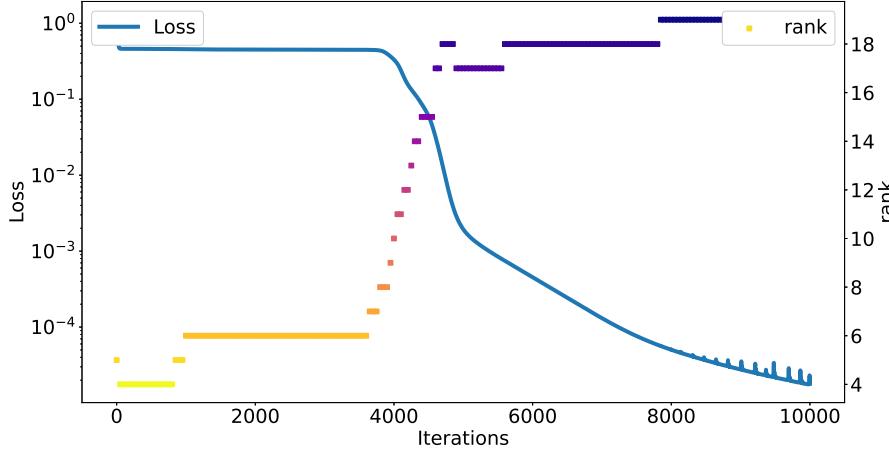


Fig. 1: Staircase phenomenon of neuron functions in training dynamics.

86 reaches a plateau, the growth in linear independence tends to stabilize. Conversely,
 87 when the linear independence increases significantly, the loss experiences a rapid de-
 88 scent. We theoretically prove that the lower bound of the loss function decreases as
 89 the ϵ -rank increases. This theoretical result holds for general deep neural networks.
 90 Consequently, achieving a sufficiently large ϵ -rank is essential for ensuring a significant
 91 reduction in the loss function.

92 This naturally raises the question: how can a set of highly linearly independent
 93 neuron functions be learned efficiently? To address this, we identify several strategies
 94 from existing techniques that enable the neuron functions with a high ϵ -rank at the
 95 early stage of training. Specifically, by designing appropriate initialization schemes
 96 and selecting well-suited network architectures, it is possible to ensure that the neu-
 97 ron functions exhibit high linear independence from the outset. Such approaches
 98 significantly accelerate the training process or improve the accuracy.

99 The main contributions of this work are summarized as follows:

- 100 1. The introduction of effective rank provides a novel perspective for under-
 101 standing the training dynamics of neural networks, revealing a staircase phenom-
 102 enon. This phenomenon is observed universally across various tasks, includ-
 103 ing function fitting, handwriting recognition, and solving partial differential
 104 equations.
- 105 2. We prove that the loss function of deep neural networks has a lower bound re-
 106 lated to the ϵ -rank. This bound decreases as the ϵ -rank increases, thereby pro-
 107 viding a theoretical explanation for the staircase phenomenon. Our analysis
 108 concludes that a sufficiently high ϵ -rank is a necessary condition for achieving
 109 a significant reduction in the loss function.
- 110 3. We investigate how ϵ -rank evolves in existing advanced methodologies. Nu-
 111 mercial examples show that these methodologies can construct neuron func-
 112 tions with a high ϵ -rank rapidly, thereby significantly accelerating the training
 113 dynamics and improving model accuracy.

114 The rest of this paper is organized as follows. In section 2, the core concept of

115 ϵ -rank is defined through eigenvalues of the Gram matrix, and the staircase phenomenon
 116 is examined across various tasks and settings. A lower bound on the loss function
 117 with respect to the ϵ -rank is given in section 3, which provides the theoretical explanation
 118 of the staircase phenomenon. The evolution of ϵ -rank under existing methods is
 119 tested through numerical experiments in section 4, which include initialization methods,
 120 specific network structures and partial of unity technique in the random feature
 121 method. Concluding remarks are given in the last section.

122 **2. Staircase Phenomenon.**

123 **2.1. Preliminary.** Before presenting the staircase phenomenon, we introduce
 124 several definitions that are extensions of linear algebra.

125 **DEFINITION 2.1.** *The n functions $f_1(x), \dots, f_n(x)$ are **linearly dependent** in
 126 domain Ω if, there exists $c_1, c_2, \dots, c_n \in \mathbb{R}$ not all zero s.t.*

127 (2.1)
$$c_1 f_1(x) + c_2 f_2(x) + \dots + c_n f_n(x) = 0, \quad \forall x \in \Omega.$$

128 If the functions are not linearly dependent, they are said to be **linearly independent**.
 129 For given n functions $f_1(x), \dots, f_n(x)$ in $L^2(\Omega)$, the mass matrix M is defined as
 130 follows

131 (2.2)
$$(M)_{ij} := \int_{\Omega} f_i(x) f_j(x) dx, \quad 1 \leq i, j \leq n. \quad \text{By } \mathbf{c}' \mathbf{M} \mathbf{c} = \sum \mathbf{g}_i \mathbf{g}_j$$

132 Obviously M is symmetric positive semi-definite.

133 **LEMMA 2.2.** *$f_1(x), \dots, f_n(x)$ in are linearly independent if and only if the rank
 134 of the mass matrix $r(M) = n$.*

135 While the concept of linear dependence is well-defined in linear algebra, few functions
 136 in real-world applications strictly satisfy the condition specified in (2.1). Consequently,
 137 a more practical and applicable indicator, extending beyond the framework
 138 of (2.1), is required.

139 **DEFINITION 2.3.** *The n functions $f_1(x), \dots, f_n(x)$ in are ϵ -**linearly dependent**
 140 in domain Ω for some $\epsilon \geq 0$ if, there exists $c_1, c_2, \dots, c_n \in \mathbb{R}$ with $\|\mathbf{c}\|^2 = 1$ s.t.,*

141 (2.3)
$$\|c_1 f_1 + c_2 f_2 + \dots + c_n f_n\|^2 \leq \epsilon.$$

142 *Otherwise they are said to be ϵ -linearly independent.*

143 Here $\|\cdot\|$ is the short note of L^2 norm, $\|u\| = \sqrt{\langle u, u \rangle} = \left(\int_{\Omega} u^2 dx \right)^{\frac{1}{2}}$. It is easy
 144 to check that $f_1(x), \dots, f_n(x)$ are ϵ -linearly independent if and only if the minimum
 145 eigenvalue of M satisfies $\lambda_{\min}(M) > \epsilon$. In the following, we intend to extend these
 146 concepts of linear independence to the neuron functions of a neural network.

DEFINITION 2.4. *For a given neural network $u(x; \theta)$ defined on $\Omega \subset \mathbb{R}^d$ as*

$$u(x; \theta) = \sum_{j=1}^n \beta_j \phi_j(x; \theta),$$

the Gram matrix M_u is defined as below

$$(M_u)_{ij} = \int_{\Omega} \phi_i(x; \theta) \phi_j(x; \theta) dx.$$

147 Straightforwardly, we have the following definition of ϵ -effective rank, ϵ -rank for
 148 short.

149 **DEFINITION 2.5.** *The ϵ -rank of a neural network $u(x, \theta)$, associated with its
 150 Gram matrix M_u , is defined as*

151 (2.4) $r_\epsilon(M_u) := |\{\lambda(M_u) > \epsilon\}|,$

152 where $|\cdot|$ denotes the cardinal number of a set.

153 The standard definitions of linear dependence and rank can be regarded as spe-
 154 cial cases corresponding to $\epsilon = 0$. For simplicity, the linear independence and rank
 155 mentioned in experiments refer to ϵ -linear independence and ϵ -rank, respectively.

156 **2.2. Staircase Phenomenon.** With the necessary groundwork established, we
 157 now focus on how the ϵ -rank of the neuron basis functions evolves throughout the
 158 training process of the neural network. Across various tasks, including function fitting,
 159 handwriting recognition, and solving partial differential equations, we consistently
 160 observe the following phenomenon.

161 ***Staircase phenomenon:*** *In training dynamics, the loss function often decreases
 162 rapidly along with a significant growth of ϵ -rank of neurons, and the evolution of the
 163 ϵ -rank over time resembles a staircase-like pattern.* The ϵ -rank, as defined in Defin-
 164 ition 2.5, quantifies the linear independence or effective features of neuron functions
 165 in the last hidden layer. We experimentally demonstrate this phenomenon under
 166 different settings. To illustrate this phenomenon, we first consider a function fitting
 167 problem, which is one of the most fundamental tasks in neural networks.

168 **Example 2.6** (Function fitting). Consider the target function composed of mul-
 169 tiple frequency components, defined as

170 (2.5) $f(x) = \cos x + \cos 2x + \cos 30x.$

171 The computational domain is $\Omega = [-1, 1]$, and the mean square error is used as the
 172 loss function.

173 This example consists of three distinct experimental settings:

174 (i) (Figure 2) Investigate the performance of neural networks with varying width
 175 and depth. The network configurations are as follows: (a) $L = 2, n = 50$. (b)
 176 $L = 2, n = 25$. (c) $L = 4, n = 50$. (d) $L = 4, n = 25$.

177 (ii) (Figure 3) Analyze the ϵ -rank of the neuron functions across different layers
 178 for a fixed network width of $n = 50$ and depth of $L = 4$.

179 (iii) (Figure 4) Test neural networks with the following different activation func-
 180 tions:

181 – ReLU: $\sigma(x) = \max(x, 0)$.

182 – ELU: $\sigma(x) = x$, if $x > 0$, and $\sigma(x) = \alpha(e^x - 1)$, if $x < 0$.

183 – Cosine: $\sigma(x) = \cos(x)$.

184 – Hyperbolic tangent: $\sigma(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$

185 Under different width and depth, the training results are presented in Figure 2.

186 The black line represents the loss function, while the scatters correspond to the ϵ -rank
 187 of the mass matrix. When the linear independence of the neuron functions does not
 188 increase, the loss function stagnates for an extended period. However, once the neuron
 189 functions become fully linearly independent, the loss function rapidly decreases to a
 190 lower level, as shown in Figure 2(a), (c) and (d). Subfigure (b) demonstrates that

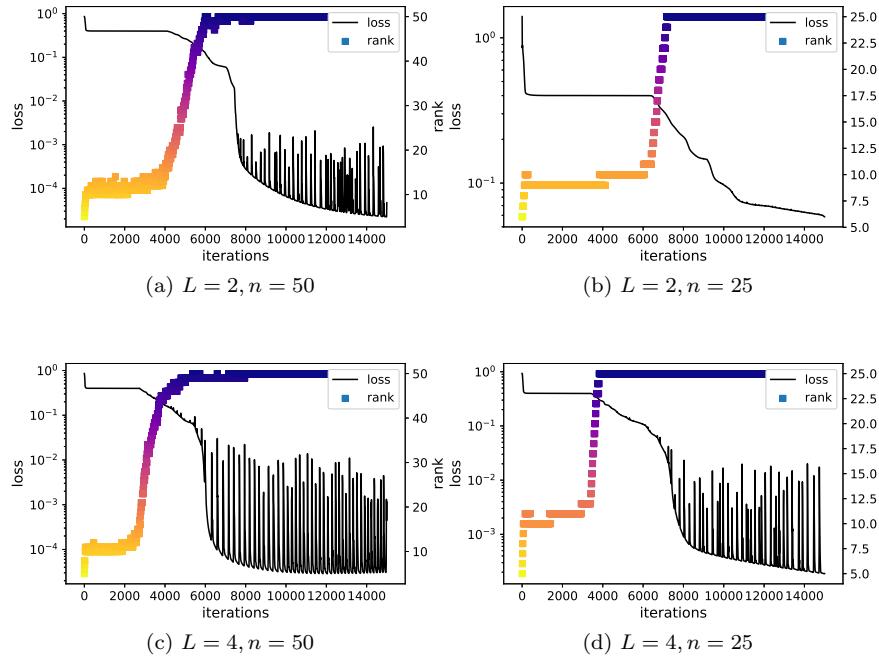


Fig. 2: (Example 2.6) Staircase phenomenon under different width and depth. The black line is the mean square error and the gradient ladder is the ϵ -rank.

shallow and narrow networks fail to approximate the target function efficiently under insufficient training. Another notable observation from Figure 2(d) is that, after attaining full rank, the loss function experiences a further sharp decline. This phase highlights a further unknown step in the learning process.

Additionally, we plot the ϵ -rank of neurons in each hidden layer for the case of $L = 4, n = 50$ in Figure 3. The staircase phenomenon is observed in most hidden layers. The results also indicate that shallow neurons exhibit fewer features compared to deeper neurons. Within the same network, the ϵ -rank of deeper neurons is consistently larger than that of shallow neurons. This observation suggests that deeper layers not only retain the linear independence of the preceding shallow layers but also further increase the complexity of the neuron functions, enabling the network to represent more intricate features. Notably, neurons in the first hidden layer fundamentally differ from that of deep layers. In the first layer, the neuron functions act as a set of basis functions that are directly formed by the activation function, without the composite transformation process that characterizes deeper networks.

The appearance of staircase phenomenon is independent of the choice of activation function. Figure 4 illustrates the evolution of the ϵ -rank during the training processes under several commonly used activation functions. The results show that while its behavior differs depending on the specific activation function used, staircase phenomenon is present across all activation functions. It can be observed that the upward trend and the peak value of the ϵ -rank vary across different activation functions. This is because neural network function classes constructed with different

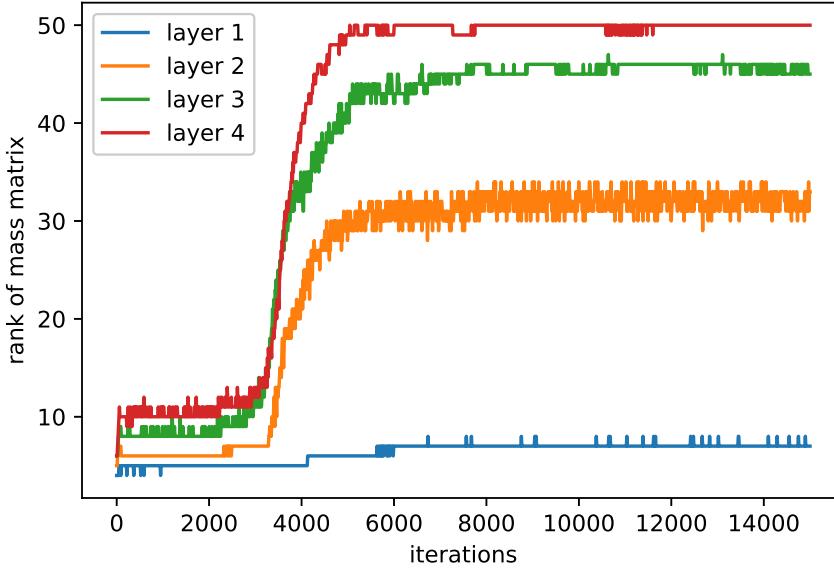


Fig. 3: (Example 2.6) The staircase phenomenon of different hidden layers in the same network

activation functions exhibit distinct approximation capabilities with respect to the target function.

Moreover, this phenomenon not only occurs in function fitting, but also in handwriting recognition and solving partial differential equations (subsection 4.1).

Example 2.7 (Handwriting recognition, Figure 5). MNIST is a widely used database of handwritten digits for training various image processing systems. The dataset contains 70,000 grayscale images of handwritten digits (0 through 9), each with a resolution of 28x28 pixels. Thus, the dimension of the input is $d = 784$. In this example, the cross entropy loss function is employed for training.

To address errors caused by high-dimensional numerical integration, we introduce an intermediate hidden layer with 10 neurons, using the neurons in this layer as sampling points for integration. As illustrated in Figure 5, the staircase phenomenon is evident in the handwriting recognition task, demonstrating that this phenomenon can also be observed in high-dimensional problems. This observation underscores the representational power of neural networks, which can effectively construct high-dimensional feature spaces, that is notably challenging in traditional scientific computing.

To gain a clearer understanding of the training mechanism, it is necessary to investigate why the staircase phenomenon occurs. Many widely used initialization methods do not ensure that the neuron functions are fully linearly independent after initialization. Therefore, the first stage of training involves separating the neuron functions **post-initialization**. This is when the staircase phenomenon typically occurs.

Existing widely used initialization methods, like Xavier or Glorot initialization

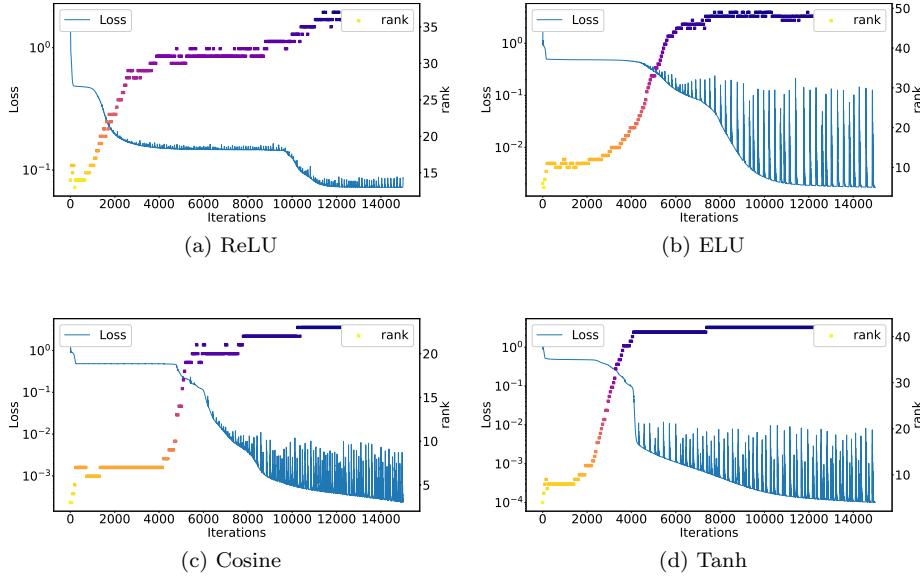


Fig. 4: (Example 2.6) Staircase phenomenon under different activation functions

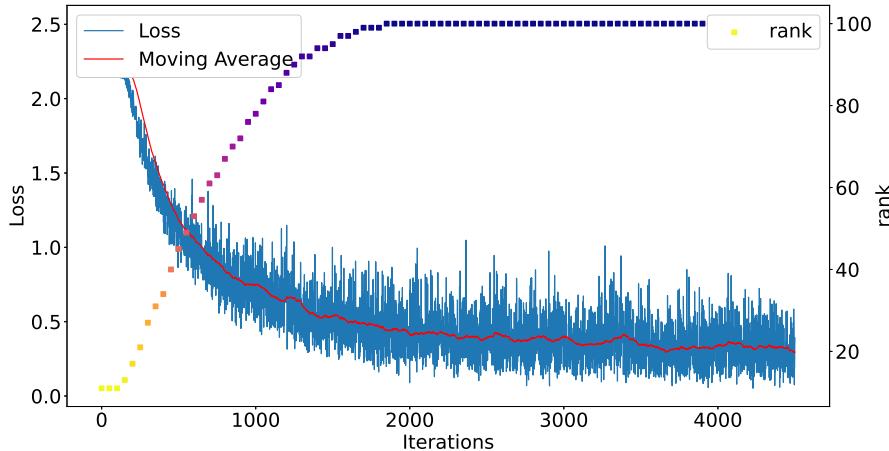


Fig. 5: (Example 2.7) Ladders phenomenon in handwriting recognition.

method [9], initialize the weights and biases as $w_j, b_j \sim U(-\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}})$. Consider a simple neuron function $\phi(x) = \sigma(wx + b)$, $x \in [-1, 1]$, with the hyperbolic tangent activation function $\sigma(x) = \tanh(x)$. Since $\sigma'(0) = 1$, the activation function behaves

238 approximately as a linear function near zero:

$$239 \quad \phi(x) = wx + b - \frac{(wx + b)^3}{3} + o((w + b)^3) \sim wx + b.$$

240 As the linear combination of linear functions is also linear, the ϵ -rank of $\{\phi_i\}_{i=1}^n$ after
241 initialization is approximately two.

242 This explains why, during the training process of function fitting, neural networks
243 often experience a plateau in the loss function that takes time to overcome. Initially,
244 this plateau arises because the initialized basis functions are not fully linearly indepen-
245 dent. This phase can be interpreted as feature extraction. From our perspective, at
246 specific stages during training, this process requires the separation of neuron functions
247 and an increase in their ϵ -rank.

248 **3. Theoretical Explanation of the Staircase Phenomenon.** In this section,
249 we demonstrate the theoretical significance of ϵ -rank and provide an explanation of
250 the staircase phenomenon. For well-posed problems, when the solution lies outside the
251 class of neural network functions, we demonstrate that an increase in ϵ -rank during
252 the training process is a necessary condition for a reduction in the loss function.

253 It is trivial that if f is a linear combination of f_1, f_2, \dots, f_n with $r(M) = p$, then
254 f can be rewritten as a linear combination of p of them. Similarly, if $r_\epsilon(M) = p$, a
255 comparable result holds. We begins with the following useful lemma constructed in
256 [14].

LEMMA 3.1. [14] Let $Q \in \mathcal{O}_{n,p}$ with $p \leq n$, and $\{Q_1, Q_2, \dots, Q_k\}$ is the set of
all p -by- p sub-matrices of Q where $k = \binom{n}{p}$. Define a vector in \mathbb{R}^k by $\sigma(Q) =$
 $(\sigma_{\min}(Q_1), \sigma_{\min}(Q_2), \dots, \sigma_{\min}(Q_k))^T$. Then

$$\inf_{Q \in \mathcal{O}_{n,p}} (\|\sigma(Q)\|_\infty) \geq \frac{1}{\sqrt{p(n-p) + \min(p, n-p)}}.$$

257 THEOREM 3.2. If $f = \sum_{j=1}^n \beta_j f_j$ with $\|\beta\|^2 \leq C$, $r_\epsilon(M_f) = p$ for some $\epsilon \geq 0$
258 and positive integer $p \leq n$, then after a reorder of set $\{f_1, \dots, f_n\} = \{\tilde{f}_1, \dots, \tilde{f}_n\}$ if
259 necessary, f can be approximated by $\tilde{f} = \sum_{j=1}^p \tilde{\beta}_j \tilde{f}_j$ with $\|f - \tilde{f}\|^2 \leq C(p+1)(n-p)^2\epsilon$.

260 *Proof.* Consider the spectral decomposition $M = Q\Lambda Q^T$, Q is orthogonal, $\Lambda =$
261 $\text{diag}([\lambda_1, \lambda_2, \dots, \lambda_n])$ is diagonal with eigenvalues $\lambda_1 \geq \dots \geq \lambda_p > \epsilon \geq \lambda_{p+1} \geq \dots \geq$
262 $\lambda_n \geq 0$. For simplicity, we denote $\beta = [\beta_1 \ \dots \ \beta_n]^T$ and $F = [f_1 \ \dots \ f_n]^T$, thus
263 $f = \beta^T F$. Let P be a permutation matrix, and denote

$$264 \quad PQ = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix} \begin{matrix} p \\ n-p \end{matrix}$$

$$265 \quad \begin{matrix} p & n-p \end{matrix}$$

$$266$$

267 as a partitioning of the matrix PQ . Now we construct an approximation of f by
268 $\tilde{f} = \tilde{\beta}^T \tilde{F}$, where

$$269 \quad \begin{aligned} \tilde{\beta} &= [I_p \ 0] P\beta - V_{12}V_{22}^{-1} [0 \ I_{n-p}] P\beta, \\ \tilde{F} &= [I_p \ 0] PF. \end{aligned}$$

To estimate L_2 error of $\|f - \tilde{f}\|^2$, we note that

$$\begin{aligned}
& \|f - \tilde{f}\|^2 \\
&= \|(P\beta)^T(PF) - ([I_p \ 0] P\beta - V_{12}V_{22}^{-1} [0 \ I_{n-p}] P\beta)^T [I_p \ 0] PF\|^2 \\
&= \|([0 \ I_{n-p}] P\beta)^T ([0 \ I_{n-p}] PF) + ([0 \ I_{n-p}] P\beta)^T V_{22}^{-T} V_{12}^T [I_p \ 0] PF\|^2 \\
&= \|([0 \ I_{n-p}] P\beta)^T V_{22}^{-T} (V_{22}^T [0 \ I_{n-p}] PF + V_{12}^T [I_p \ 0] PF)\|^2 \\
&= \|([0 \ I_{n-p}] P\beta)^T V_{22}^{-T} (PQ [0 \ I_{n-p}]^T)^T PF\|^2 \\
&= \|([0 \ I_{n-p}] P\beta)^T V_{22}^{-T} [0 \ I_{n-p}] Q^T F\|^2 \\
&\leq \|\beta\|^2 \|V_{22}^{-T}\|^2 (\lambda_{p+1} + \dots + \lambda_n) \\
&\leq C \|V_{22}^{-T}\|^2 (n-p)\epsilon.
\end{aligned}$$

270 It remains to control the term $\|V_{22}^{-T}\|^2$. By Lemma 3.1, for any orthogonal matrix Q ,
271 there exists a permutation P , such that $\|V_{22}^{-T}\|^2 \leq (p+1)(n-p)$. \square

272 It is worth noting that the bound established in the theorem is quite loose. The
273 final inequality in the proof straightforwardly bounds $\lambda_{p+1} + \dots + \lambda_n$ by $(n-p)\epsilon$
274 despite the potential for **rapid decay** of the eigenvalues in practice. Moreover, the
275 bound in Lemma 3.1 is not sharp, except for $p = 1$ and $p = n-1$. We conjecture that
276 $\frac{1}{\sqrt{n}}$ provides the sharp bound for all p , supported by extensive numerical experiments
277 that have yet to produced a counterexample.

278 We then apply the theorem to the neural networks. The L -layer neural network
279 is represented as follows:

$$\begin{aligned}
\mathcal{F}_n &= \left\{ \sum_{i=1}^n \beta_j \phi_j(x; \theta) \mid \phi_j(x; \theta) \in \mathcal{H}_L, \beta_j \in \mathbb{R}, j = 1, \dots, n \right\}, \\
280 \quad (3.1) \quad \mathcal{H}_k &= \left\{ \sigma(w_k \cdot y(x) + b_k) \mid y(x) \in \mathbb{R}^{n_{k-1}}, y_j(x) \in \mathcal{H}_{k-1}, \right. \\
&\quad \left. w_k \in \mathbb{R}^{n_{k-1}}, b_k \in \mathbb{R} \right\}, \quad k = 1, \dots, L, \quad \text{[yellow speech bubble icon]} \\
&\mathcal{H}_0 = \{x \in \Omega \subset \mathbb{R}^d\}.
\end{aligned}$$

281 where $\{\beta_j\}_{j=1}^n$ and $\theta = \{(W_k, B_k)\}_{k=1}^L$ are trainable coefficients, and σ is the activation
282 function satisfying the universal approximation theorem of neural networks [15].
283 The two-layer (shallow) neural network is a special case when $L = 1$.

284 Consider the following loss function:

$$285 \quad (3.2) \quad \min_{u \in \mathcal{F}_n} \mathcal{L}(u) = \|\mathcal{G}(u) - f\|^2, \quad \text{[yellow speech bubble icon]}$$

286 where $f \in L^2(\Omega)$ represents the target function or data. In this work, we always
287 assume that the exact solution u^* does not belong to the function class \mathcal{F}_n . Obviously,
288 with standard definition of the linearly independence, the Gram matrix of a optimizer
289 $u_n^* \in \mathcal{F}_n$ should be full rank. Otherwise, some redundant neurons in the last layer can
290 be deleted. More concisely, $r(M_{u_n^*}) = n$. Hence, for a wider network we can always
291 find a better approximation, i.e.,

$$292 \quad \text{dist}(u^*, \mathcal{F}_n) < \text{dist}(u^*, \mathcal{F}_m), \quad m < n,$$

293 where $\text{dist}(u, A) = \min_{v \in A} \|u - v\|$. However, the situation will become quite different
 294 if we consider the concept of the ϵ -rank. We get a more precise relationship between
 295 **the loss function and the ϵ -rank**.

296 **THEOREM 3.3.** *Given the problem $\mathcal{G}(u) = f$ and \mathcal{G}^{-1} being the solution operator,
 297 assume that the problem satisfies the following **stability condition**, for any u, v ,*

298 (3.3)
$$\|\mathcal{G}^{-1}(u) - \mathcal{G}^{-1}(v)\| \leq C_S \|u - v\|.$$

299 Let u_n be an arbitrary approximation in \mathcal{F}_n with the ϵ -rank equalling to p , i.e.,

$$u_n(x; \theta) = \sum_{j=1}^n \beta_j \phi_j(x; \theta),$$

300 where $\|\beta\|^2 \leq C$ and $r_\epsilon(M_{u_n}) = p$. Then

301 (3.4)
$$\sqrt{\mathcal{L}(u_n)} \geq \frac{1}{C_s} \left(\text{dist}(u^*, \mathcal{F}_p) - \sqrt{C(p+1)(n-p)^2 \epsilon} \right),$$
 

302 where $u^* = \mathcal{G}^{-1}(f)$ is the exact solution, $\mathcal{L}(u) = \|\mathcal{G}(u) - f\|^2$ is the loss function.

303 *Proof.* By Theorem 3.2, there exists a $u_p \in \mathcal{F}_p$ satisfying $\|u_p - u_n\|^2 \leq C(p + 1)(n - p)^2 \epsilon$. A triangular inequality

$$\begin{aligned} \text{dist}(u^*, \mathcal{F}_p) &\leq \|u^* - u_p\| \\ &\leq \|u_p - u_n\| + \|u_n - u^*\| \\ &\leq \sqrt{C(p+1)(n-p)^2 \epsilon} + \|u_n - u^*\| \\ &= \sqrt{C(p+1)(n-p)^2 \epsilon} + \|\mathcal{G}^{-1}(\mathcal{G}(u_n)) - \mathcal{G}^{-1}(f)\| \\ &\leq \sqrt{C(p+1)(n-p)^2 \epsilon} + C_S \|\mathcal{G}(u_n) - f\| \end{aligned}$$

306 gives the desired inequality. \square

307 *Remark 3.4.* The stability assumption (3.3) is reasonable for well-posed problems.
 308 For instance, in the function fitting problems, $\mathcal{G} = \mathcal{I}$, $C_S = 1$, and the loss function
 309 is $\mathcal{L}(u) = \|u - f\|^2$. In the case using PINN to solve Poisson equation $-\Delta u = f$,
 310 $C_S = \|(-\Delta)^{-1}\|$ is uniformly bounded.

311 *Remark 3.5.* When the ϵ -rank of the neural network approximator $u_n \in \mathcal{F}_n$ is
 312 $r_\epsilon(M_{u_n}) = p$, the result of the theorem can be expressed as

313
$$\sqrt{\mathcal{L}(u_n)} \geq \frac{\text{dist}(u^*, \mathcal{F}_p)}{C_S} - O(\sqrt{\epsilon}).$$

314 Recall that ϵ is a fixed hyperparameter, and it is chosen sufficiently small, which yields
 315 the loss function has a lower bound in terms of $\text{dist}(u^*, \mathcal{F}_p)$. During the training
 316 process, to minimize the loss function $\mathcal{L}(u)$, there must be a decrease in $\text{dist}(u^*, \mathcal{F}_p)$,
 317 implying an increase in the ϵ -rank of the neuron functions.

318 *Remark 3.6.* If ϵ is sufficiently small and the loss function is minimized to an
 319 optimal level while p remains small relative to n , then Theorem 3.3 offers an alternative
 320 explanation: p neurons can approximate the solution well, and more features are
 321 unnecessary. This is one of the reasons why **neurons pruning** [37, 25] is feasible in
 322 computation. 

323 **4. ϵ -rank in Existing Methods.** This section presents how the ϵ -rank evolves
 324 in various existing methodologies. A considerable number of methods facilitate the lin-
 325 ear independence of neuron functions during the initial stages of the training process.
 326 These approaches have been demonstrated to accelerate of the training process and
 327 enhance the accuracy of the resulting models. Based on this, it is beneficial to ensure
 328 that the neuron functions exhibit a relatively high ϵ -rank at the outset.

329 The neural network structure is defined as (1.1). Unless otherwise mentioned, the
 330 activation function is hyperbolic tangent function $\sigma(x) = \tanh(x)$. L^2 norm is used to
 331 measure errors between predicted solution u and exact solution or reference solution
 332 u^* .

$$333 \quad e = \|u - u^*\|, \quad \tilde{e} = \frac{\|u - u^*\|}{\|u^*\|},$$

334 where $\|u\| = \left(\int_{\Omega} u^2 dx \right)^{\frac{1}{2}}$ is the short note of L^2 norm.

335 In numerical calculations, we extend the ϵ -linear independence to the discrete
 336 form. Given n functions discretized on m nodes

$$337 \quad D = \begin{pmatrix} \phi_1(x_1) & \cdots & \phi_n(x_1) \\ \phi_1(x_2) & \cdots & \phi_n(x_2) \\ \vdots & \ddots & \vdots \\ \phi_1(x_m) & \cdots & \phi_n(x_m) \end{pmatrix},$$

338 the mass matrix is computed by $M = D^T W D$, where W is the weight matrix. The
 339 ϵ -linear independence of these n functions is

$$340 \quad r_{\epsilon}(M) = |A|, \quad A = \{|\lambda(M)| > \epsilon\},$$

341 where $|A|$ is the cardinal number of A , and the tolerance is given $\epsilon = 10^{-6}$.

342 The rank of mass matrix, $r_{\epsilon}(M)$ is employed to measure the linear independence
 343 of the basis functions.

344 In low-dimensional cases, M is approximated using numerical integration, while
 345 in high dimensions, M is approximated by Monte Carlo integration. For simplicity,
 346 we generate one set of integration data points $\{x\}_{k=1}^m$, which can be Gaussian integral
 347 points or uniform mesh for $d = 1, 2$. Then

$$348 \quad (4.1) \quad (M)_{ij} \approx \sum_{k=1}^m w_k \phi_i(x_k) \phi_j(x_k), \quad \text{numerical integration}$$

349 where w_k are the integral weights. For example, $w_0 = w_m = \frac{1}{2}$ and $w_i = 1, i =$
 350 $2, \dots, m-1$ is the trapezoidal formulation.

351 The notations are listed in Table 1.

352 **4.1. Deterministic Initialization.** This subsection evaluates the feasibility of
 353 directly constructing highly linearly independent neuron functions through initializa-
 354 tion.

355 Example 4.1 (function fitting with initialization, Figure 6). In this example, we
 356 consider a function fitting problem where the target function is also defined as (2.5)

$$357 \quad u(x) = \cos(x) + \cos(2x) + \cos(30x), \quad x \in [-1, 1].$$

Table 1: The List of Notations

Notation	Stands for ...
L	Depth of hidden layers
n	Width of hidden layers
N	Number of total parameters
m	Sample size
d	Dimension of the input
ϕ	The neurons of the output layer
β	Coefficients of the output layer
$M(\phi)$	The mass matrix of basis functions $\{\phi_j\}_{j=1}^n$
$r_\epsilon(M)$	The ϵ -rank of the mass matrix
ϵ	Tolerance of eigenvalues

358 We compare two initialization methods: deterministic and random initialization. For
 359 the deterministic initialization, the first layer of the neural network is initialized as:

360 (4.2)
$$y_1 = \sigma(w_0 x + b_0),$$

361 where the weights and biases are given by $(w_0)_j = \frac{n}{2}$, $(b_0)_j = \frac{n}{2} - j$, $j = 1, \dots, n$.

362 As discussed in section 2, a set of linearly independent neuron functions is im-
 363 portant for neural network performance. A straightforward method to improve the
 364 ϵ -rank of neurons is to expand the range of the uniform distribution. For example,
 365 set $\theta \sim U(-m, m)$. While this approach can enhance the linear independence of the
 366 neuron basis functions, it is not commonly used in practice due to the potential issues
 367 it introduces. As mentioned in [9], such an initialization strategy can lead to problems
 368 like exploding gradients and the saturation of activation functions, which negatively
 369 affect the training process.

370 Inspired by traditional numerical methods, we propose an alternative initialization
 371 method for the first layer of the neural network when $d = 1$, which guarantees a
 372 sufficiently high ϵ -rank of neuron functions. Specifically, the initialization for the first
 373 hidden layer is given as (4.2), which can be rewritten in the form of

374 (4.3)
$$(y_1)_j = \tanh\left(\frac{n}{2}(x - x_j)\right), \quad j = 1, \dots, n, \quad \text{初始值如此所示 , 实现了高epsilon-rank}$$



375 where $\{x_j\}$ are the uniform grids on $[-1, 1]$.

376 The result is shown in Figure 6. This figure clearly illustrates that once the neu-
 377 ron functions exhibit sufficient linear independence, the loss function will be rapidly
 378 optimized. Comparing the blue curve (loss = 10^{-5}) in Figure 6(a) and the orange
 379 curve (loss = 10^{-4}) in Figure 6(b), even a shallow and narrow network performs better
 380 than a deeper and wider network. This indicates that a good initialization method
 381 can greatly reduce training time and improve training accuracy.

382 We now demonstrate that the staircase phenomenon also arises when solving
 383 partial differential equations and that appropriate initialization techniques can signif-
 384 icantly enhance performance. Since the work of [29], physics-informed neural networks
 385 (PINN) have achieved remarkable success in the field of computational science. Nu-
 386 merous studies have highlighted the advantages of neural network based algorithms

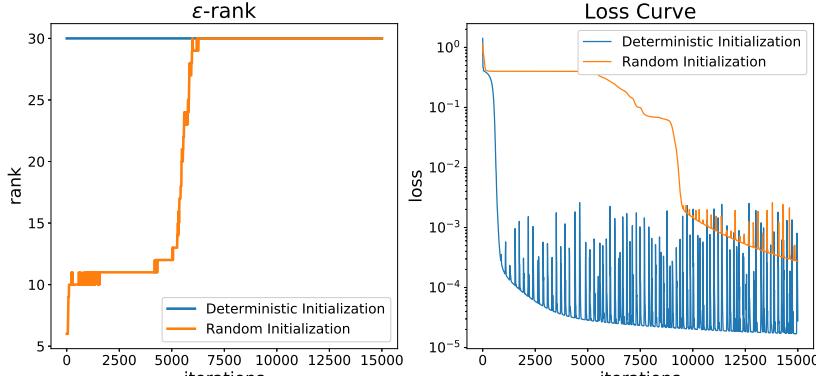
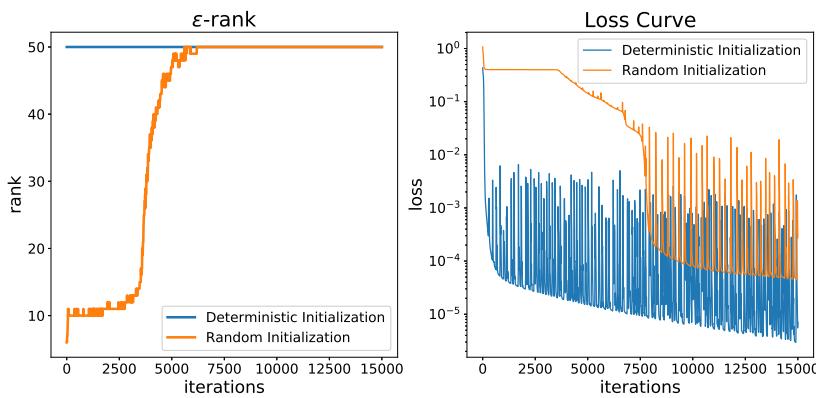
(a) $L = 2, n = 30$ (b) $L = 4, n = 50$

Fig. 6: (Example 4.1) The training process of neural networks with default settings and deterministic initialization. The left figure shows the linear independence and the right figure plots the losses. The blue curve gives the result of deterministic initialization method and the orange curve is under default settings.

387 for partial differential equations in high dimensional problems [31, 8, 7], irregular
388 domains [38, 33] and systems with complex mechanisms [22, 20].

389 Consider the following boundary value problem:

390 *Example 4.2* (Solving Poisson's equation by PINN, Figure 7).

$$391 \quad \begin{cases} -\Delta u = f, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \end{cases}$$

392 where $\Omega = \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]^2$, $f(x, y) = 8 \sin 2x \sin 2y$. The analytic solution of this differen-
393 tial equation is $u(x, y) = \sin 2x \sin 2y$. The loss function is defined as

394 (4.4)
$$\mathcal{L}(u) = \|\Delta u + f\|_{L^2(\Omega)}^2 + \|u\|_{L^2(\partial\Omega)}^2.$$

395 The previously used initialization method becomes ineffective in this context, as
 396 the problem is two-dimensional. In [41], the authors proposed a method for generating
 397 uniformly distributed neurons in shallow networks to ensure equal expressive power
 398 across all regions of the domain. Inspired by this approach, we can separate the neuron
 399 functions in the first hidden layer by employing a uniformly distributed initialization
 400 method. This method re-parameterizes the weight and bias of each neuron in the first
 401 hidden layer as:

$$402 \quad (4.5) \quad \sigma(w_j^T x + (b_0)_j) = \sigma(\gamma_j(a_j^T x + r_j)),$$

403 where w_j^T is the j -th rows of W_0 , $\|a_j\|^2 = 1$, and $\gamma_j \geq 0$. $\{a_j\}_{j=1}^n$ are initialized
 404 by uniformly sampled on the unit sphere, and $\{r_j\}_{j=1}^n$ are initialized by uniformly
 405 sampled on a bounded positive real line related to Ω . This initialization method
 406 generate neurons with uniform hyperplane density in the region, termed as uniform
 407 density initialization (UDI).

408 The result is presented in Figure 7, which clearly demonstrate that solving PDEs
 409 with neural networks also exhibits the staircase phenomenon. Furthermore, the figure
 410 highlights that an effective initialization technique, which ensures a high ϵ -rank, can
 significantly accelerate the training process.

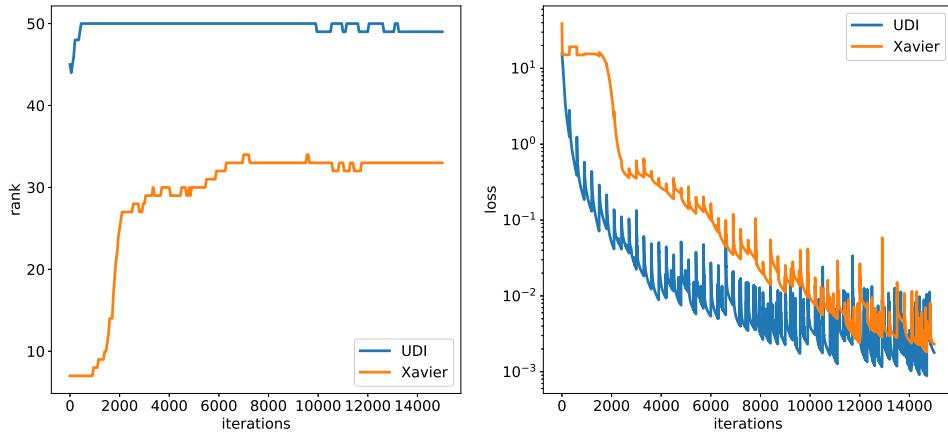


Fig. 7: (Example 4.2) The training process of solving 2-D Poisson's equation with default Xavier initialization and uniformly density initialization (UDI). The left figure shows the ϵ -rank and the right figure shows losses. The blue curve gives the result of uniformly density initialization and the red curve is under Xavier initialization.

411

412 **4.2. Partial of Unity.** Next, we evaluate the ϵ -rank in two methods that do
 413 not involve training process. Both extreme learning machine (ELM) [17] and random
 414 features [28] are widely used techniques in deep learning. Notably, neither method
 415 involves training the hidden layers, offering computationally efficient solutions. In
 416 these approaches, the linear independence of the neuron functions depends solely on
 417 the initialization and network structure employed.

418 An important improvement is the partition of unity method (PoU) technique,
 419 employed in the random feature method (RFM) [2] and local extreme learning machine
 420 [6]. In RFM, the approximate solution is expressed as a linear combination of random

421 features combined with the PoU, as follows:

$$422 \quad u_R(x) = \sum_{i=1}^m \psi_i(x) \sum_{j=1}^{J_R} u_{ij} \phi_{ij}(x),$$

423 where u_{ij} are unknown coefficients. In RFM, N points $\{x_i\}_{i=1}^N$ are chosen from Ω ,
 424 typically uniformly distributed. Then Ω is decomposed to N disjoint subdomains
 425 $\{\Omega_i\}_{i=1}^N$ with $x_i \in \Omega_i$. For each Ω_i , a PoU function ψ_i is constructed with support
 426 Ω_i , i.e., $\text{supp}(\psi_i) = \Omega_i$. The commonly used PoU function is

$$427 \quad \psi_i(x) = \mathbb{I}_{\Omega_i}(x).$$

428 Since $|\Omega_i \cap \Omega_j| = 0$, it is clear that $\{\psi_i \sum_{j=1}^{J_R} u_{ij} \phi_{ij}\}_{i=1}^N$ are ϵ -linearly independent when
 429 $\|\psi_i \sum_{j=1}^{J_R} u_{ij} \phi_{ij}\|^2 > \epsilon$. The extreme learning machine is modeled as

$$430 \quad u_E(x) = \sum_{j=1}^{J_E} u_j \phi_j(x),$$

431 which can be seen as a random feature method with no subdomains ($N = 1$).

432 *Example 4.3* (Two dimensional function fitting, Figure 8).

$$433 \quad u^*(x, y) = \cos x \cos y + \cos 10x \cos 10y, \quad \Omega = [-1, 1]^2.$$

434 In this example, we compare the performance of modeling with and without the
 435 partition of unity (PoU) technique, regarded as the RFM and ELM respectively. The
 436 number of neurons is set to $n = 900$. In the RFM, these 900 neurons are divided into
 437 3×3 sub-intervals, i.e., $i = 9, J_R = 100$ and in the ELM, $J_E = 900$. The coefficients
 438 of the output layer in both methods are determined using the least squares method.

439 The results, presented in Figure 8, demonstrate that, for the same number of
 440 neurons, the RFM achieves greater linear independence due to the compact support
 441 in each subdomain, resulting in higher accuracy. This example clearly illustrates
 442 that, under identical configurations, achieving a high linear independence through
 443 specific techniques can significantly enhance network performance. Furthermore, an
 444 approximate inverse proportional relationship between the ϵ -rank and the error is
 445 observed.

446 **4.3. ResNet.** The network structure has a significant impact on the linear in-
 447 dependence of neuron functions. The Residual Network (ResNet), is a deep neural
 448 network architecture introduced by [12]. ResNet has been widely adopted in the field
 449 of deep learning, particularly for the training of very deep networks.

450 The typical structure of the ResNet is the residual block, which is given as

$$451 \quad y = R(x) = x + \sigma(W_1 \sigma(W_2 x + b_2) + b_1).$$

452 The shortcut connection allows the input of the block to bypass the transformations
 453 and connect directly to its output. This shortcut provides a direct path for the
 454 gradient, facilitating more effective backpropagation and addressing the degradation
 455 problem, where deeper networks may perform worse than their shallower counterparts.

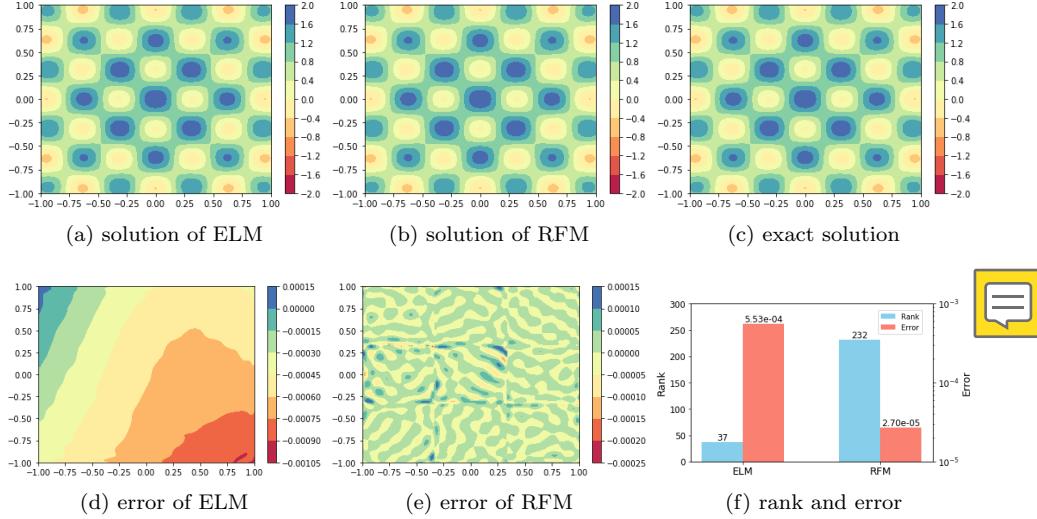


Fig. 8: (Example 4.3) (a)-(e) are the solutions and point-wise errors of random feature method and extreme learning machine method. The last subfigure (f) shows the rank and L^2 error of two methods.

When the neuron functions in deeper layers are connected to the neuron functions in shallower layers via a residual block, i.e.,

$$\phi^{L+1}(x) = R(\phi^L(x)),$$

this architecture demonstrates an additional advantage: it helps sustain the growth of the ϵ -rank.

Example 4.4 (Function fitting with ResNet, Figures 9 and 10). This example examines the ϵ -rank in each layer of the ResNet compared to MLP. To ensure a comparable number of parameters and to make each layer of neuron functions observable, we employ a one-layer residual block. The ResNet structure is defined as follows:

$$(4.6) \quad \begin{cases} y_0 = x, \\ y_{k+1} = y_k + \sigma(W_k y_k + b_k), & k = 0, \dots, L-1, \\ y = \beta \cdot y_L. \end{cases}$$

The problem is the same function fitting problem as Example 2.6.

In Figure 9, we observe that the ϵ -rank of ResNet is initially higher and grows faster to full rank compared to the MLP. Furthermore, as shown in Figure 10, the residual block structure ensures greater rank growth in the deeper neuron functions.

This example demonstrates that the linear independence of neuron functions varies across different network structures. Selecting a network architecture that promotes linear independence among neuron functions enables the capture of more features, thereby improving performance.

5. Concluding Remarks. In summary, this research provides a novel perspective on the training dynamics of deep neural networks by drawing connections to

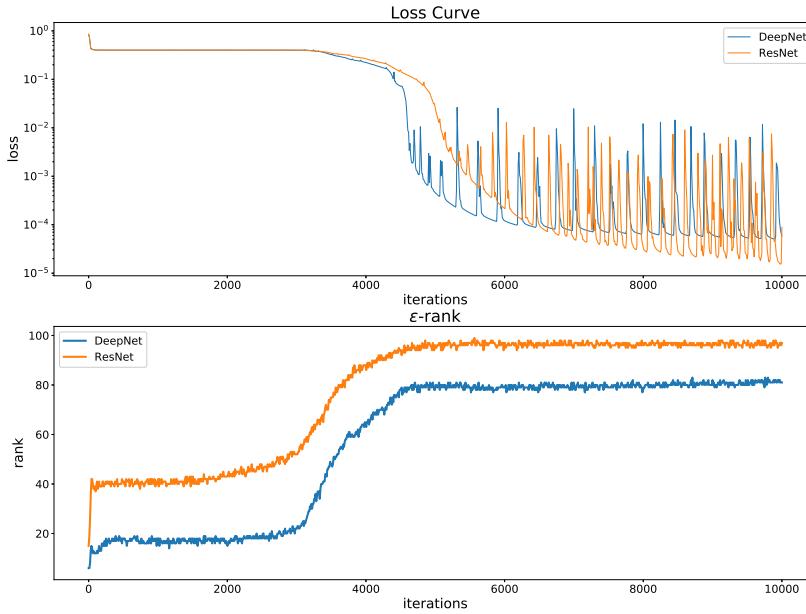


Fig. 9: (Example 4.4) The training result between ResNet and fully connected neural network.

476 traditional numerical analysis. A key finding of our study is the identification of the
 477 *staircase phenomenon*, which describes a stepwise increase in the linear independence
 478 of neuron functions during the training process, typically associated with rapid de-
 479 creases in the loss function. This finding highlights the importance of establishing
 480 a diverse and robust set of neuron functions in the early stages of training, which
 481 promotes both efficiency and convergence in model optimization.

482 Theoretical analyses and numerical experiments confirm that a set of linearly
 483 independent basis neuron functions is essential for effectively minimizing the loss
 484 function of neural networks. The training process can be significantly accelerated by
 485 leveraging appropriate techniques, such as deterministic initialization methods,
 486 constructing efficient network architectures, and employing proper domain partitioning.
 487 These strategies have shown effective in promoting the linear independence of neuron
 488 functions, providing insight into the success of certain neural network approaches.

489 This study offers a deeper understanding of the mechanisms underlying deep
 490 learning by bridging neural network framework with traditional numerical methods.
 491 It provides a solid foundation for future innovations in network initialization, training
 492 methodologies, and the design of more efficient models.

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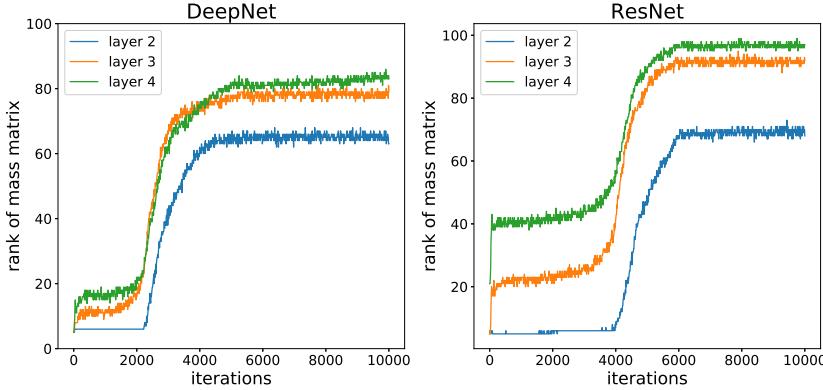


Fig. 10: (Example 4.4) The ϵ -rank for each layer of neuron functions in DeepNet and ResNet.

496

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