

Growing Networks by Folding on Typical Instances (Neural Networks Were Not Intended to Be Large in Scale from the Beginning)

Jimmy KANG

November 1, 2024

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- The black box nature of the training process weakens the **interpretability** of neural network models in understanding of the mechanisms behind their decision-making.
- The existing training strategy initializes **over-parameterized** models and allows representations to be learned in an anarchic manner from large amounts of data.
 - found to **underutilize the approximability** of the model
 - **decision criteria** are arranged in an unordered and susceptible manner

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Published as a conference paper at ICLR 2022

GRADMAX: GROWING NEURAL NETWORKS USING GRADIENT INFORMATION

Utku Evci, Bart van Merriënboer, Thomas Unterthiner,
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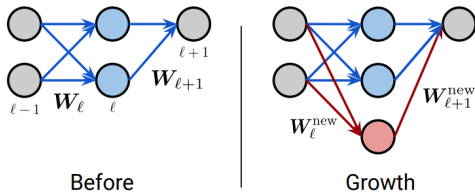
ABSTRACT

The architecture and the parameters of neural networks are often optimized independently, which requires costly retraining of the parameters whenever the architecture is modified. In this work we instead focus on growing the architecture without requiring costly retraining. We present a method that adds new neurons during training without impacting what is already learned, while improving the training dynamics. We achieve the latter by maximizing the gradients of the new weights and efficiently find the optimal initialization by means of the singular value decomposition (SVD). We call this technique Gradient Maximizing Growth (GradMax) and demonstrate its effectiveness in variety of vision tasks and architectures¹.

1 INTRODUCTION

The architecture of deep learning models influences a model's inductive biases and has been shown to have a crucial effect on both the training speed and generalization (d'Áscoli et al., 2019; Neyshabur, 2020). Searching for the best architecture for a given task is an active research area with diverse approaches, including neural architecture search (NAS) (Elsken et al., 2019), pruning (Liu et al., 2018), and evolutionary algorithms (Stanley & Miikkulainen, 2002). Most of these approaches are costly, as they require large search spaces or large architectures to start with. In this

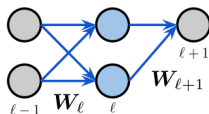
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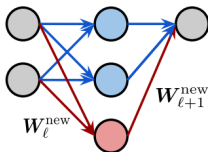
$$W_\ell^+ = \begin{bmatrix} W_\ell \\ W_\ell^{\text{new}} \end{bmatrix}$$

$$W_{\ell+1}^+ = \begin{bmatrix} W_{\ell+1} & W_{\ell+1}^{\text{new}} \end{bmatrix}.$$

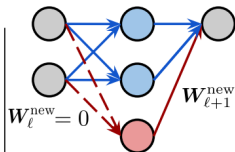
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Before

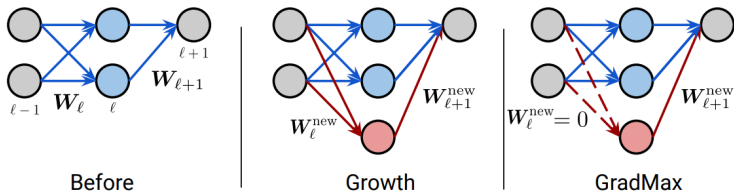


Growth



GradMax

Baseline: GradMax (Evci, et al., 2022)



$$\arg \max_{\mathbf{W}_{\ell+1}^{\text{new}}} \left\| \mathbf{W}_{\ell+1}^{\text{new}, \top} \mathbb{E}_D \left[\frac{\partial L}{\partial \mathbf{z}_{\ell+1}} \mathbf{h}_{\ell-1}^\top \right] \right\|_F^2, \quad \text{s.t.} \quad \|\mathbf{W}_{\ell+1}^{\text{new}}\|_F \leq c.$$

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Growing neural networks: When, where and how? Algorithms for growing neural networks start training with a smaller *seed architecture*. Then over the course of the training new neurons are added to the seed architecture, either increasing the width of the existing layers or creating new layers. Algorithms for growing neural networks should address the following questions:

1. **When** to add new neurons? For instance, some methods (Liu et al., 2019; Kilcher et al., 2019) require the training loss to plateau before growing, whereas others grow using a predefined schedule.
2. **Where** to add new capacity? We can add new neurons to the existing layers or create new layers among the existing ones.
3. **How** to initialize the new capacity?

In this work we mainly focus on the question of **how** and introduce a new initialization method for the new neurons. Our approach can also be used to guide when and where to grow new neurons. However, in order to make our comparison with other initialization methods fair we keep the growing schedule (**where** and **when**) fixed.

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Preliminaries - The Manifold Hypothesis

- DNNs can be seen as to approximate data distributions or decision boundaries by learning **manifolds** in high dimensional feature spaces (Bengio, Mesnil, et al., 2013; Bengio, Courville, and Vincent, 2013);

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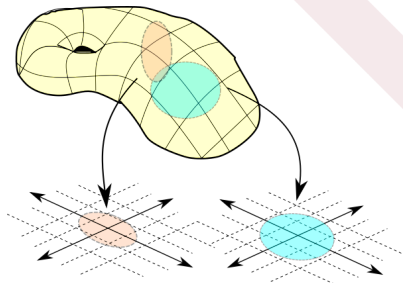
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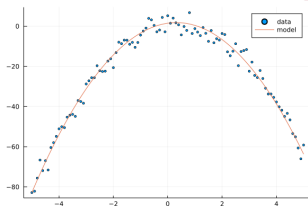
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Rates of approximation by RallII shallow neurons

Rates of approximation by rectified shallow neural networks

Tong Mao¹, Ding-Xian Zhou^{2,3}

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Several networks activated by the rectified linear unit (ReLU) have been shown to be the optimal structure of deep learning. The importance of approximating functions from hidden spaces in these networks is crucial for understanding the efficiency of the deep learning algorithm through the universal approximation property. In this paper, we first prove that the ReLU network is the best in the setting of deep neural networks with many layers of hidden neurons, it is still open for shallow networks. We then only use one hidden layer of neurons to show how to approximate functions from hidden spaces in these networks with uniform approximation by these networks. We then show that ReLU shallow neural networks with hidden neurons can uniformly approximate functions from the hidden spaces of the universal space (called ReLU universal space) when $n \geq 2$. The ReLU space is narrower to the optimal one (Gao's) when $n \geq 2$. The space ReLU is wider to the optimal one (Gao's) when $n = 1$.

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Proposition 1

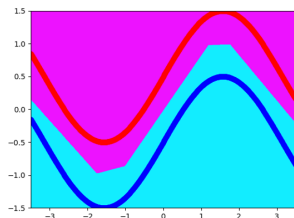
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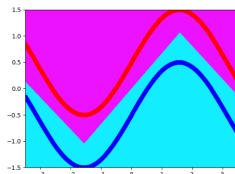
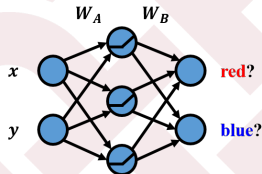
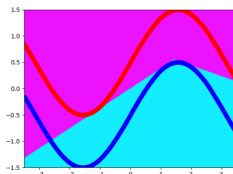
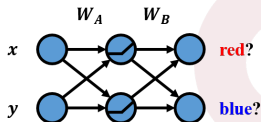
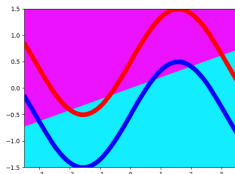
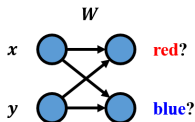


Preliminaries - Growing DNNs Increase Non-linearity

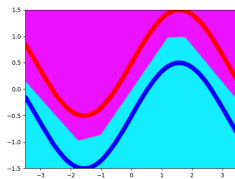
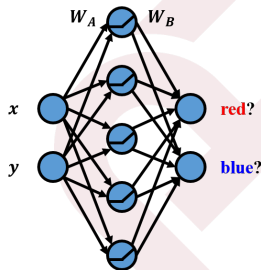
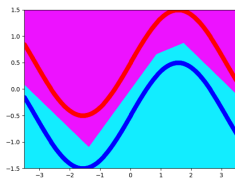
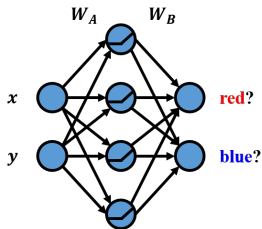
Observation 1

Growing a DNN by adding new node(s) to broaden a specific layer introduces new dimension(s) to the latent feature space associated with that layer, which is, in nature, increasing the non-linearity of the low-dimensional projections of the manifold to enhances the network's capacity to model complex patterns.

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- ④ Specifically, the model's capability (i.e., approximatability) can be increased by introducing non-linearity to its complexity,
- ⑤ which, can be achieved by breaking / folding the corresponding activated linear segment that leads to the typical mis-prediction.

Definitions

Definition (Activated Linear Segment)

For manifolds in high-dimensional spaces that are approximated by ReLU-based MLPs, their projections onto the input space are locally linear. In classification tasks, these projections are the decision boundaries, whereas in prediction tasks, they are the regression curves. Each piece of linear segments of these projections results from a composition of linear transformations governed by a specific activation pattern of ReLU units. These segments can thus be called "activated linear segments".

Definition (Fold Point)

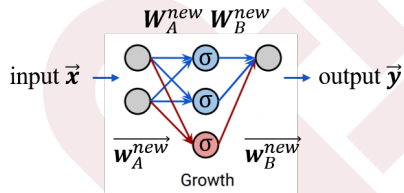
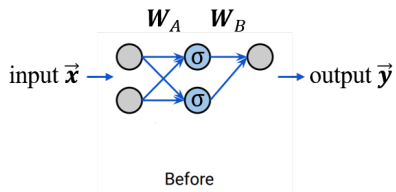
The transition points between two contiguous activated linear segments, where the activation pattern changes, are referred to as "fold points".

Definitions

Definition (Typical Mis-predicted Instance)

Among all input data that is wrongly predicted by an model, the single input data instance that can be represents a certain kind of mistakes that the model cannot distinguish is called a "typical mis-predicted instance".

Notations & Symbols



$$W_A^{new} = \begin{bmatrix} W_A \\ \overrightarrow{w_A^{new}} \end{bmatrix}$$

$$W_B^{new} = \begin{bmatrix} W_B & \overrightarrow{w_B^{new}} \end{bmatrix}$$

Determining Values for New Parameters

Lamma 1

$$\frac{d\mathcal{L}}{d\vec{x}} = (W_B \sigma(\cdot)' W_A)^T \frac{d\mathcal{L}}{d\vec{y}} + (w_B^{\vec{new}} \cdot \frac{d\mathcal{L}}{d\vec{y}}) w_A^{\vec{new}}$$

Theorem 3

$w_A^{\vec{new}}$ directly affect the direction of $\frac{d\mathcal{L}}{d\vec{x}}$ by specifying the direction of its component vector, while $w_B^{\vec{new}}$ indirectly affect $\frac{d\mathcal{L}}{d\vec{x}}$ by determining the norm of its component vector.

Determining Values for New Parameters

Lamma 2

$w_A^{\vec{n}^{ew}}$ directly determines which input domains can activate the newly added node

Theorem 4

$w_A^{\vec{n}^{ew}}$ determines the location of the fold point after adding a new node.

Proposed Method

Algorithm: Grow by Folding

initialize training dataset $\mathbb{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$, where $\mathbf{x}_i \sim \mathbb{D}$ ($i \in \{1, 2, \dots, n\}$, \mathbb{D} is the input space)

initialize shallow ReLU MLP model f with parameters $\mathbf{W}_A, \mathbf{b}_A, \mathbf{W}_B, \mathbf{b}_B$

do loop: train f on \mathbb{X} until converge

find the most typical mis-predicted instance and a fold point on the decision boundary:

$\mathbf{x}_t, \mathbf{x}_f = \text{fold_point_search}(\mathbb{X}, f)$, where $\mathbf{x}_f \sim \mathbb{D}$

calculate new parameters for the broaden model:

$\mathbf{W}_A^{new}, \mathbf{b}_A^{new}, \mathbf{W}_B^{new} = \text{hidden_layer_broaden}(\mathbf{x}_t, \mathbf{x}_f, f)$

create new model and apply new parameters as initial values:

$f_{\mathbf{W}_A, \mathbf{b}_A, \mathbf{W}_B, \mathbf{b}_B} \leftarrow f_{\mathbf{W}_A^{new}, \mathbf{b}_A^{new}, \mathbf{W}_B^{new}, \mathbf{b}_B}$

$f_{\mathbf{W}_A, \mathbf{b}_A, \mathbf{W}_B, \mathbf{b}_B} \leftarrow \text{equivalent_network_deepening}(f_{\mathbf{W}_A, \mathbf{b}_A, \mathbf{W}_B, \mathbf{b}_B})$

Proposed Method

Algorithm: Fold Point Search

input training dataset \mathbb{X}

input shallow ReLU MLP model f with parameters W_A, b_A, W_B, b_B

find the most typical mis-predicted instance:

$$\mathbf{x}_t = \text{find_typical_mis_predicted_instance}(\mathbb{X}, f)$$

find the activated linear segment of model f given \mathbf{x}_t as input:

$$W_{\text{activated}}, b_{\text{activated}} = \text{find_activate_linear_segment}(\mathbf{x}_t, W_A, b_A, W_B, b_B)$$

decision boundary regarding \mathbf{x}_t can be defined by:

$$\{\mathbf{d}_1, \mathbf{d}_2, \dots, \mathbf{d}_\infty\} \text{ s.t. } W_{\text{activated}}\mathbf{x}_i + b_{\text{activated}} = \mathbf{c}, \text{ where } \mathbf{c} \text{ is a uniform vector}$$

find the fold point \mathbf{x}_f on the decision boundary that is closest to \mathbf{x}_t :

$$\mathbf{x}_f = \min_{d \in \{\mathbf{d}_1, \mathbf{d}_2, \dots, \mathbf{d}_\infty\}} \|\mathbf{d} - \mathbf{x}_t\|^2$$

output $\mathbf{x}_t, \mathbf{x}_f$

Proposed Method

Algorithm: Find Typical Mis-Predicted Instance

input training dataset \mathbb{X}

input shallow ReLU MLP model f with parameters W_A, b_A, W_B, b_B

sample subset $\mathbb{S} = \{\mathbf{x}_a, \mathbf{x}_b, \dots, \mathbf{x}_m\}$ from \mathbb{X}

feed \mathbb{S} into the model f and calculate their corresponding **values of loss function** $\mathbb{L} = \{l_a, l_b, \dots, l_m\}$

performing **weighted k-means clustering** on \mathbb{S} using corresponding \mathbb{L} as weights and get clusters $\{\mathbb{C}_1, \mathbb{C}_2, \dots, \mathbb{C}_k\}$

calculate average loss for instances in each clusters $\{l_{\mathbb{C}_1}, l_{\mathbb{C}_2}, \dots, l_{\mathbb{C}_k}\}$

find the cluster \mathbb{C}_i that has the highest average loss $l_i = \max(\{l_{\mathbb{C}_1}, l_{\mathbb{C}_2}, \dots, l_{\mathbb{C}_k}\})$

find instance $\mathbf{x}_t = \min_{\mathbf{x}_i \in \mathbb{C}_i} \|\mathbf{x}_i - \mathbf{x}_c\|^2$, where \mathbf{x}_c is the centroid of \mathbb{C}_i

output \mathbf{x}_t

Proposed Method

Algorithm: Hidden Layer Broaden

input typical mis-predicted point x_t

input fold point on the decision boundary x_f

input shallow ReLU MLP model f_{W_A, b_A, W_B, b_B} with parameters W_A, b_A, W_B, b_B

ensure $\forall x: W_B^{new} W_A^{new} x = W_B W_A x$:

set $W_B^{new} = [W_B \quad \mathbf{0}]$

set $b_A^{new} = \begin{bmatrix} b_A \\ 0 \end{bmatrix}$

set $W_A^{new} = \begin{bmatrix} W_A \\ W_A^+ \end{bmatrix}$ s.t.:

ensure the grown new model fold only at point x_f :

$$W_A^{new} x_f + b_A^{new} = \mathbf{0}$$

apply GradMax to W_A^{new}

$$\max_{W_A^{new}} \|\mathbb{E}_{\mathbb{D}} \nabla W_A^{new}\|_F^2$$

align gradient direction with $W_A^{new}(x_t - x_f)$

$$\max_{W_A^{new}} \frac{\nabla W_A^{new} x_t \cdot W_A^{new}(x_t - x_f)}{\|\nabla W_A^{new} x_t\| \cdot \|W_A^{new}(x_t - x_f)\|}$$

output $W_A^{new}, b_A^{new}, W_B^{new}$

Supplementary Details

1 "Dead Layer" Problem



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 - Batch Normalization



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- ① "Dead Layer" Problem
 - Batch Normalization
- ② Optimization Problem of Fold Point Search Algorithm

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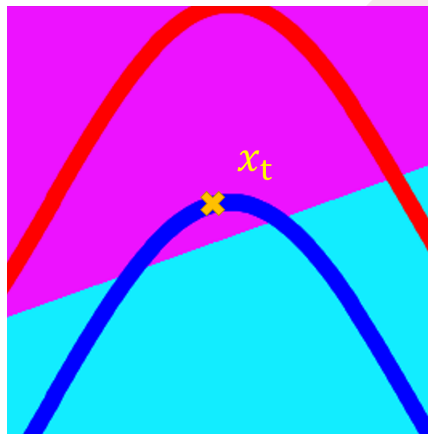
① "Dead Layer" Problem

- Batch Normalization

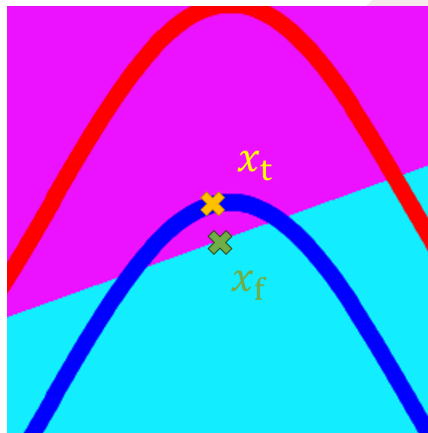
② Optimization Problem of Fold Point Search Algorithm

- given the equation of decision boundary: $w \cdot x + b = 0$, the closest point on the decision boundary can be found by $x_t - ((w \cdot x_t) + b) * (w / (w \cdot w))$

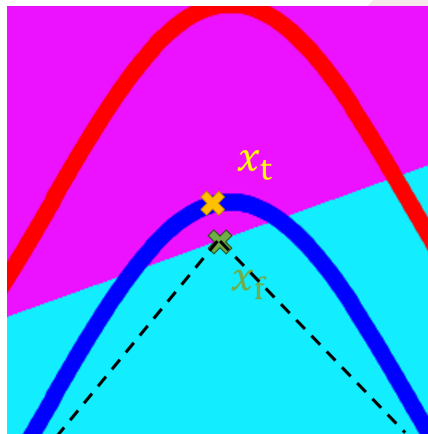
Example



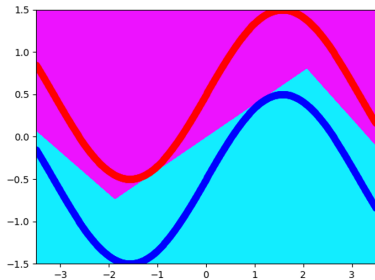
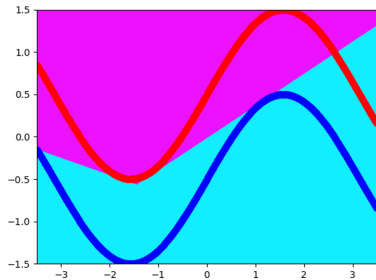
Example



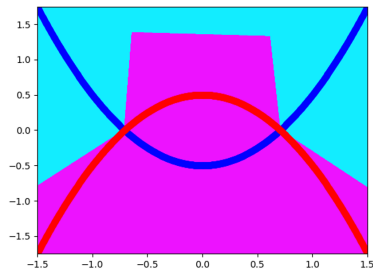
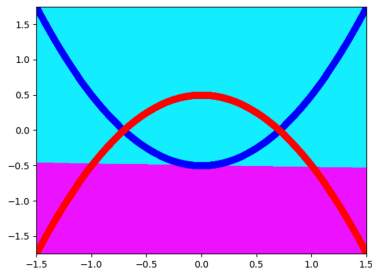
Example



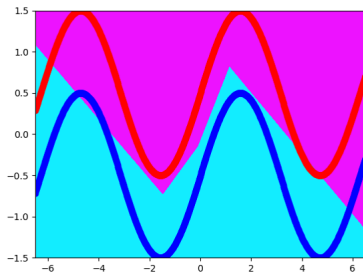
Binary Classification: Sine



Binary Classification: Overlap Quadratic



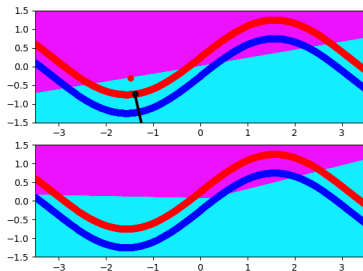
Utilization of Approximatability



- random initialized: **65** / 1000
- grow from 2-2-2 to 2-3-2: **360** / 1000

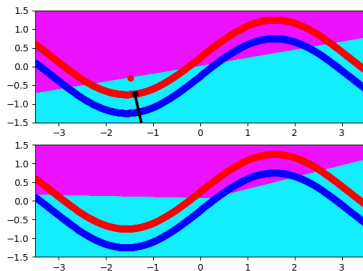
Next Milestones

- 1 due to the difference in updating speeds between the old and new parameters, the proposed direction along $\vec{x}_t - \vec{x}_f$ is not the most ideal gradient direction for updates



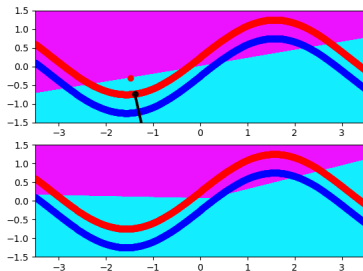
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- 2 Folding point does not lie on the effective activated linear segment



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- 1 due to the difference in updating speeds between the old and new parameters, the proposed direction along $\vec{x}_t - \vec{x}_f$ is not the most ideal gradient direction for updates
- 2 Folding point does not lie on the effective activated linear segment
- 3 Constrained Optimization Difficulty



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Thank you!

