Testing Neural Networks

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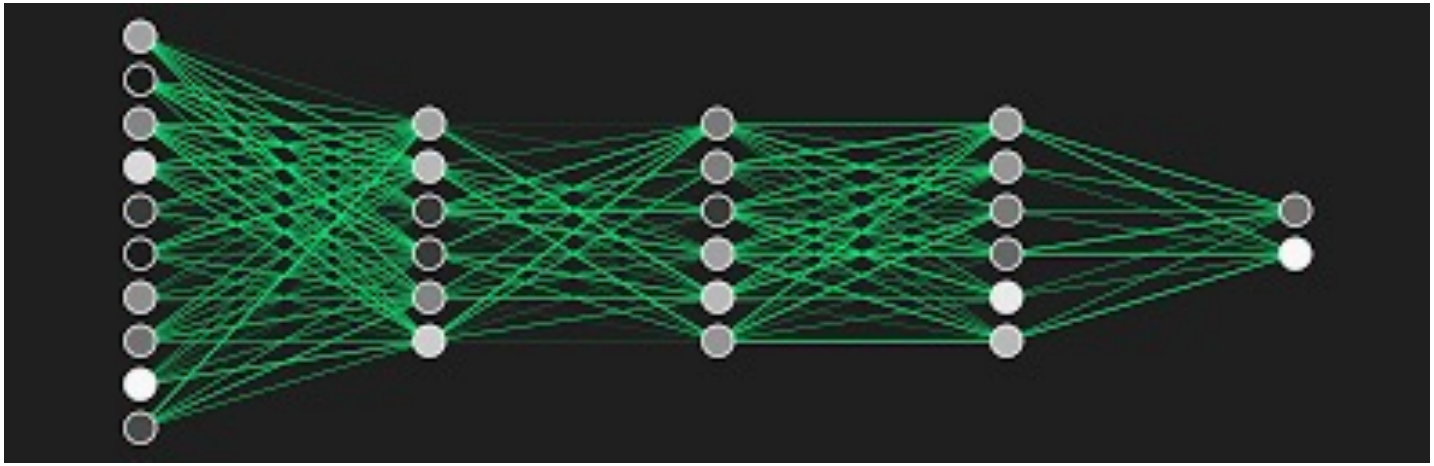
Central question

Does a given neural network compute in a robust way?



Testing a Neural Network

We will view a (trained, feedforward) neural network as a circuit:

- receives an input vector and
- computes an output

A neural network may be viewed as computing a function f of the inputs

Testing a Neural Network

Goal: formulate an approach that allows us to obtain
a mathematical understanding of the correspondence
of the (local) structure of the networks
with the function of its input it computes.

Our method of choice: framework of **property testing**

Underlying idea behind property testing:

- solve a *relaxed decision problem* by inspecting only a small part of the input
  - for example, by sampling

Property Testing

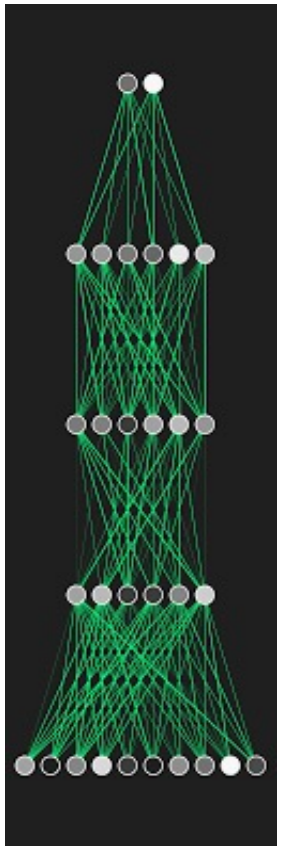
- Distinguish inputs that have specific property
  from those that are far from having the property (Rubinfeld-Sudan'96)

Benefits:

- May be a natural question to ask
- May be just as good when data constantly changing
- Gives fast sanity check to rule out very "bad" inputs (i.e., restaurant bills) or to decide when expensive processing is worth it

Testing a Neural Network

Underlying idea behind property testing: solve a relaxed decision problem by inspecting only a small part of the input (for example, by sampling).



A **property testing** algorithm is given

- query access to an object and
- the objective is to
  - accept objects that have a certain property of interest and
  - reject objects that are ***far*** from having that property.

In this talk:

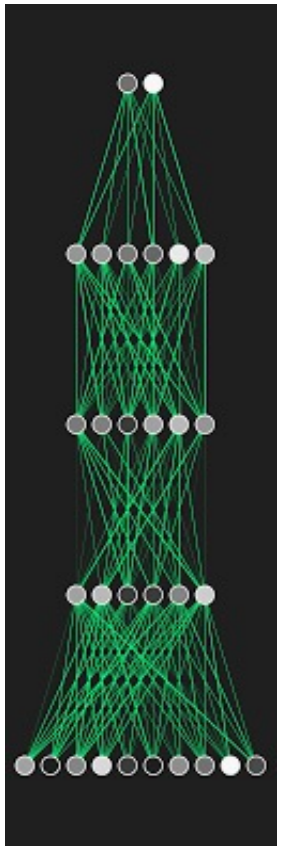
- objects = neural networks
- properties = functions or properties of functions

Testing a Neural Network

Why property testing?

- Not necessarily because neural networks are massive and we need sublinear-time algorithms
- Our view: property testing is a tool to reveal relations between the local structure of an object and its global structure
  - this in turn: can provide combinatorial insights about the structure of an object

- Our goal: improve our understanding of the relation between the network structure and the computed function

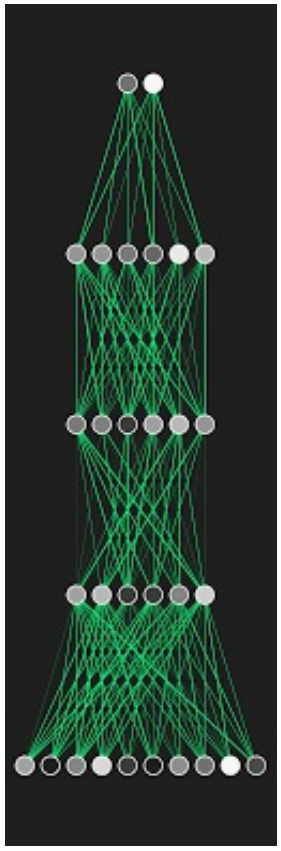


Testing a Neural Network

Why property testing?

- *Relaxed decision* setting in property testing has some appealing properties in the context of understanding neural networks:
  - typically, we'd like a neural network to be robust to small changes in the network;
  - to cope with risks of adversarial attacks
  - to accommodate network training of *dropout* used to improve generalization

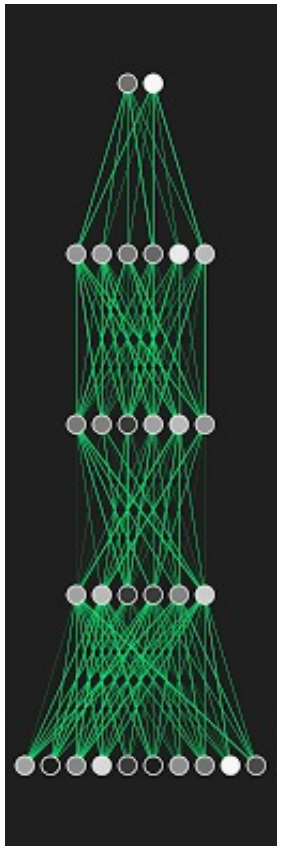
    e.g., a random fraction of input nodes is dropped during training for each training example



Testing a Neural Network

We introduce a property testing model for a fully connected feedforward network with
ReLU activation function (without bias) and hidden layers

- We will view the network as a circuit that computes a Boolean function
- Our objective: design property testing algorithms that
  - sample weights of the network and
  - accept, if the network computes a certain function and
  - reject, if the network is (ε, δ)-far from computing the function



Network is (ε, δ)-far from computing the function f if

- one has to change the network in more than an ε-fraction of its size
- to obtain a function that differs from the target function on $< \delta$-fraction of inputs

Testing a Neural Network

We introduce a property testing model for a fully connected feedforward network with
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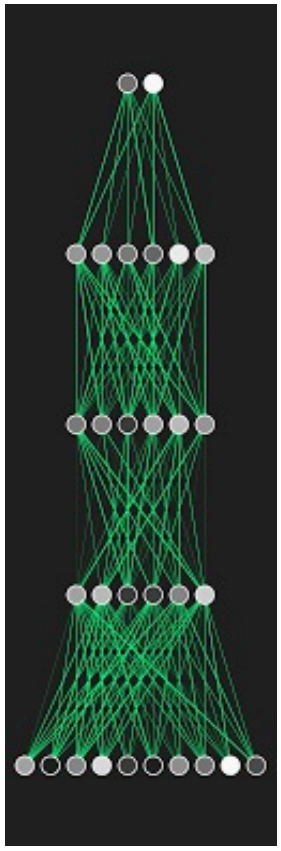

We will not consider a bias in the activation function

- we believe the main challenge is to understand the non-linearity of the ReLU function;
- one can easily simulate a bias in a network by allowing some inputs that are always 1 (and in practice, a network that is trained without bias will typically learn the bias)

Testing a Neural Network

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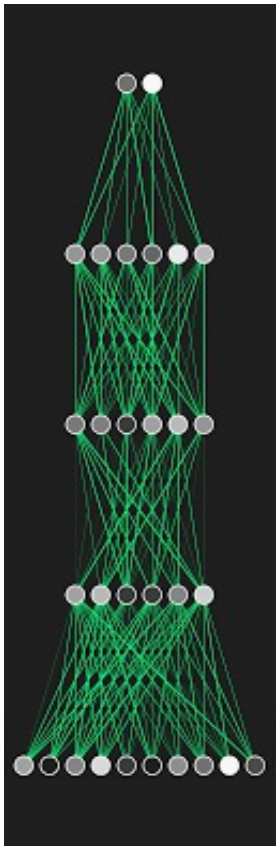
We will assume most of the time that the number of input neurons and neurons at the hidden layer will be polynomially related (in practice, they are typically within a constant factor of each other)



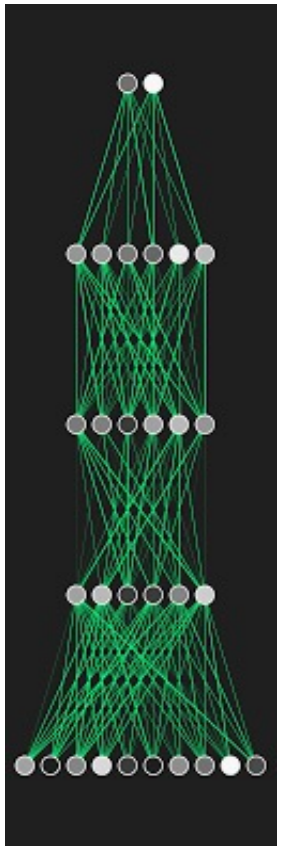
Testing a Neural Network

Main conceptual contribution:

- a model that allows a nontrivial study of neural networks from the lens of property testing

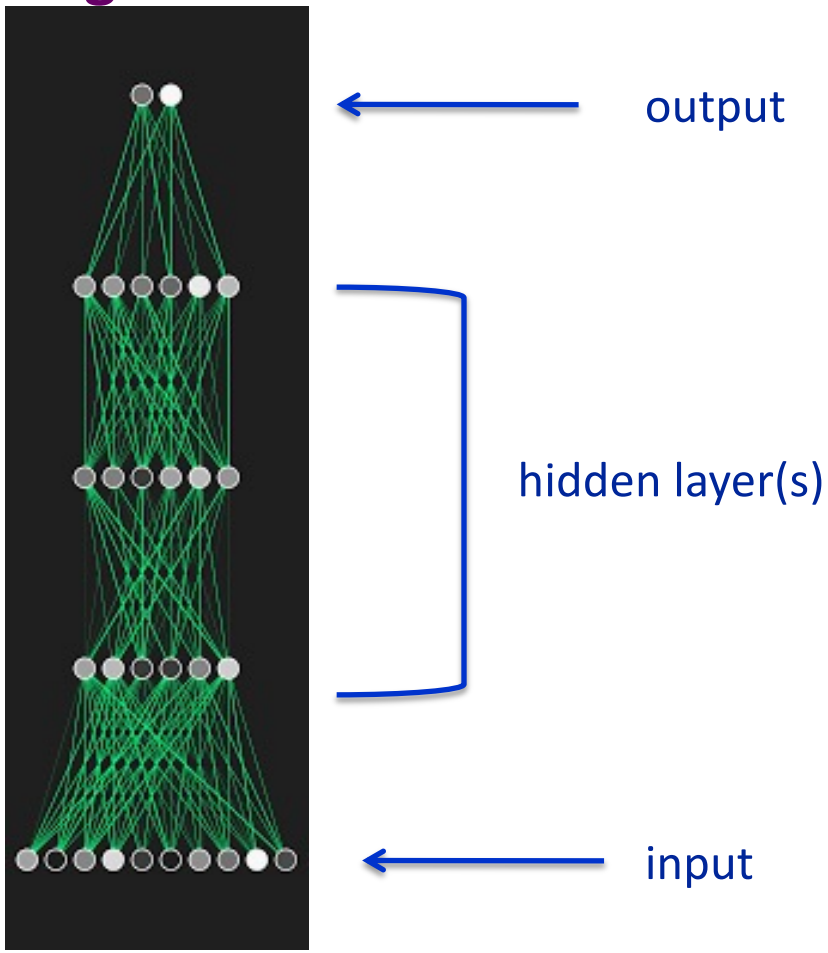
Main technical contribution:

- study of basic Boolean functions and properties
- showing that some of them can be efficiently tested



Testing a Neural Network

- Underlying model:



A simple feedforward network with ReLU activation function

We consider a feedforward network with one hidden layer and ReLU activation function.

- The network is fully connected,
- has n input nodes labeled $\{1, \ldots, n\}$,
- a hidden layer with m nodes labeled $\{1, \ldots, m\}$, and
- one output node.

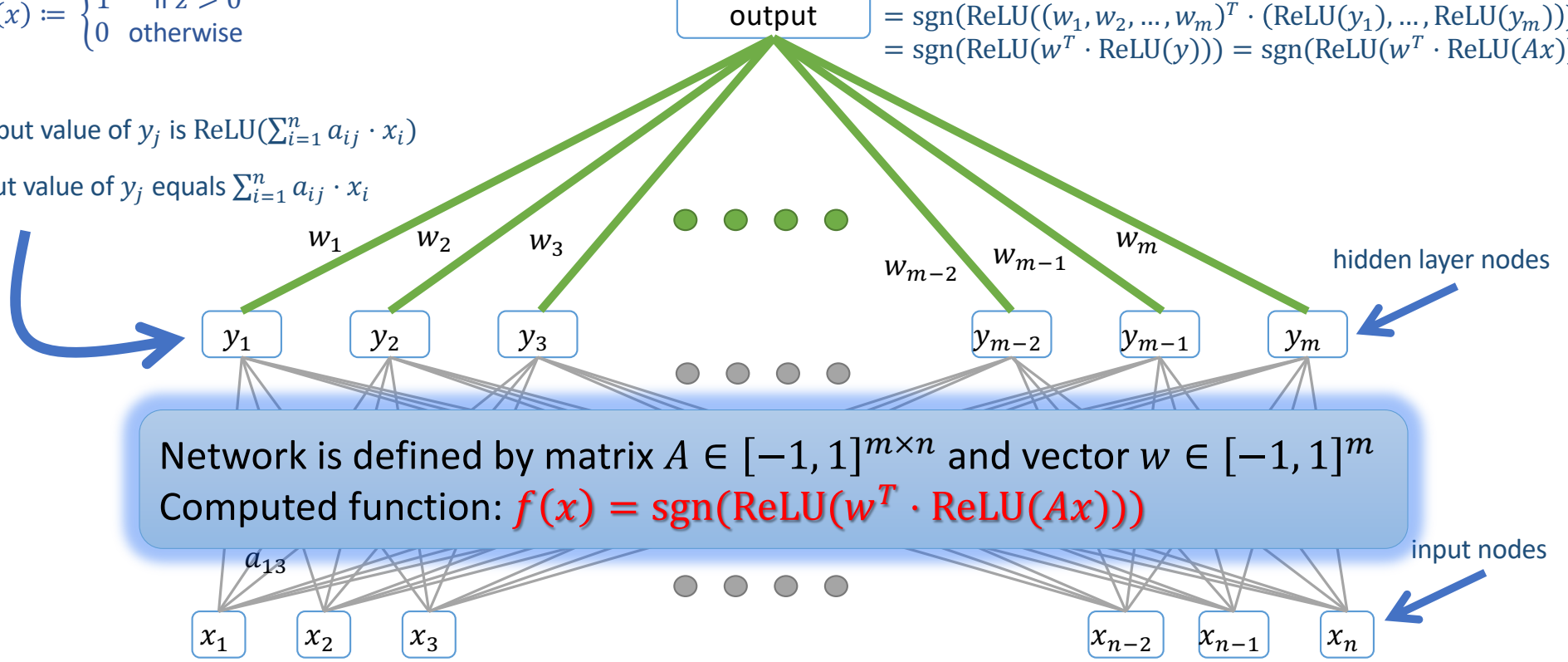
output value is equal to sign of $\mathrm{ReLU}(\sum_{j=1}^{m} w_j \cdot y_j)$

$$\mathrm{sgn}(x) := \begin{cases} 1 & \text{if } z > 0 \\ 0 & \text{otherwise} \end{cases}$$

output $= \mathrm{sgn}(\mathrm{ReLU}((w_1, w_2, \dots, w_m)^T \cdot (\mathrm{ReLU}(y_1), \dots, \mathrm{ReLU}(y_m))))$
$= \mathrm{sgn}(\mathrm{ReLU}(w^T \cdot \mathrm{ReLU}(y))) = \mathrm{sgn}(\mathrm{ReLU}(w^T \cdot \mathrm{ReLU}(Ax)))$

output value of y_j is $\mathrm{ReLU}(\sum_{i=1}^{n} a_{ij} \cdot x_i)$

input value of y_j equals $\sum_{i=1}^{n} a_{ij} \cdot x_i$



$a_{ij}, w_i \in [-1,1]$

ReLU activation function: $ReLU(u) = \max\{0, u\}$

output value is equal to sign of $\mathrm{ReLU}(\sum_{j=1}^{m} w_j \cdot y_j)$

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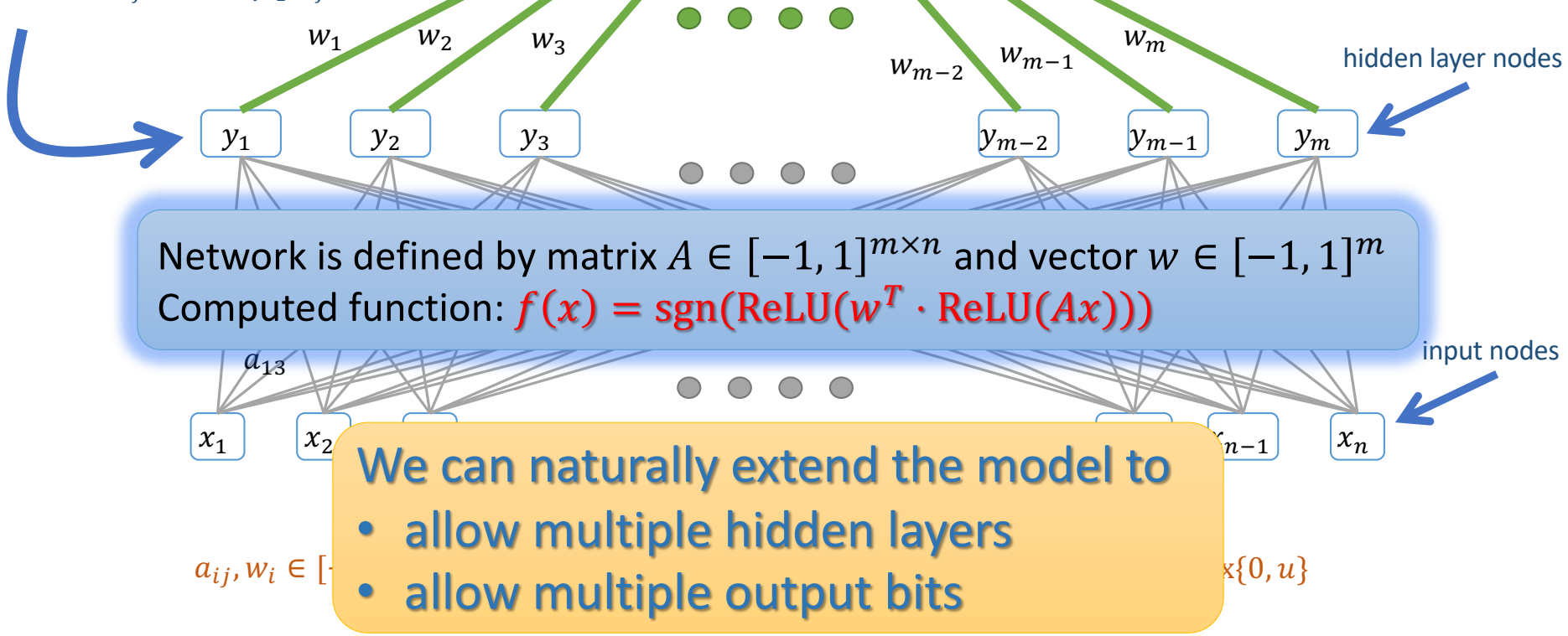


Network is defined by matrix $A \in [-1,1]^{m \times n}$ and vector $w \in [-1,1]^m$
Computed function: $f(x) = \mathrm{sgn}(\mathrm{ReLU}(w^T \cdot \mathrm{ReLU}(Ax)))$

We can naturally extend the model to

- allow multiple hidden layers
- allow multiple output bits

$a_{ij}, w_i \in [$ … $x\{0, u\}$

ReLU network as a binary classifier

We interpret the network as a binary classifier:

- the network assigns each input vector to one of two classes, which we define as 0 and 1.

If the output value of the network is ≤ 0 we assign class 0, if it is > 0 we assign class 1.

We focus on the setting when $x \in \{0,1\}^n$ is a binary vector.

ReLU network is defined by a pair (A, w) where $A \in [-1,1]^{m \times n}$ and $w \in [-1,1]^m$

➔ the neural network defines a function $f : \{0,1\}^n \to \{0,1\}$ that computes

$$f(x) = \mathrm{sgn}(\mathrm{ReLU}(w^T \cdot \mathrm{ReLU}(Ax)))$$

Testing a Neural Network

Properties of Boolean functions:

A property of Boolean functions is a family $P = \bigcup_{n\in\mathbb{N}} P_n$,

- where P_n is a set of Boolean functions $f: \{0,1\}^n \to \{0,1\}$

ReLU network being far from computing a function:

Let (A, w) be a ReLU network with n input nodes and m hidden layer nodes.

(A, w) is called (ε, δ)-close to computing a function $f: \{0,1\}^n \to \{0,1\}$, if

- one can change the matrix A in $\leq \varepsilon nm$ places and the weight vector w in $\leq \varepsilon m$ places
- to obtain a ReLU network that computes a function g such that

$$\Pr[g(x) \neq f(x)] \leq \delta,$$

where x is chosen uniformly at random from $\{0,1\}^n$.

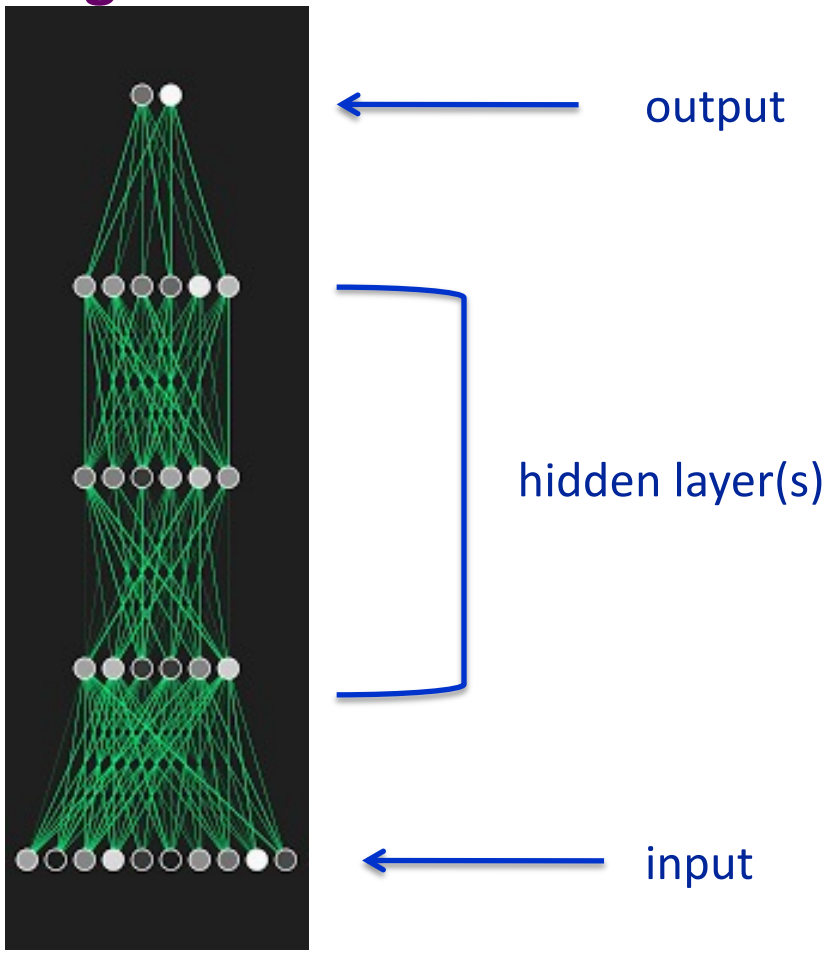
If (A, w) is not (ε, δ)-close to computing f ➔ (A, w) is (ε, δ)-far from computing f

Testing a Neural Network

Network is (ε, δ)-close to computing a function f :

we can edit the network to

- make it to compute f on $(1-\delta)$-fraction of the inputs
- by modifying an ε-fraction of weights at every layer



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If (A, w) is not (ε, δ)-close to computing f ➔ (A, w) is (ε, δ)-far from computing f

Testing a Neural Network

Properties of Boolean functions:

Extension to properties of functions

A property of Boolean functions is a family $P = \bigcup_{n\in\mathbb{N}} P_n$,

- where P_n is a set of Boolean functions $f: \{0,1\}^n \to \{0,1\}$

ReLU network being far from computing a function:

Let (A, w) be a ReLU network with n input nodes and m hidden layer nodes.

(A, w) is (ε, δ)-close to computing a function $f: \{0,1\}^n \to \{0,1\}$ with property P, if

- one can change the matrix A in $\leq \varepsilon nm$ places and the weight vector w in $\leq \varepsilon m$ places
- to obtain a ReLU network that computes a function g such that

$$\Pr[g(x) \neq f(x)] \leq \delta,$$

where x is chosen uniformly at random from $\{0,1\}^n$.

If (A, w) is not (ε, δ)-close to computing f ➔ (A, w) is (ε, δ)-far from computing f with P

Testing a Neural Network

Property $P = \bigcup_{n \in \mathbb{N}} P_n$ of Boolean functions is testable with query complexity $q(\varepsilon, \delta, n, m)$

- if for every $n, m \in N$, $\varepsilon, \delta \in (0, 1)$
- there exists an algorithm that
- receives parameters $n, m, \varepsilon, \delta$ as input and
- is given query access to a ReLU network with n input nodes and m hidden layer nodes,
- that queries the ReLU network in at most $q(\varepsilon, \delta, n, m)$ many places,
- accepts with probability at least $2/3$ if the network computes a function from P_n, and
- rejects with probability at least $2/3$ every network that computes a function that is (ε, δ)-far from P_n.

A tester that accepts every function from P with probability 1 is called one-sided tester.

If the function q depends only on ε and δ we just say that the property P is testable.

Testing a Neural Network: What can we show?

Our key findings:

- study of basic functions
  - understanding testability of constant 0-function, OR-function, and near-constant functions – for one and multiple hidden layer networks
- distribution-free model is too strong
- we can test functions faster than in the vanilla testing algorithm
- …

Testing a Neural Network: does it compute constant 0 function?

- We consider most basic functions – to understand which models are suitable
- Determining whether a network computes the constant 0-function is NP-hard

Testing a Neural Network: does it compute constant 0 function?

Vanilla testing algorithm:

- Sample many inputs at random and check if the network computes 0 on all of them

- There are networks that are is (ε, δ)-far from computing the constant 0-function (for constant ε and $\delta = 2^{-\Theta(n)}$) that require $2^{\Omega(n)}$ samples

- In our model: we can do it MUCH better

Testing a Neural Network: constant 0-function

Theorem: Let (A, w) be a ReLU network with n input nodes and m hidden layer nodes.

Let $e^{-n/16} \leq \delta < 1$ and let $0 < \varepsilon, \lambda < 1/2$.

Then A sample nodes and evaluate the restricted network with a suitable bias at the output node whether it computes the constant 0-function

- acc ion;
- rejects with prob $\geq 1 - \lambda$, if the ReLU network (A, w) is (ε, δ)-far from computing the 0-function;

Furthermore, the algorithm queries $O(\log^2(1/\varepsilon\lambda)/\varepsilon^6)$ entries from A and w.

Algorithm 1: AllZeroTester$(\varepsilon, \delta, \lambda, n, m)$

1 Sample $s = \lceil \frac{2^{20}}{\varepsilon^2} \cdot \ln(1/\varepsilon\lambda) \rceil$ nodes from the input layer and $t = \lceil \frac{2^{30}}{\varepsilon^4} \cdot \ln(1/\varepsilon\lambda) \rceil$ nodes from the hidden layer uniformly at random without replacement.

2 Let $S \in \mathbb{N}_0^{n \times n}$ and $T \in \mathbb{N}_0^{m \times m}$ be the corresponding sampling matrices.

3 **if** there is $x \in \{0,1\}^n$ with $\frac{nm}{st} \cdot w^T \cdot \mathrm{ReLU}(TASx) - \varepsilon nm/8 > 0$ **then reject**;

4 **else accept**.

Dependence $e^{-n/16} \leq \delta$ can be "moved" into the query complexity if n and m are polynomially related.

Testing a Neural Network: constant 0-function

Theorem: Let (A, w) be a ReLU network with n input nodes and m hidden layer nodes.

Let $e^{-n/16} \leq \delta < 1$ and let $0 < \varepsilon, \lambda < 1/2$.

Then AllZeroTester$(\varepsilon, \delta, \lambda, n, m)$ with query access to A and w

- accepts with prob $\geq 1 - \lambda$ if the ReLU network (A, w) computes the 0-function;
- rejects with prob $\geq 1 - \lambda$ if the ReLU network (A, w) is (ε, δ)-far from computing

1) if the network is (ε, δ)-far from computing the constant 0-function then there exists an input $x \in \{0,1\}^n$ on which the network has an output value of $\Omega(\varepsilon nm)$
   - sampling a constant number of hidden layer nodes one can approximate the output value for this particular x with sufficient accuracy so that the output value is $\Omega(\varepsilon nm)$
2) we can also sample a constant number of input nodes and approximate the value at the sampled hidden layer nodes in such a way that the value at the output node is positive

3 **if** there is $x \in \{0,1\}^n$ with $\frac{nm}{st} \cdot w^T \cdot \mathrm{ReLU}(TASx) - \varepsilon nm/8 > 0$ **then reject**;
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Algorithm accepts a network that computes the constant 0-function?
Claim: for all input vectors x the sampled network computes the constant 0-function.
Consider the sample from the input nodes as being fixed
Restricting our network to the sampled input nodes can also be done by restricting the input to vectors x that are 0 for all input nodes that do not belong to the sample.
➔ our sampling approach = only sampling from the hidden layer
➔ concentration bound + union bound over all ➔ proof

4 else accept.

Dependence $e^{-n/16} \leq \delta$ can be "moved" into the query complexity if n and m are polynomially related.

Testing a Neural Network: constant 0-function

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Let $e^{-n/16} \leq \delta < 1$ and let $0 < \varepsilon, \lambda < 1/2$.

Then AllZeroTe

A similar result can be shown for the OR-function

- accepts with prob $\geq 1 - \lambda$ if the ReLU network (A, w) computes the 0-function;
- rejects with prob $\geq 1 - \lambda$, if the ReLU network (A, w) is (ε, δ)-far from computing the 0-function;

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Dependence $e^{-n/16} \leq \delta$ can be "moved" into the query complexity if n and m are polynomially related.

Testing a Neural Network: constant 0-function

Algorithm above has two-sided error (may err while accepting and rejecting)

Can we do the same with 1-sided error?

Theorem: Any tester for the constant 0-function that has one-sided error has query complexity of $\Omega(m)$.

Similar results can be shown for the OR-function

At t

Follows from the fact that if too few weights are specified, one can always "complete" the network in such a way that it computes the constant 0-function

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1 Sample $s = \lceil \frac{2^{20} \log m}{\varepsilon^2} \cdot \ln(\frac{1}{\lambda}) \rceil$ nodes from the input layer uniformly at random without replacement.

2 Let $S \in \mathbb{N}_0^{n \times n}$ be the corresponding sampling matrix.

3 **if** there is $x \in \{0,1\}^n$ with $w^T \cdot \mathrm{ReLU}(ASx) > 0$ **then reject**;

4 **else accept**.

Testing a Neural Network: 0 and OR are central …

Theorem: Let (A, w) be a ReLU network with n input nodes and m hidden layer nodes.

Let $0 < \delta \leq 1/2$ and let $\varepsilon \geq 2\sqrt{\frac{\log(1/\delta)}{n}}$.

Then (A, w) is (ε, δ)-close to computing the OR-function or it is (ε, δ)-close to computing the constant 0-function.

This does not imply that all functions are pairwise $(2\varepsilon, 2\delta)$-close as our distance measure does not satisfy the triangle inequality.

Testing a Neural Network: 0 and OR are central …

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Let $0 < \delta \leq 1/2$ and let $\varepsilon \geq 2\sqrt{\frac{\log(1/\delta)}{n}}$.

Then (A, w) is (ε, δ)-close to computing the OR-function or it is (ε, δ)-close to computing the constant 0-function.

Corollary: Every property that contains the constant 0-function and the OR-function is trivially testable.

A Boolean function f is ***monotone***, if for every $x, y \in \{0,1\}^n$, $x \leq y$ implies $f(x) \leq f(y)$.

A Boolean function is ***symmetric***, if its value does not depend on the order of its arguments.

Corollary: Monotone/symmetric functions are testable.

Testing monotone properties

We consider also monotone properties.

A property P is monotone, if it is closed under flipping bits in the truth table of any function from the property from 0 to 1.

One can think of monotone properties as being defined by the set of minimal functions under the operation of flipping zeros to ones. We call such a set a generator.

Theorem: Every monotone property is testable with query complexity logarithmically on the size of the generator.

ReLU networks with multiple output bits

- Our main focus was on a Boolean functions
- We can extend some of the study to multiple output bits

For a vector $u = (u_1, \dots, u_r)$, let $\mathrm{sgn}(u) = (\mathrm{sgn}(u_1), \dots, \mathrm{sgn}(u_r))$

Definition: A ReLU network with n input nodes, m hidden layer nodes and r output node is a pair (A, W) where $A \in [-1, 1]^{m \times n}$ and $W \in [-1, 1]^{m \times r}$. The function $f: \{0,1\}^n \to \{0,1\}^r$ computed by a ReLU network (A, W) is defined as

$$f(x) := \mathrm{sgn}(\mathrm{ReLU}(W^T \cdot \mathrm{ReLU}(Ax)))$$

- All networks are close to a near-constant function
- Testing a near-constant function can be done with constant query complexity

Since for input 0, the output must be 0 ➔ near-constant function = constant except for input 0

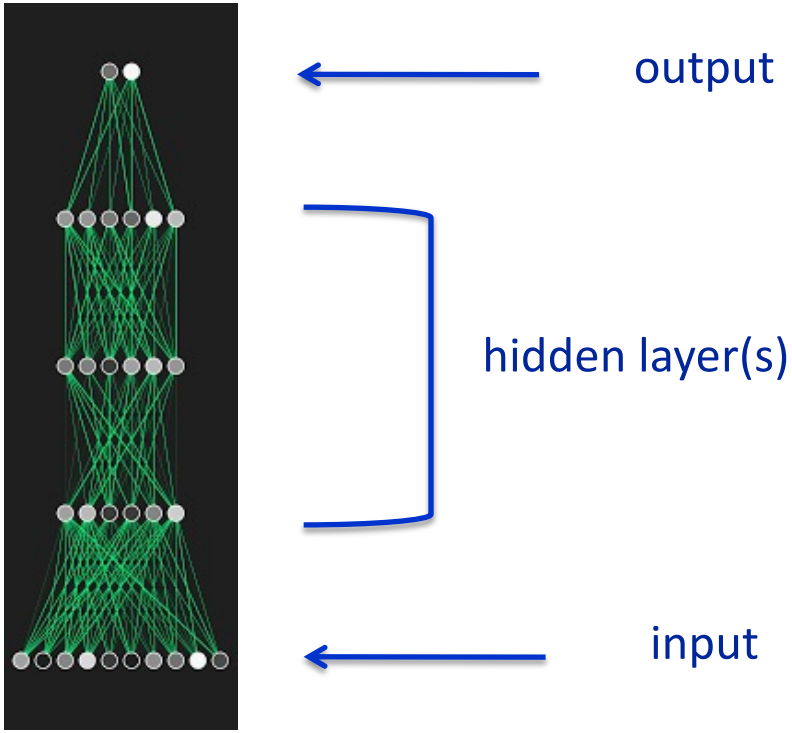
ReLU networks with multiple hidden layers

- Our main focus was on a Boolean functions with one hidden layer
- We can extend some of the study to multiple hidden layers

Network is (ε, δ)-close to computing a function f :

we can edit the network to

- make it to compute f on $(1-\delta)$-fraction of the inputs
- by modifying an ε-fraction of weights at every layer



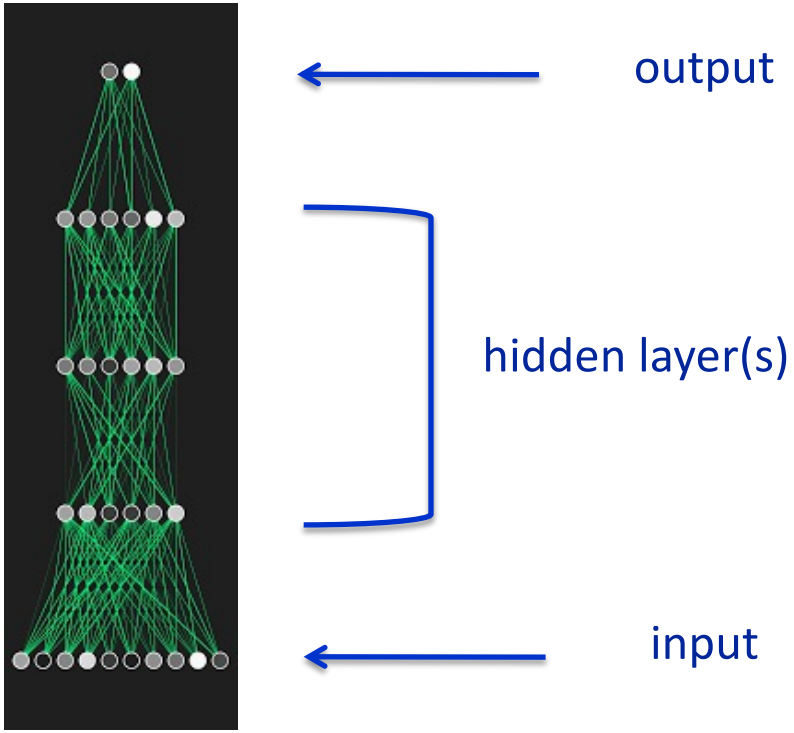
ReLU networks with multiple hidden layers and multiple output bits

- Testing a near-constant function can be done with constant query complexity

Network is (ε, δ)-close to computing a function f :

we can edit the network to

- make it to compute f on $(1-\delta)$-fraction of the inputs
- by modifying an ε-fraction of weights at every layer



Distribution-free model?

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Theorem: For every constant $k > 0$, every property tester for the constant 0-function in the distribution-free model has query complexity $\Omega(n^{1-1/k})$

Distribution-free model:

- an unknown distribution D over $\{0,1\}^n$
- query access: $\mathrm{query}(i, j)$ – sample input $y_i \in \{0,1\}^n$ according to D and return jth bit of y_i

(A, w) is called (ε, δ)-close to computing a function $f: \{0,1\}^n \to \{0,1\}$, if

- one can change the matrix A in $\leq \varepsilon nm$ places and the weight vector w in $\leq \varepsilon m$ places
- to obtain a ReLU network that computes a function g such that

$$\Pr[g(x) \neq f(x)] \leq \delta,$$

where x is chosen at random according to distribution D.

Distribution-free model?

Our ma… respect to the s…

Theorem: For every constant $k > 0$, every property tester for the constant 0-function in the distribution-free model has query complexity $\Omega(n^{1-1/k})$

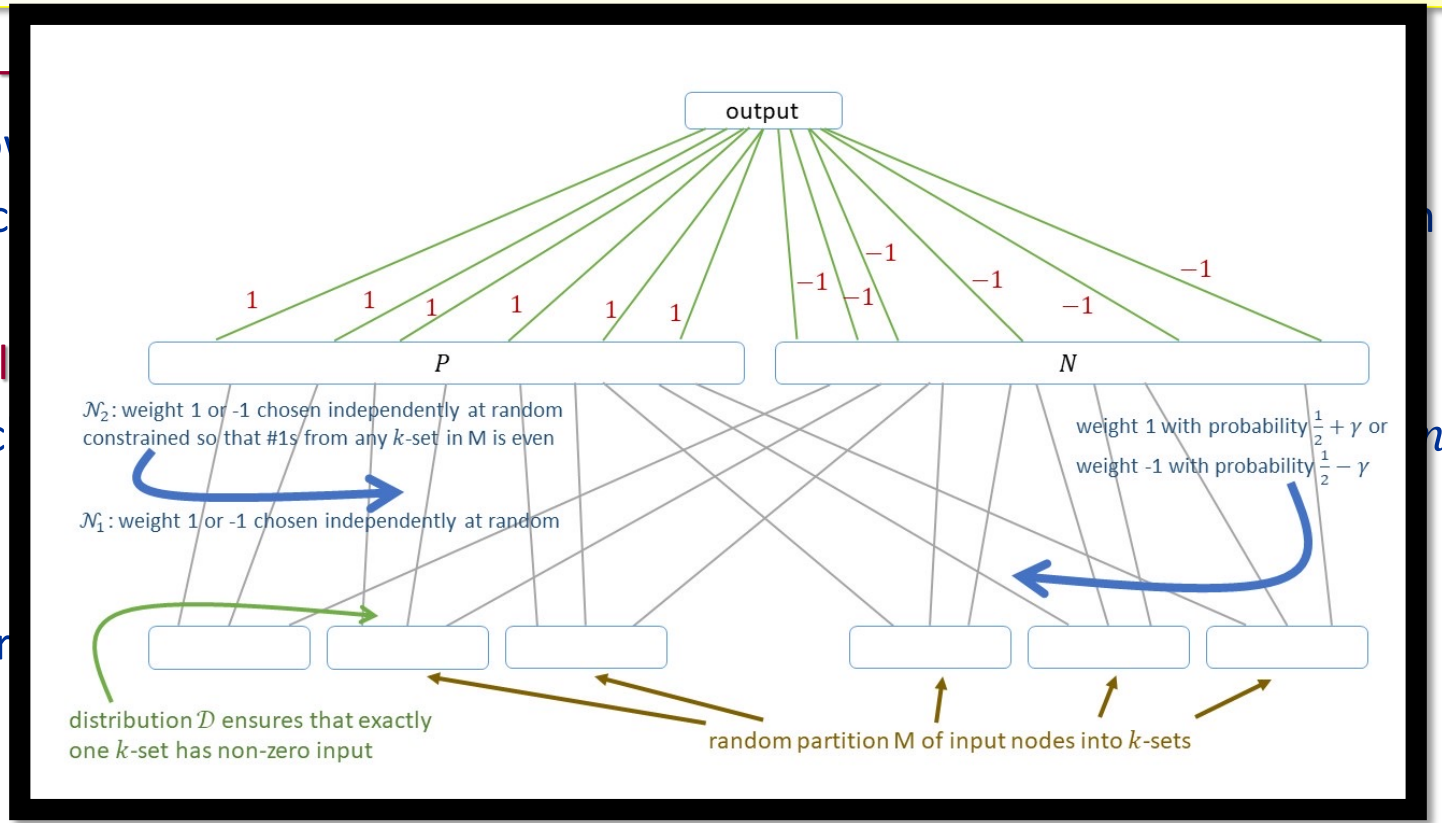
Distribution-…

- an unkno…
- query acc… jth bit of y_i

(A, w) is call…

- one can c… places
- to obtain …

wher…



Summary

- We introduced a property testing model to study neural networks
- Gave some first results in this model

- Large number of open questions regarding ReLU networks
  - query complexity of testing dictatorship and juntas
  - classify constant time testable properties with one- and two-sided error
  - extend the results to inputs over the reals
  - going beyond ReLU networks
  - …

THANK YOU!