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 $\mathbb{C}^N$

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Outline

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

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- Neural networks (particularly, *linear networks*)

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- Neural network training as a minimization problem in real analysis

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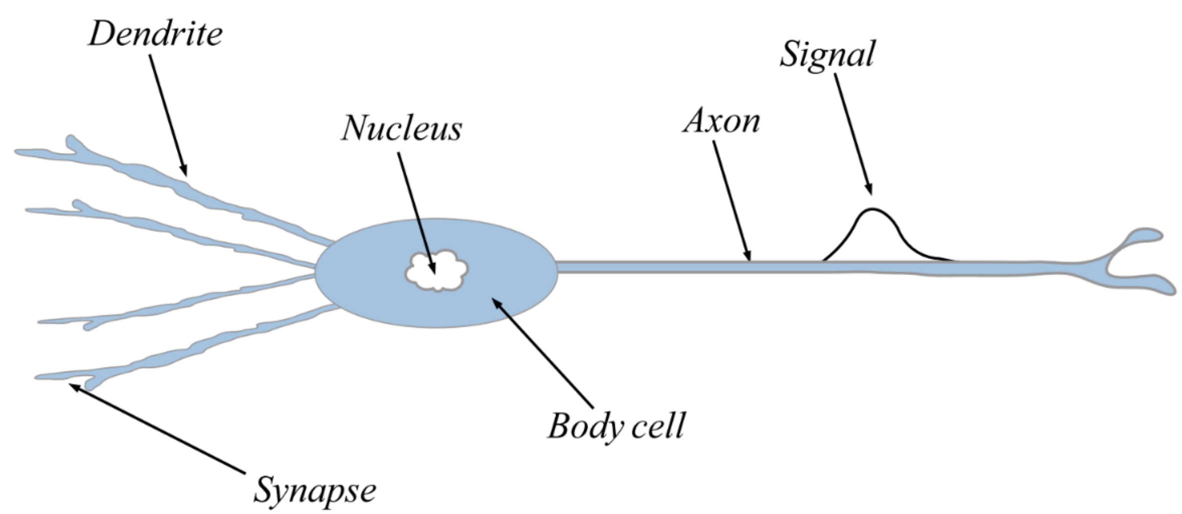
- Neural networks (particularly, *linear networks*)
- Neural network training as a minimization problem in real analysis
- Neural network training as solving polynomial systems in algebraic geometry
- Results and contributions

Neural Networks

Neuron

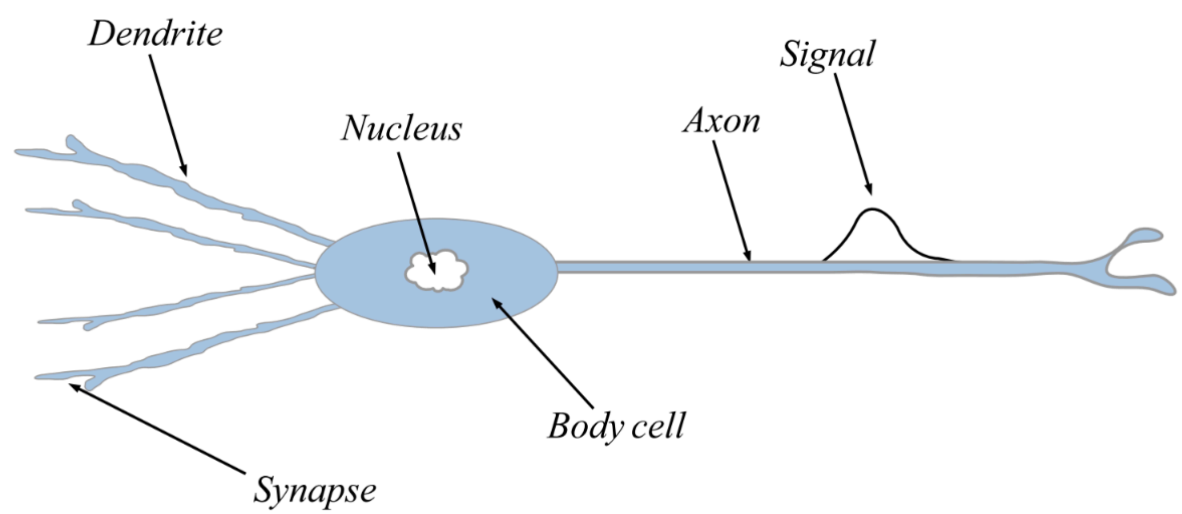
Neural Networks

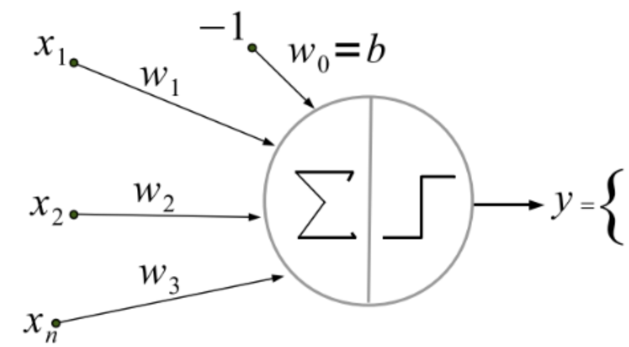
Neuron



Neural Networks

Neuron





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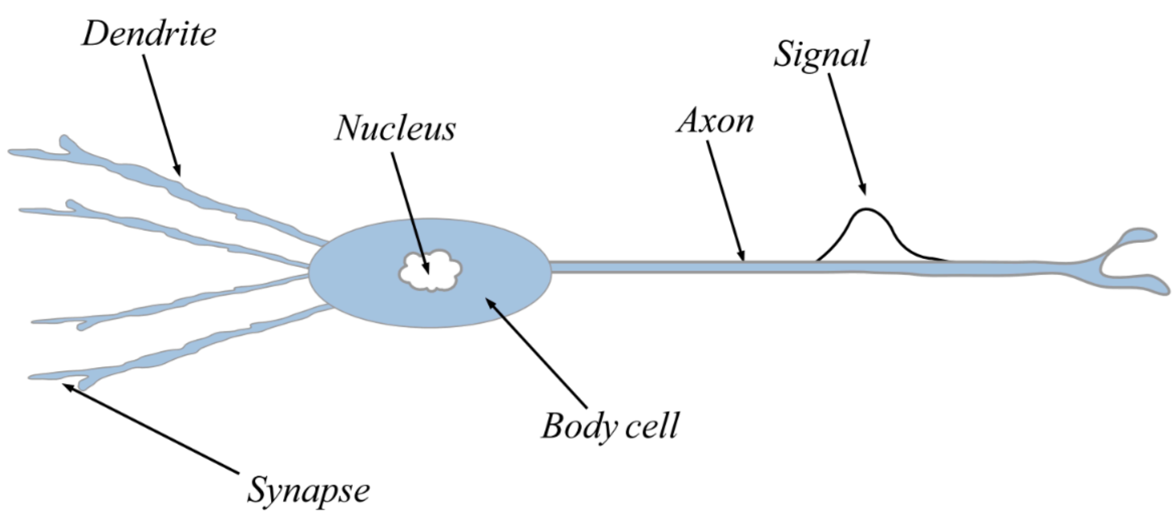

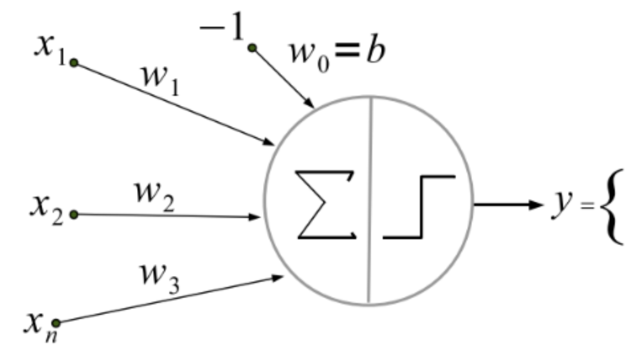

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Neural Networks

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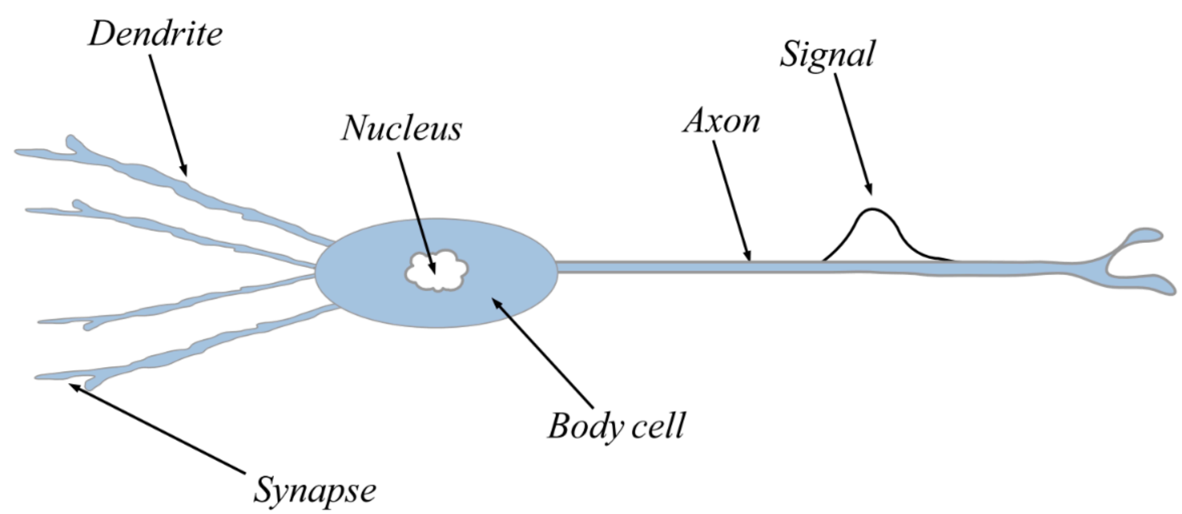

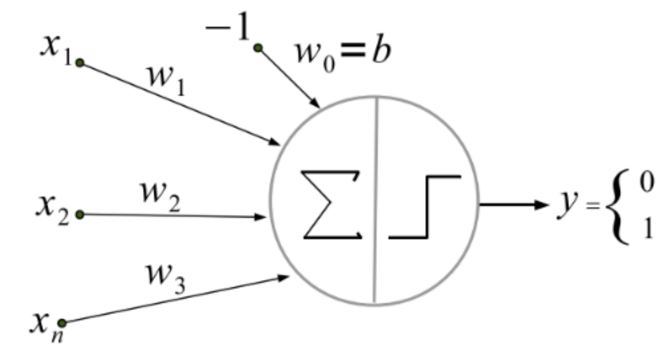

- $f_w(x_1, \ldots, x_n) = \phi\left(\sum_{j=1}^{n} w_j x_j - b\right)$ **(output function)**

Neural Networks

Neural network

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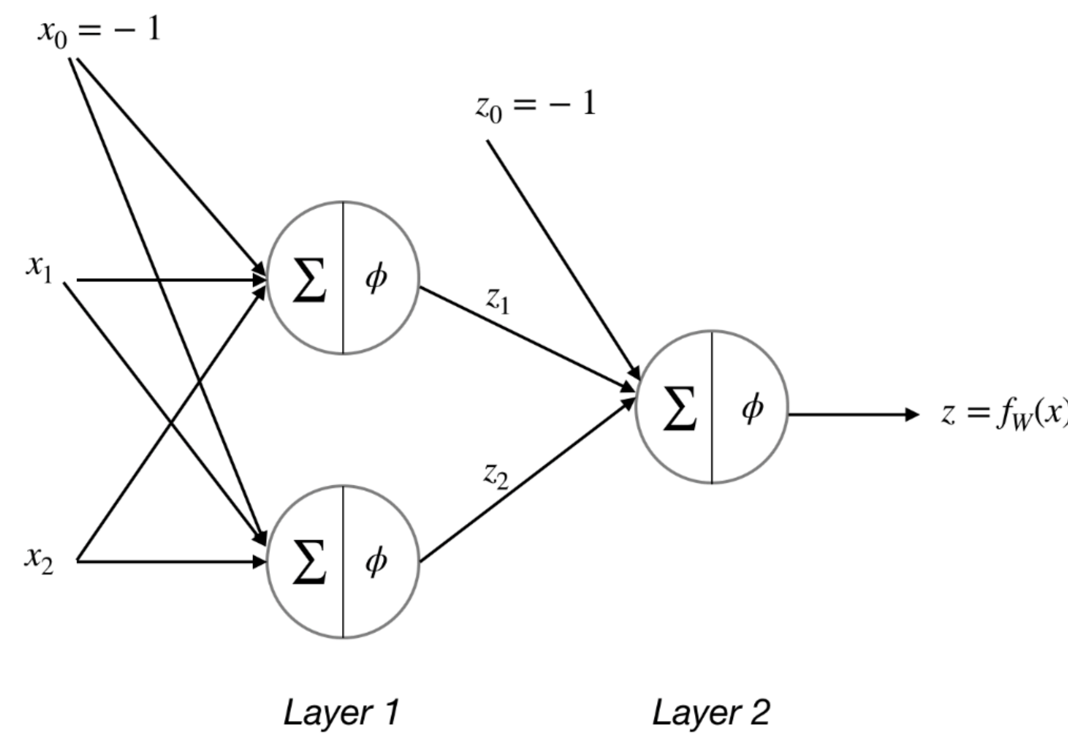
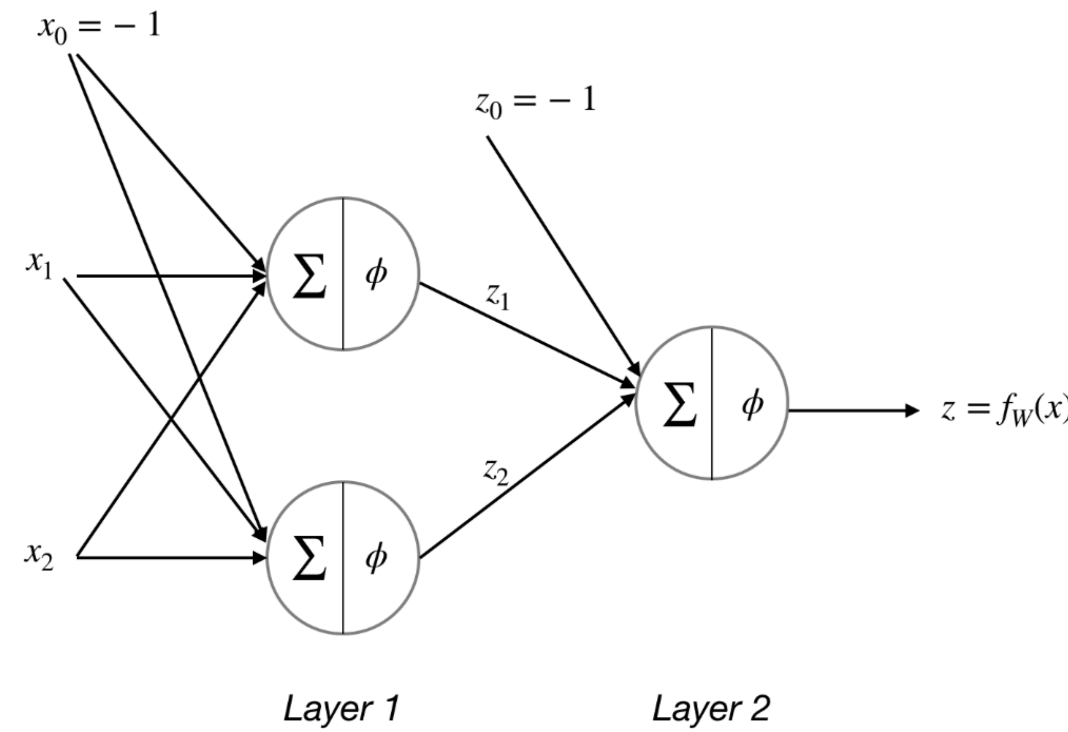


Neural Networks

Neural network

- The weight matrix of the ith layer

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



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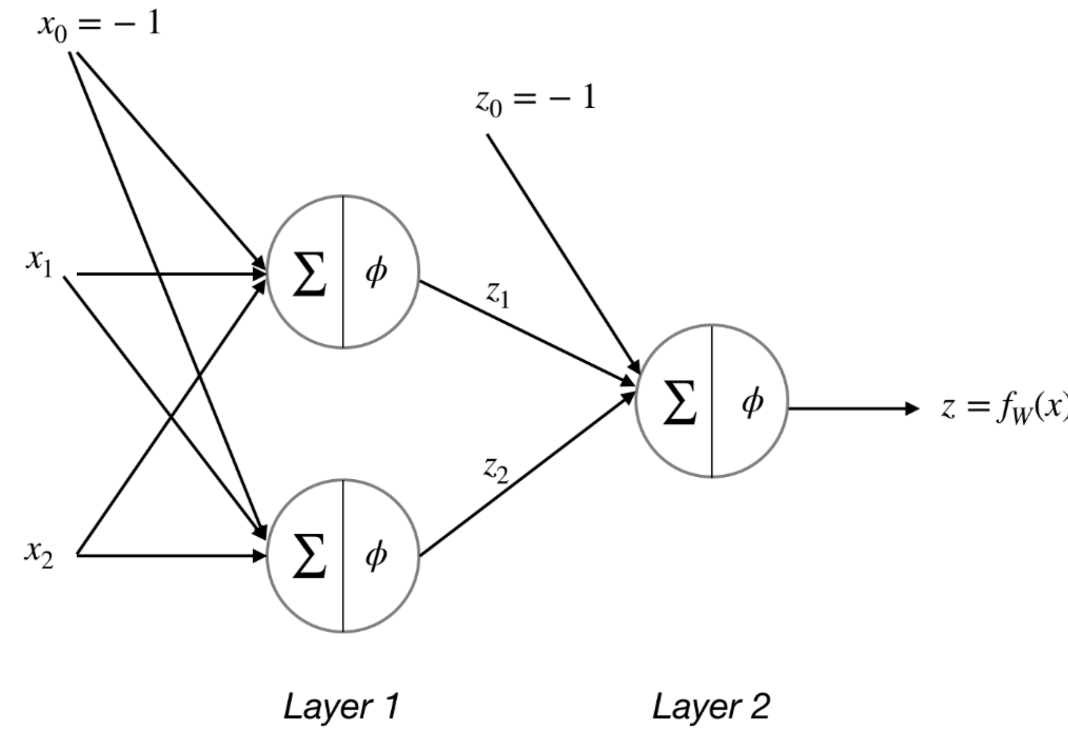

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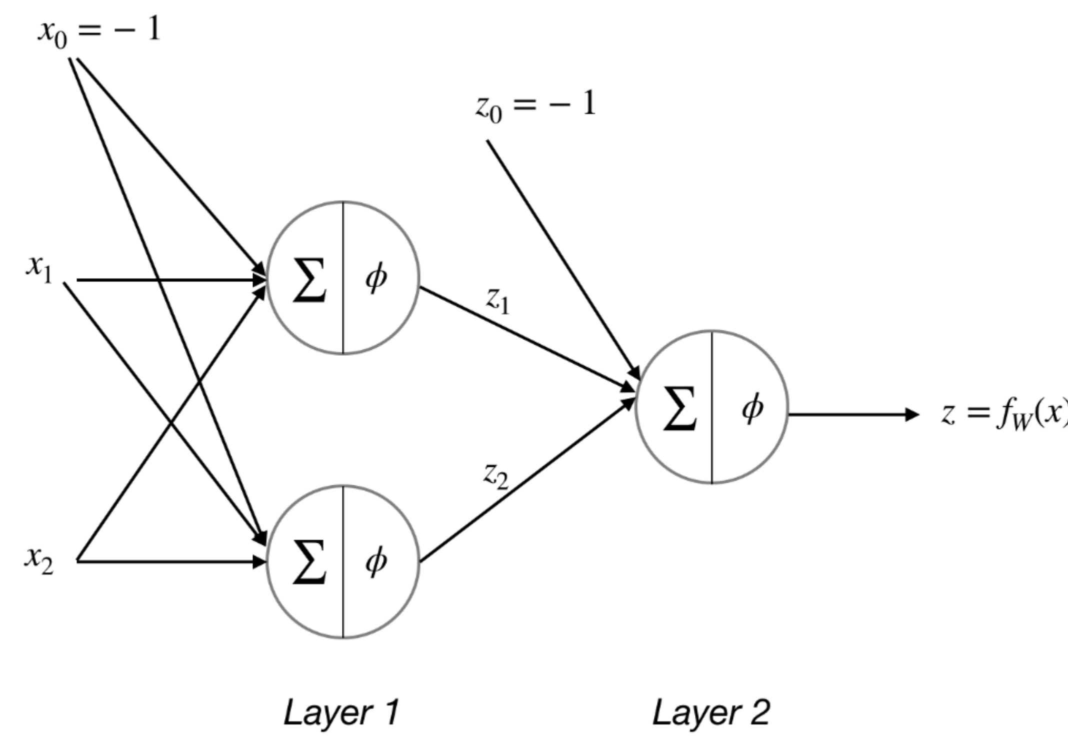

- Output of the ith layer

$$z^{(i)} = \phi\left(W_i \begin{bmatrix} -1 \\ z^{(i-1)} \end{bmatrix}\right)$$

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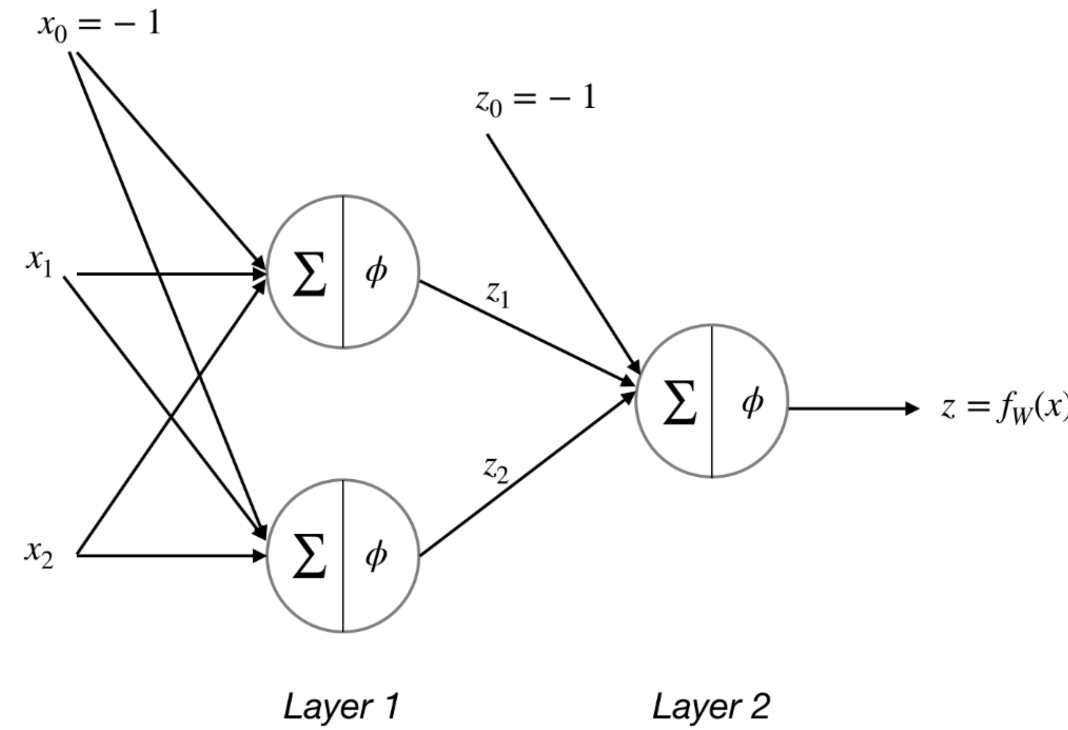

- Output of the ith layer

$$z^{(i)} = \phi\Big(W_i \begin{bmatrix} -1 \\ z^{(i-1)} \end{bmatrix}\Big)$$

- Output of the network

$$f_W(x) = z^{(H+1)} = \phi\Big(W_{H+1} \begin{bmatrix} -1 \\ z^{(H)} \end{bmatrix}\Big) \tag{2}$$

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Linear network

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- Drop the bias term b
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We want to use f_W to approximate some function $y : \mathbb{R}^n \longrightarrow \mathbb{R}^p$

Neural Networks

Training a linear network

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

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Not convex

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

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Motivation for an algebraic geometry view

Neural Networks

Training a linear network

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

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We introduce the following relaxations:

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

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We solve:

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

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Polynomial system

Neural Networks

Training a linear network

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

Solutions are precisely the critical points

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

Solutions are precisely the critical points

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

$$W_1 = [\alpha_1, \alpha_2]$$

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Example 1.2 (A 4-weight network). Let us consider a 2-layer network with

$$W_1 = [\alpha_1, \alpha_2] \quad W_2 = \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} \quad X = \left(\begin{smallmatrix} 1 & 2 \\ 3 & 4 \end{smallmatrix}\right), Y = \left(\begin{smallmatrix} 1 & 3 \\ 2 & 4 \end{smallmatrix}\right).$$

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

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

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

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Nice polynomial system

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- $\nabla \mathcal{L}(W) = \nabla \mathcal{L}(\alpha_1, \alpha_2, \beta_1, \beta_2) = 0$ gives

Nice polynomial system

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

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Algebraic Geometry

Main Ideas

Algebraic Geometry

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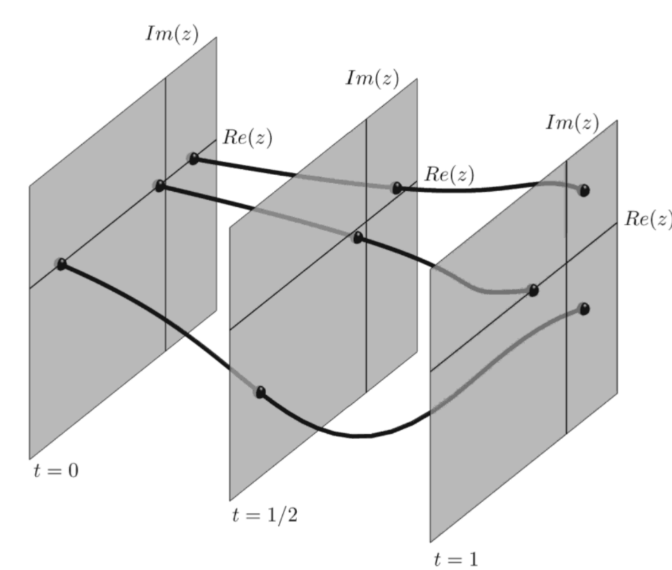

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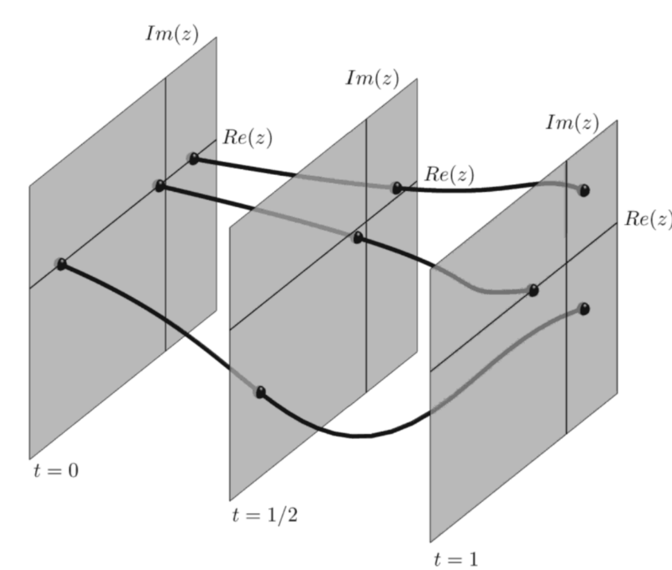

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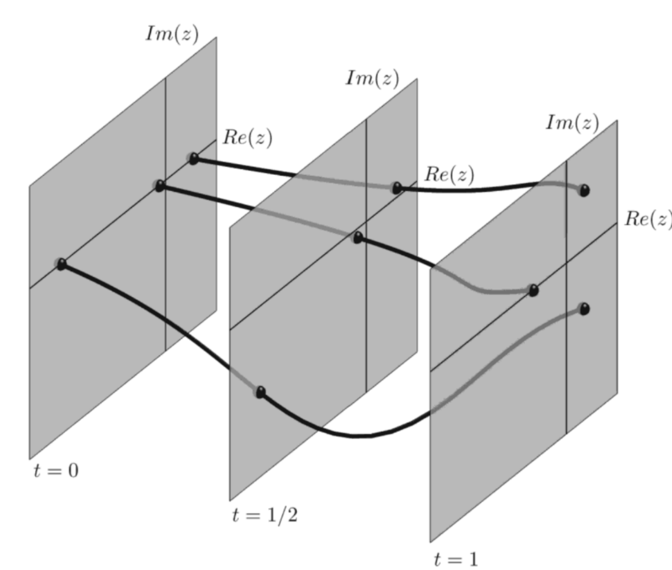

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Theorem 2.22 (Bernstein's Theorem). *Let $f_1, ..., f_N \in \mathbb{C}[x_1, ..., x_N]$ be Laurent polynomials with Newton polytopes $Q_1, ..., Q_N$. The number of isolated solutions of the system $f_1(x) = ... = f_N(x) = 0$ in $(\mathbb{C}^*)^N$ is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

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Results

Number of complex critical points

Critical points with all non-zero weights

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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* $b_{1,1}, \ldots, b_{p,d} \in \mathbb{C}^*$.

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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*

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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.

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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 $s = 1, \ldots, n$.*

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,*

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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,*

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```
###################### di=2, H=1, m=1, dx=2, dy=2 ####################

W2 W1
0 1  0 0
0 1  1 1
subspace dim: 4
solution count: 8

W2 W1
1 1  1 1
1 1  1 1
subspace dim: 8
solution count: 16

W2 W1
1 0  1 1
1 0  0 0
subspace dim: 4
solution count: 8

W2 W1
0 0  0 0
0 0  0 0
subspace dim: 0
solution count: 1
```

Further research

3. run experiments to check if increasing m causes BBK bound to be attained? for what value of m for a given architecture?

4. Conversely, can we show that the BKK bound is never reached? Even though our systems are non-generic, we might be able to solve the corresponding facial system may have no solutions, in which case, the BKK bound is a strict bound.

5. prove zero patterns for $H > 1$

6. extend table for H = 1, m=1 but higher values if d_x, d_y, d_i by solving reduced systems.

Recap

$\mathscr{B}_{\mathbb{C}}$ $\mathscr{B}_{\mathbb{C}^*}$

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  - New upper bounds $\mathscr{B}_{\mathbb{C}}, \mathscr{B}_{\mathbb{C}^*}$ on the number of complex critical points of 1-hidden layer networks

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  - Structure in the location of complex critical points with some zero weights