Critical Points of Deep Linear Networks in $\mathbb{C}^N$

Thesis Defense Presentation

by

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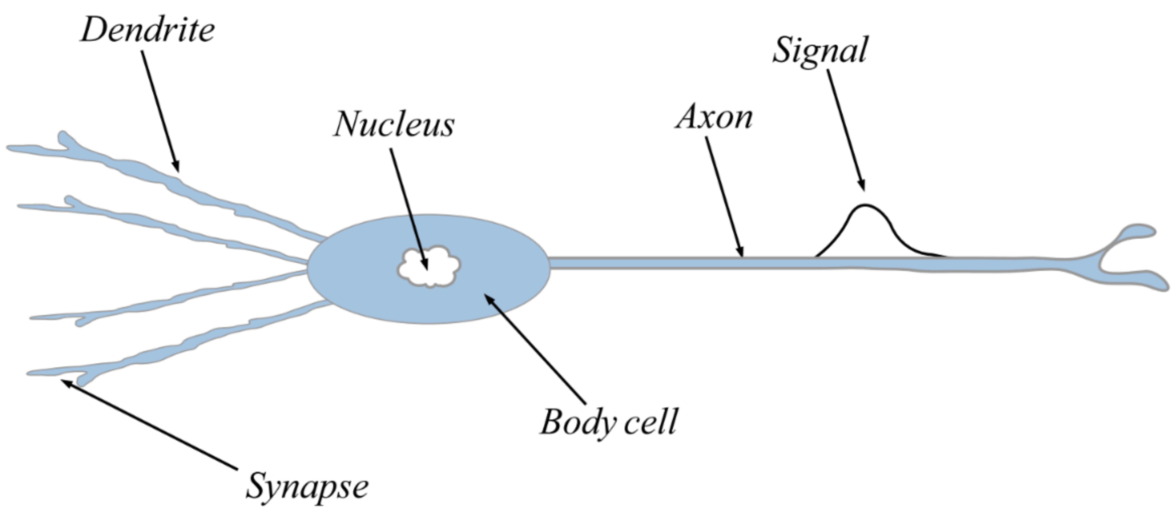
Critical Points of Deep Linear Networks in $\mathbb{C}^N$

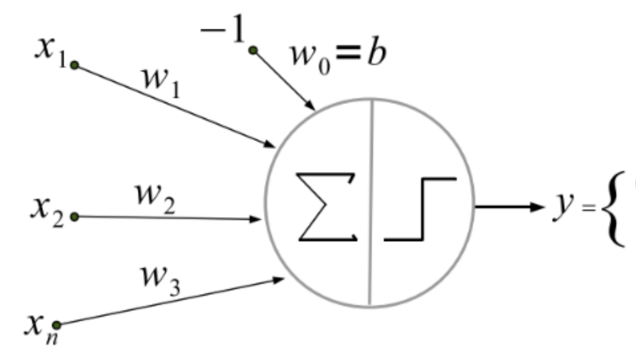
Outline

- Neural networks (particularly, *linear networks*)
- Neural network training as a minimization problem in real analysis
- Neural network training as solving polynomial systems in algebraic geometry
- Results:
    - New upper bounds $\mathscr{B}_{\mathbb{C}}, \mathscr{B}_{\mathbb{C}^*}$ on the number of complex critical points of 1-hidden layer networks
    - Structure in the location of complex critical points

Neural Networks

Neuron



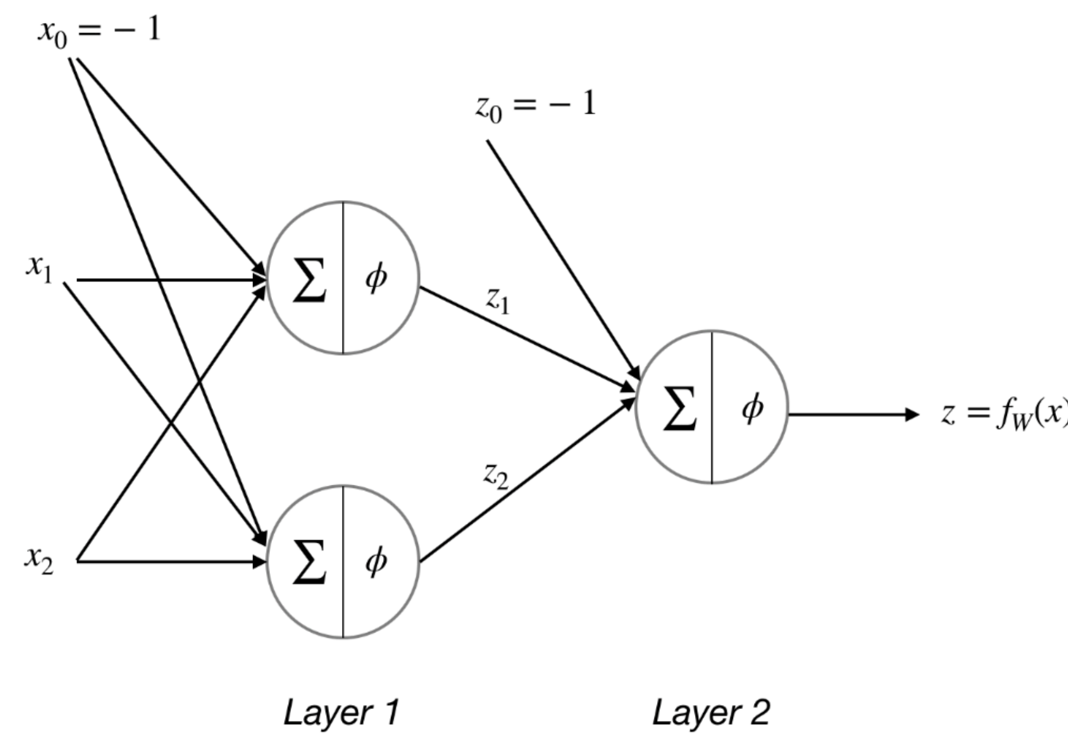


- $f_w(x_1, ..., x_n) = \phi\left(\sum_{j=1}^{n} w_j x_j - b\right)$ **(output function)**

Image source: Ovidiu Calin. *Deep Learning Architectures - A Mathematical Approach*. Springer Series in the Data Sciences. Springer Cham, 2020. isbn: 978-3-030-36720-6.

Neural Networks

Neural network



- The weight matrix of the ith layer

$$W_i = \begin{pmatrix} w_{i11} & \cdots & w_{i1n} \\ \vdots & & \vdots \\ w_{ir1} & \cdots & w_{irn} \end{pmatrix}$$

We drop the bias term b and choose $\phi = \mathbf{I}$ Neuron output $f_w(x_1, ..., x_n) = \sum_{j=1}^{n} w_j x_j$

This simplifies the network output function:

Linear Network

$$\boxed{f_W(x) = W_{H+1} W_H \cdots W_2 W_1 x} \tag{2}$$

We want to use f_W to approximate some function $y : \mathbb{R}^n \longrightarrow \mathbb{R}^p$

Neural Networks

Training a linear network

Minimization problem in real analysis

- Error (or *loss*), $\mathcal{L} : \mathbb{R}^n \longrightarrow \mathbb{R}$ defined by:

$$\mathcal{L}(W) = \frac{1}{2} \sum_{i=1}^{m} ||W_{H+1} W_H ... W_2 W_1 x^{(i)} - y^{(i)}||^2 \tag{3}$$

- We want to solve the minimization problem:

$$\min_{W \in \mathbb{R}^N} \; \mathcal{L}(W) \tag{4}$$

Not convex

Neural Networks

Training a linear network

Non-convexity of $\mathcal{L}(W)$ presents challenges

1. Hard to guarantee that all local minima have been found by the algorithm.
2. Hard to make assertions about the number and location of minima before hand.

Motivation for an algebraic geometry view

Neural Networks

Training a linear network

From a problem in Real Analysis to a problem in Algebraic Geometry

We introduce the following relaxations:

- $\min_{W \in \mathbb{R}^N} \ \mathcal{L}(W) \longrightarrow \nabla \mathcal{L}(W) = 0$
- $W \in \mathbb{R}^N \longrightarrow W \in \mathbb{C}^N$

We solve:

$$\boxed{\nabla \mathcal{L}(W) = 0, \quad W \in \mathbb{C}^N} \tag{5}$$

Polynomial system

Neural Networks

Training a linear network

From a problem in Real Analysis to a problem in Algebraic Geometry

Example 1.2 (A 4-weight network). Let us consider a 2-layer network with $W_1 = [\alpha_1, \alpha_2]$ $W_2 = \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix}$

- $\mathcal{L}(W) = \mathcal{L}(\alpha_1, \alpha_2, \beta_1, \beta_2) = \frac{1}{2}\sum_{i=1}^{2} ||W_2 W_1 x^{(i)} - y^{(i)}||^2$
- $\nabla\mathcal{L}(W) = \nabla\mathcal{L}(\alpha_1, \alpha_2, \beta_1, \beta_2) = 0$ gives

Nice polynomial system

- **Square**
- **Sparse**
- **Deg 2H + 1**

Solutions are precisely the critical points

$$\boxed{\begin{aligned} 5\alpha_1\beta_1^2 + 5\alpha_1\beta_2^2 + 11\alpha_2\beta_1^2 + 11\alpha_2\beta_2^2 - 7\beta_1 - 10\beta_2 &= 0 \\ 11\alpha_1\beta_1^2 + 11\alpha_1\beta_2^2 + 25\alpha_2\beta_1^2 + 25\alpha_2\beta_2^2 - 15\beta_1 - 22\beta_2 &= 0 \\ 5\alpha_1^2\beta_1 + 22\alpha_1\alpha_2\beta_1 + 25\alpha_2^2\beta_1 - 7\alpha_1 - 15\alpha_2 &= 0 \\ 5\alpha_1^2\beta_2 + 22\alpha_1\alpha_2\beta_2 + 25\alpha_2^2\beta_2 - 10\alpha_1 - 22\alpha_2 &= 0 \end{aligned}} \tag{1.13}$$

Algebraic Geometry

Main Ideas

Algebraic geometry provides results and methods to analyze and solve systems of polynomial equations. In particular, it provides us ways to:

1. exploit the monomial structure of a polynomial system to place upper bounds on the number of complex solutions **beforehand**

adresses challenge 2

2. use these upper bounds to algorithmically find **all** complex solutions

adresses challenge 1

Homotopy continuation

Tighter upper bounds lead to faster solutions

Question: How to find a good upper bound for our system

Algebraic Geometry

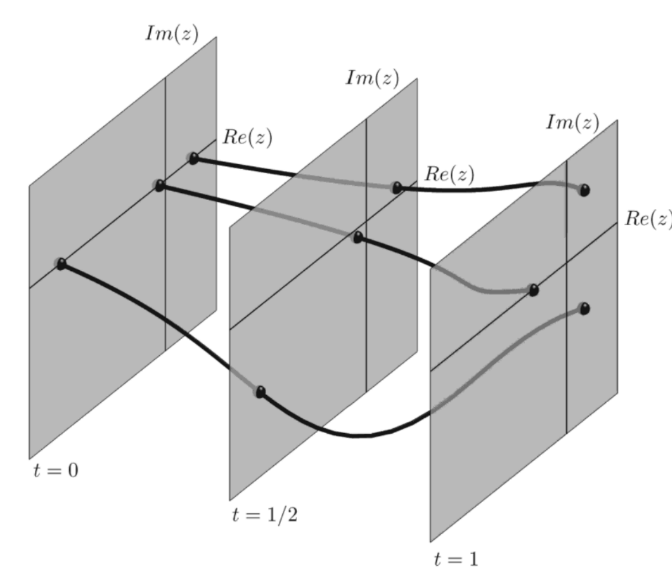
Main Ideas

Homotopy Continuation

- Suppose we want to solve the system $F(x) = [f_1(x), ..., f_N(x)] = 0$ **Target system**
- We generate another polynomial system $G(x) = [g_1(x), ..., g_N(x)] = 0$ **Start system**
- $G(x) = 0$ is guaranteed to have at least as many isolated solutions as $F(x) = 0$ and these solutions are known beforehand
- We define a parameterized family of systems:

Homotopy

$$H(x, t) = tG(x) + (1 - t)F(x), \quad t \in [0, 1]$$



A tighter upper bound means fewer paths to track and therefore provides a more efficient way to solve the target system

Image source: Daniel J. Bates et al. *Numerically solving polynomial systems with Bertini*. Vol 25 of Software, Environments and Tools. SIAM, 2013. isbn: 978-1-611972-69-6

Algebraic Geometry

Main Ideas

Well known upper bounds

Theorem 2.13 (Classical Bezout Bound). *Let $f_1, ..., f_N$ be polynomials in $\mathbb{C}[x_1, ..., x_N]$. Then the number of isolated solutions of the system $f_1(x) = ... = f_N(x) = 0$ is bounded above by the product $deg(f_1) \cdots deg(f_N)$.*

Theorem 2.22 (Bernstein's Theorem). *Let $f_1, ..., f_N \in \mathbb{C}[x_1, ..., x_N]$ be Laurent polynomials with Newton polytopes $Q_1, ..., Q_N$. The number of isolated solutions of the system $f_1(x) = ... = f_N(x) = 0$ in $(\mathbb{C}^*)^N$ is bounded above by the mixed volume $\mathcal{M}(Q_1, ..., Q_N)$.*

Question: Can we do better? Yes!

Results

Number of complex critical points

Critical points with all non-zero weights

Proposition 3.6 (upper bound on solutions in $(\mathbb{C}^*)^N$, $\mathcal{B}_{\mathbb{C}^*}$)**.** *Consider a linear network with* $H = 1$, $m = 1$, $d_x = n$, $d_y = p$ *and* $d_1 = d$. *Let* $(W_1, W_2) = \left(\begin{pmatrix} a_{1,1} & \cdots & a_{1,n} \\ & \vdots & \\ a_{d,1} & \cdots & a_{d,n} \end{pmatrix}, \begin{pmatrix} b_{1,1} & \cdots & b_{1,d} \\ & \vdots & \\ b_{p,1} & \cdots & b_{p,d} \end{pmatrix} \right)$ *denote a solution to the gradient polynomial system (3.1). Then, there are at most*

$$\mathcal{B}_{\mathbb{C}^*} = (4p)^d$$

solutions for which $a_{1,1}, \ldots, a_{d,n} \in \mathbb{C}^*$ *and* $b_{1,1}, \ldots, b_{p,d} \in \mathbb{C}^*$.

Results

Number of complex critical points

All critical points

Theorem 3.9 (upper bound on complex critical points, $\mathcal{B}_{\mathbb{C}}$). *Consider a linear network with $H = 1$, $m = 1$, $d_x = n$, $d_y = p$ and $d_1 = d$. This network has at most*

$$\mathcal{B}_{\mathbb{C}} = (1 + 4p)^d$$

complex critical points.

No	d	d_x	d_y	N	CBB	BKK	$\mathcal{B}_{\mathbb{C}}$	$\mathcal{B}_{\mathbb{C}^*}$	$N_{\mathbb{C}}$	$N_{\mathbb{C}^*}$	$max\{N_{\mathbb{R}}\}$
1	1	1	1	2	9	5	5	4	5	4	3
2	1	2	1	3	27	9	5	4	5	4	3
3	1	3	1	4	81	13	5	4	5	4	3
4	1	1	2	3	27	9	9	8	9	8	3
5	1	2	2	4	81	33	9	8	9	8	3
6	1	3	2	5	243	73	9	8	9	8	3
7	1	1	3	4	81	13	13	12	13	12	3
8	1	2	3	5	243	73	13	12	13	12	3
9	1	3	3	6	729	245	13	12	13	12	3
10	2	1	1	4	81	25	25	16	9	0	4
11	2	2	1	6	729	81	25	16	9	0	5
12	2	3	1	8	6561	169	25	16	9	0	5
13	2	1	2	6	729	81	81	64	33	16	9
14	2	2	2	8	6561	1089	81	64	33	16	9
15	2	3	2	10	59049	5329	81	64	33	16	9
16	2	1	3	8	6561	169	169	144	73	48	9
17	2	2	3	10	59049	5329	169	144	73	48	9
18	2	3	3	12	531441	60025	169	144	73	48	9
19	3	1	1	6	729	125	125	64	13	0	7
20	3	2	1	9	19683	729	125	64	13	0	7
21	3	3	1	12	531441	2197	125	64	13	0	7
22	3	1	2	9	19683	729	729	512	73	0	19
23	3	2	2	12	531441	35937	729	512	73	0	19
24	3	3	2	15	14348907	389017	729	512	73	0	19
25	3	1	3	12	531441	2197	2197	1728	245	64	27
26	3	2	3	15	14348907	389017	2197	1728	245	64	27

Table 3.1: Case: $H = 1, m = 1$. Comparison of upper bounds on the number of complex critical points of a linear network. $d =$ number of neurons in each layer, $d_x =$ input dimension and $d_y =$ output dimension. $N =$ total number of weights in the network. CBB and BKK refer to the classical Bezout bound and the BKK bound respectively. $\mathcal{B}_{\mathbb{C}}$ and $\mathcal{B}_{\mathbb{C}^*}$ refer to the new bounds on the number of critical points in $(\mathbb{C})^N$ and $(\mathbb{C}^*)^N$ respectively. $N_{\mathbb{C}}$ and $N_{\mathbb{C}^*}$ refer to the actual number of critical points in $(\mathbb{C})^N$ and $(\mathbb{C}^*)^N$ respectively. $max\{N_{\mathbb{R}}\}$ = maximum number of real solutions observed within each sample.

Results

Location of complex critical points

Critical points with some zero weights lie on particular coordinate subspaces

Proposition 3.1 (no stray zeros in W_1). *Consider a linear network with $H = 1, m = 1, d_x = n, d_y = p$ and $d_1 = d$. Let $(W_1, W_2) = \left(\begin{pmatrix} a_{1,1} & \cdots & a_{1,n} \\ & \vdots & \\ a_{d,1} & \cdots & a_{d,n} \end{pmatrix}, \begin{pmatrix} b_{1,1} & \cdots & b_{1,d} \\ & \vdots & \\ b_{p,1} & \cdots & b_{p,d} \end{pmatrix} \right)$ denote a solution to the regularized gradient polynomial system (3.1). If $a_{i,j} = 0$, then $a_{i,s} = 0$ for all $s = 1, ..., n$.*

Proposition 3.3 (no stray zeros in W_2). *Consider a linear network with $H = 1, m = 1, d_x = n, d_y = p$ and $d_1 = d$. Let $(W_1, W_2) = \left(\begin{pmatrix} a_{1,1} & \cdots & a_{1,n} \\ & \vdots & \\ a_{d,1} & \cdots & a_{d,n} \end{pmatrix}, \begin{pmatrix} b_{1,1} & \cdots & b_{1,d} \\ & \vdots & \\ b_{p,1} & \cdots & b_{p,d} \end{pmatrix} \right)$ denote a solution to the regularized gradient polynomial system (3.1). Then,*

$$b_{k,i} = 0 \implies b_{\cdot,i} = 0$$

Results

Location of complex critical points

Critical points with some zero weights lie on particular coordinate subspaces

Proposition 3.2 (null rows of W_1 match null columns of W_2). *Consider a linear network with* $H = 1$, $m = 1$, $d_x = n$, $d_y = p$ *and* $d_1 = d$. *Let* $(W_1, W_2) = \left(\begin{pmatrix} a_{1,1} & \cdots & a_{1,n} \\ & \vdots & \\ a_{d,1} & \cdots & a_{d,n} \end{pmatrix}, \begin{pmatrix} b_{1,1} & \cdots & b_{1,d} \\ & \vdots & \\ b_{p,1} & \cdots & b_{p,d} \end{pmatrix} \right)$ *denote a solution to the regularized gradient polynomial system (3.1). Then,*

$$a_{i,\cdot} = 0 \iff b_{\cdot,i} = 0$$

Results

Location of complex critical points

Critical points with some zero weights lie on particular coordinate subspaces

W1		W2		
0	0	0	*	8 solutions
*	*	0	*	
*	*	*	0	8 solutions
0	0	*	0	
*	*	*	*	16 solutions
*	*	*	*	
0	0	0	0	1 solution
0	0	0	0	

Figure 3.1: Case: $H = 1$, $m = 1$, $d = 2$, $d_x = 2$, $d_y = 2$ (corresponds to line no. 14 in Table 3.1. Number of solutions corresponding to each zero-pattern occurring in the weight matrices W_1 and W_2. * represents a non-zero entry.

Recap

- Neural networks (particularly, *linear networks*)
- Neural network training as a minimization problem in real analysis
- Neural network training as solving polynomial systems in algebraic geometry
- Results:
  - New upper bounds $\mathscr{B}_{\mathbb{C}}, \mathscr{B}_{\mathbb{C}^*}$ on the number of complex critical points of 1-hidden layer networks
  - Structure in the location of complex critical points with some zero weights

Further research

- Are $\mathcal{B}_{\mathbb{C}^*}$ and $\mathcal{B}_{\mathbb{C}}$ ever attained? Maybe for large m?
- Conversely, can we show that $\mathcal{B}_{\mathbb{C}^*}$ and $\mathcal{B}_{\mathbb{C}}$ are never attained?
- Prove zero patterns hold for $H > 1$.