Representational Capabilities of Feed-forward and Sequential Neural Architectures

Clayton Sanford

Ph.D. Thesis Defense

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April 17, 2024

Public talk

- Machine learning and neural networks background
- Dissertation contributions overview
- Vignette #1: Random feature models
- Vignette #2: Transformers and sequential models
- Acknowledgements

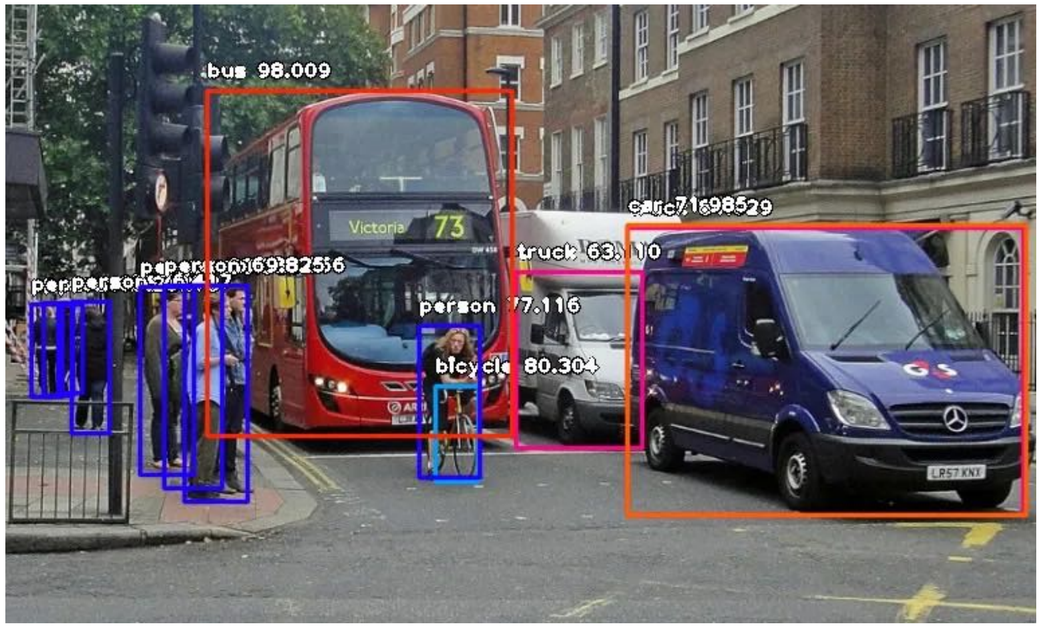
What is machine learning?

Algorithms that make decisions based on data,
without explicit programming.

What is machine learning?

Examples

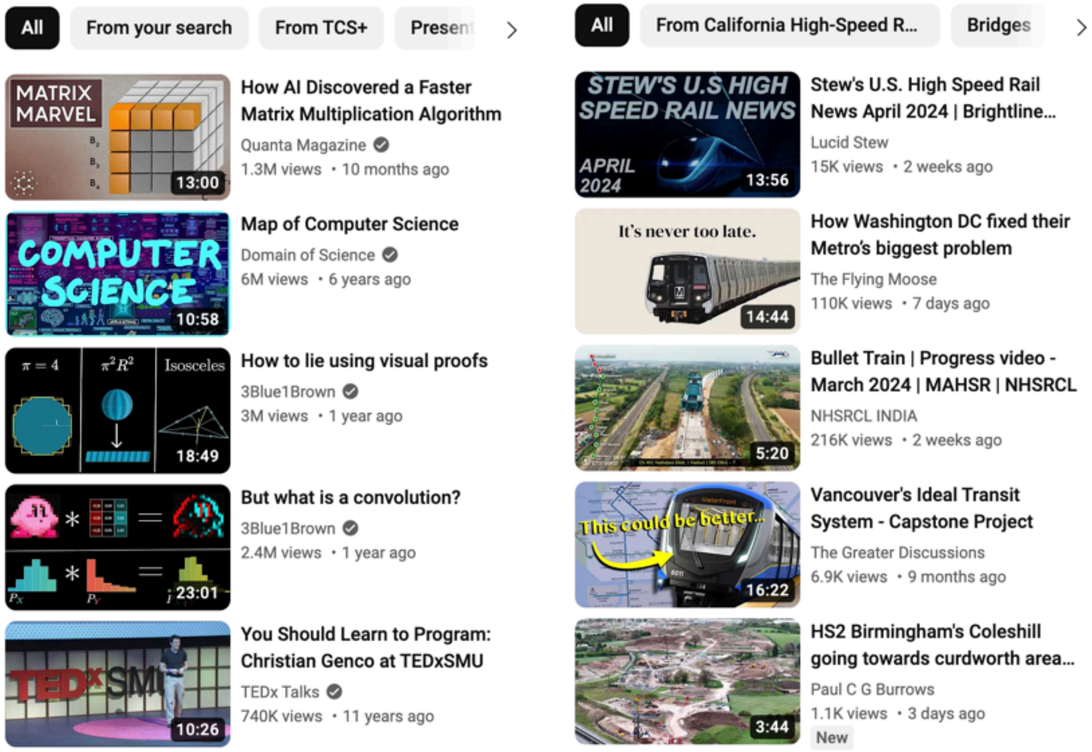
- Object recognition



What is machine learning?

Examples

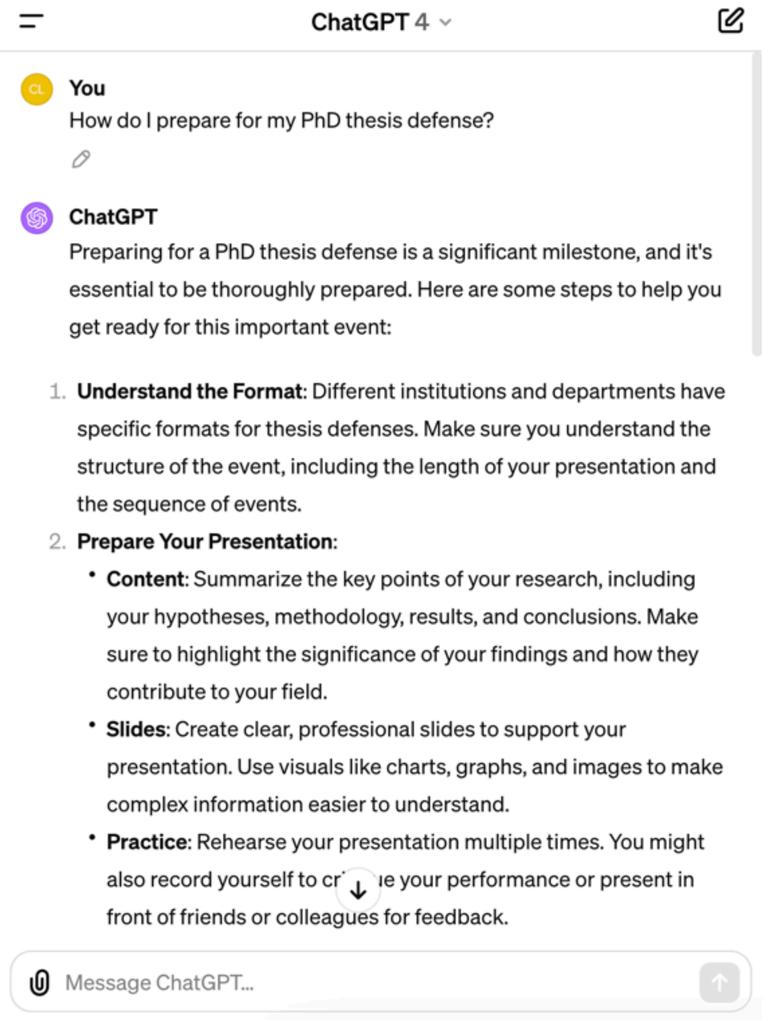
- Object recognition
- Content recommendation



What is machine learning?

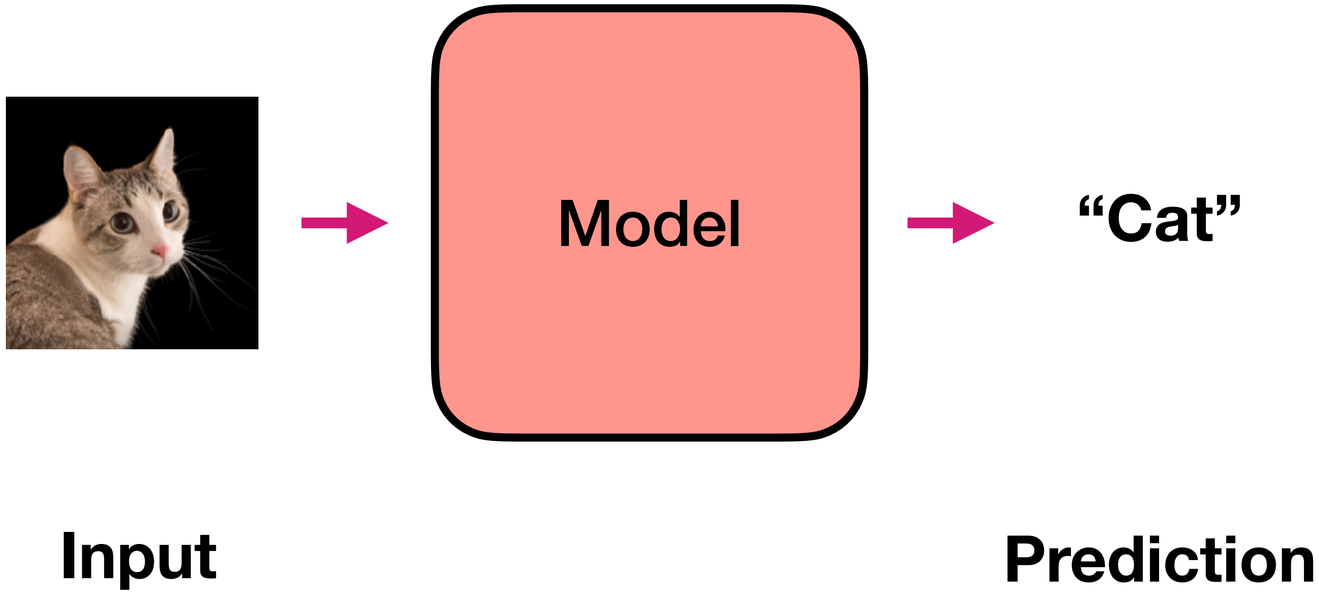
Examples

- Object recognition
- Content recommendation
- Large language models



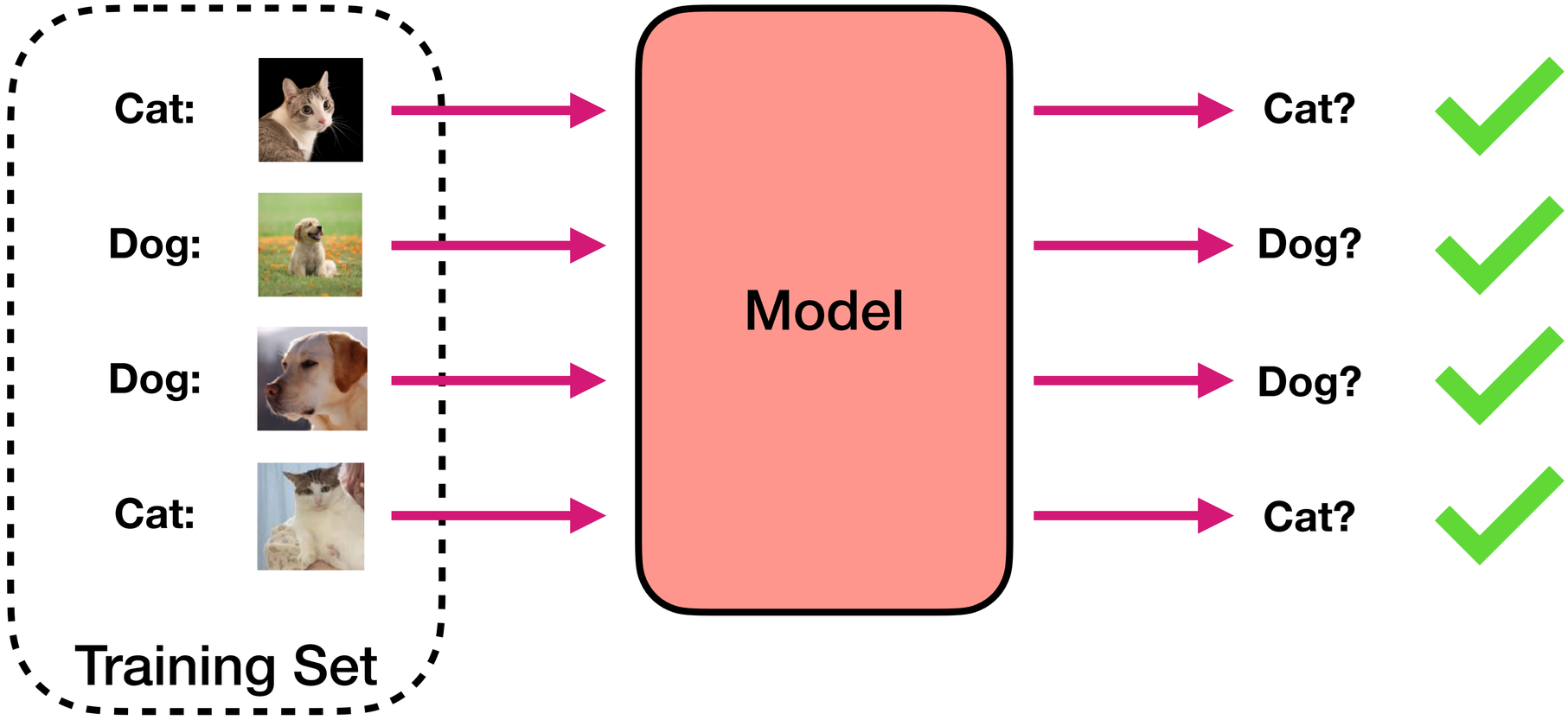
How does ML work?

Goal: Model that correctly maps inputs to labels.



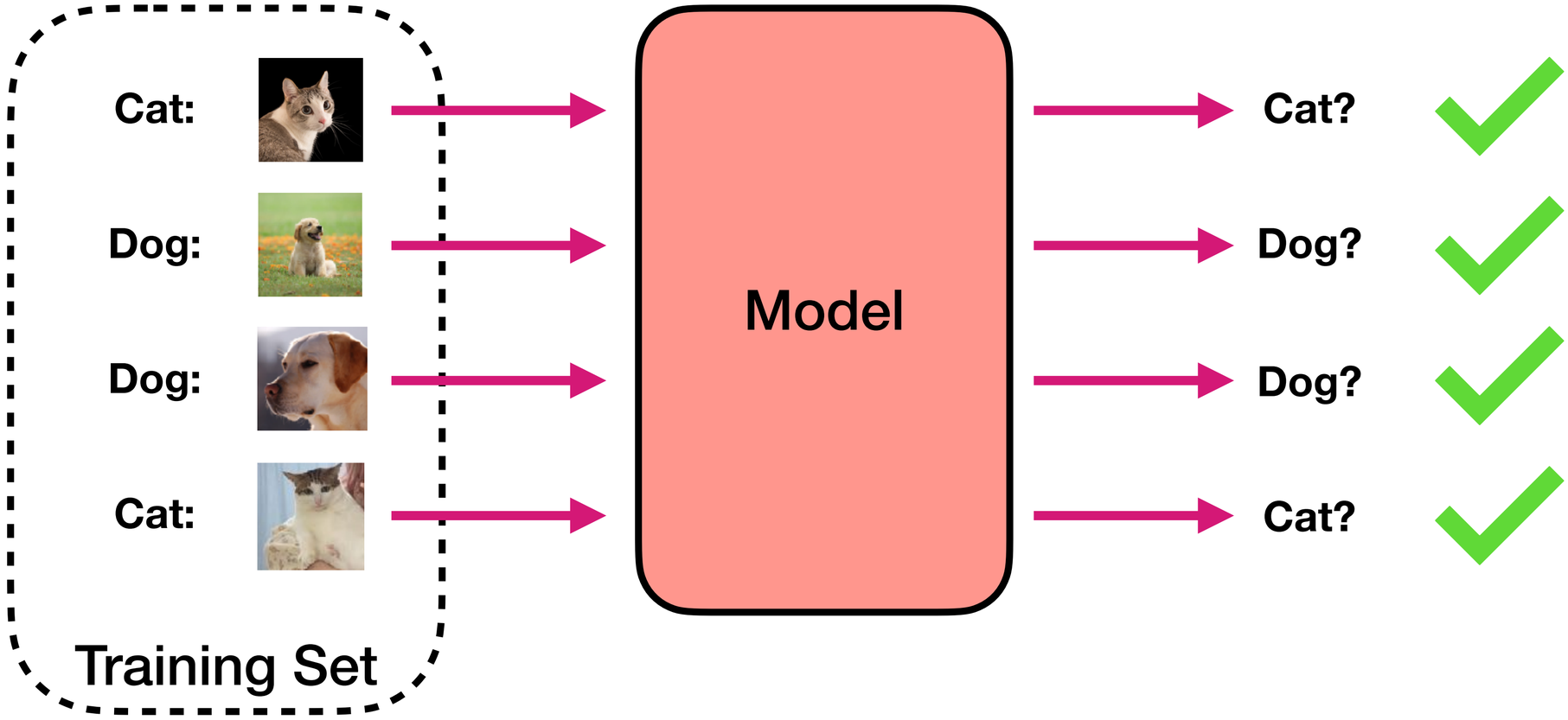
How does ML work?

Approach: Choose a model that correctly classifies training set.



How does ML work?

Challenge: How to find a “pixels to cat/dog” mathematical function?

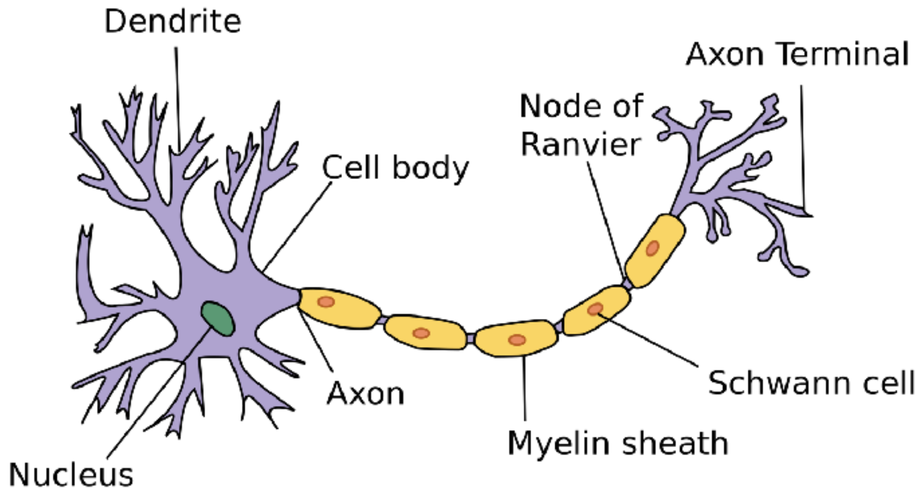


Neural network models

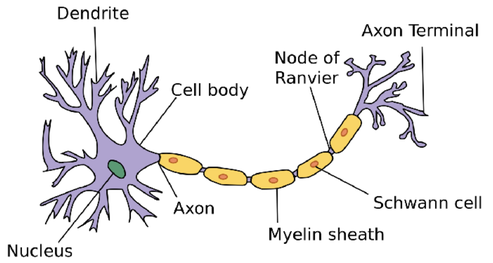
Model

A **neural network** f is a biologically inspired mathematical function.

An **architecture** $\mathscr{F}$ is a family of neural networks with similar structure.



Neural network models

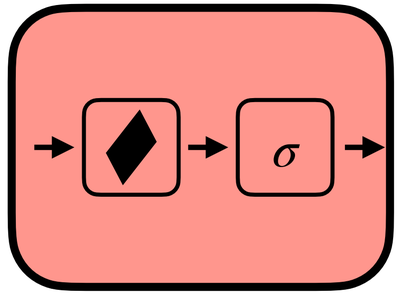


Model

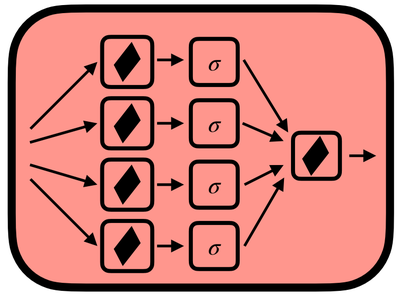
Architecture $\mathscr{F}$ of **networks** f.

Perceptron: $f(x) = \sigma(w^\mathsf{T} x + b)$.

- Parameters: w, b.
- Threshold activation $\sigma : \mathbb{R} \to \mathbb{R}$.

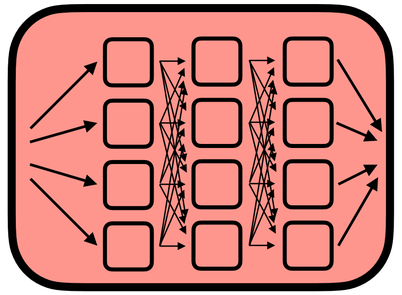


Two-layer perceptron: $f(x) = \sum_{i=1}^{m} u_i \sigma(w_i^\mathsf{T} x + b_i)$



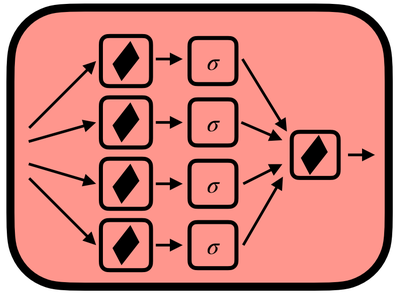
- Parameters: w, b, u.

Multi-layer perceptron:



Complete ML pipeline

1. Choose an architecture $\mathscr{F}$.



Complete ML pipeline

"Cat"

1. Choose an architecture $\mathscr{F}$.

2. Find network $f \in \mathscr{F}$ that fits labeled dataset $(x_1, y_1), \ldots, (x_n, y_n)$,
   i.e. choose f such that $f(x_i) \approx y_i$.

f

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Complete ML pipeline

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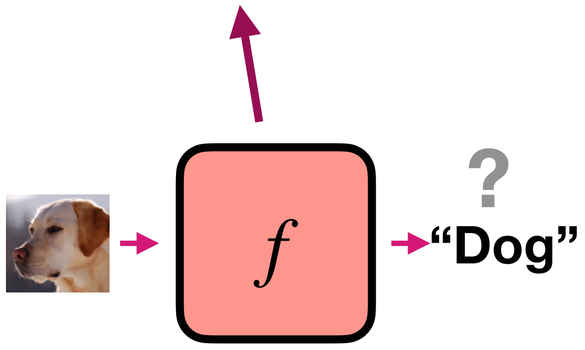
3. Deploy trained network f to new data, use $f(x_{\text{test}})$ as prediction.



Theoretical questions about ML

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   Is $\mathscr{F}$ expressive enough for the data? [**Representation**]

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   Can f be found efficiently? [**Optimization**]

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   Does high training accuracy mean high test accuracy? [**Generalization**]

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3. Deploy trained network f to new data, use $f(x_{\text{test}})$ as prediction.
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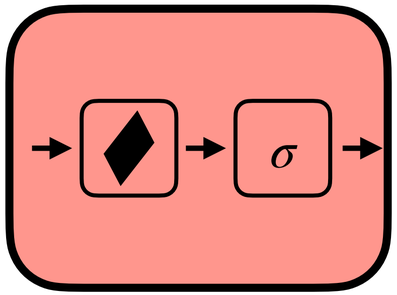
Vignette #0

Perceptron [Rosenblatt ’58]:

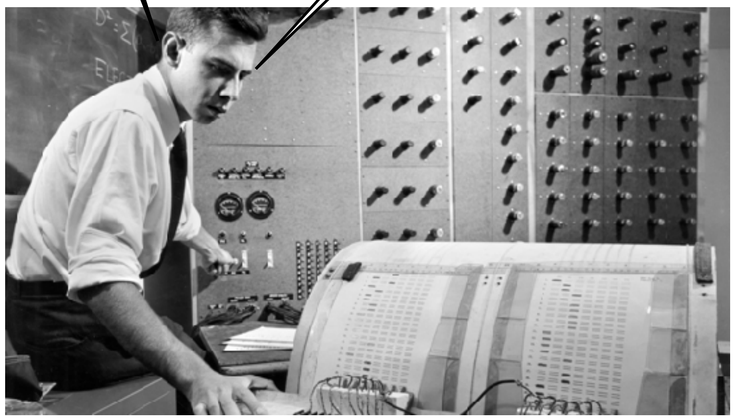
$$f(x) = \sigma(w^\top x + b).$$

- Parameters: w, b.
- Threshold activation $\sigma : \mathbb{R} \to \mathbb{R}$.



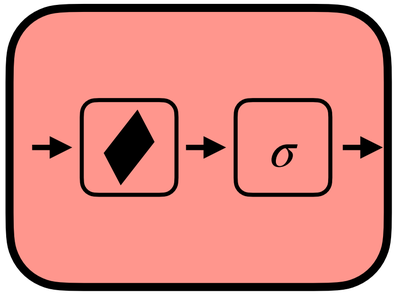
“walk, talk, see, write, reproduce itself and be conscious of its existence”

“learn, make decisions, and translate languages”



Frank Rosenblatt

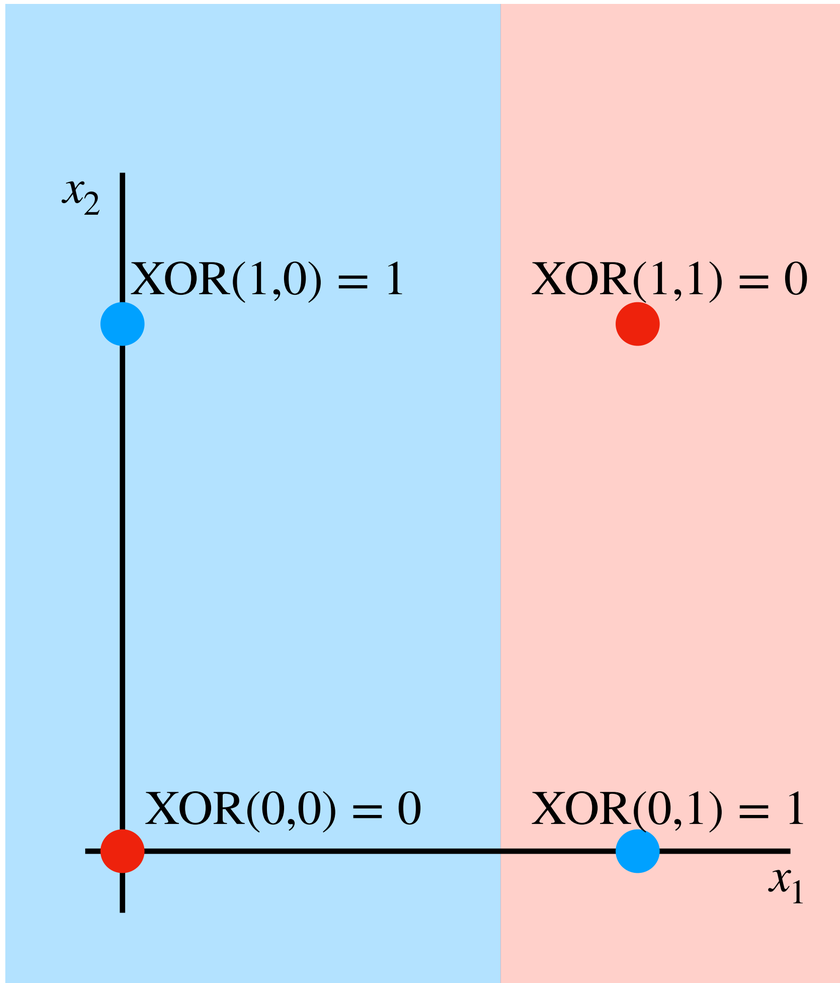
Vignette #0: Perceptrons



$$f(x) = \sigma(w^\top x + b).$$

Papert and Minsky ’69:

- Perceptrons only work for linearly separable data.
- **Negative result:** No Perceptron f_θ computes XOR.



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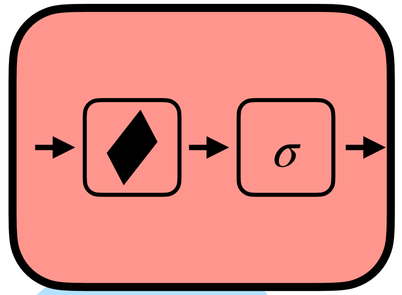

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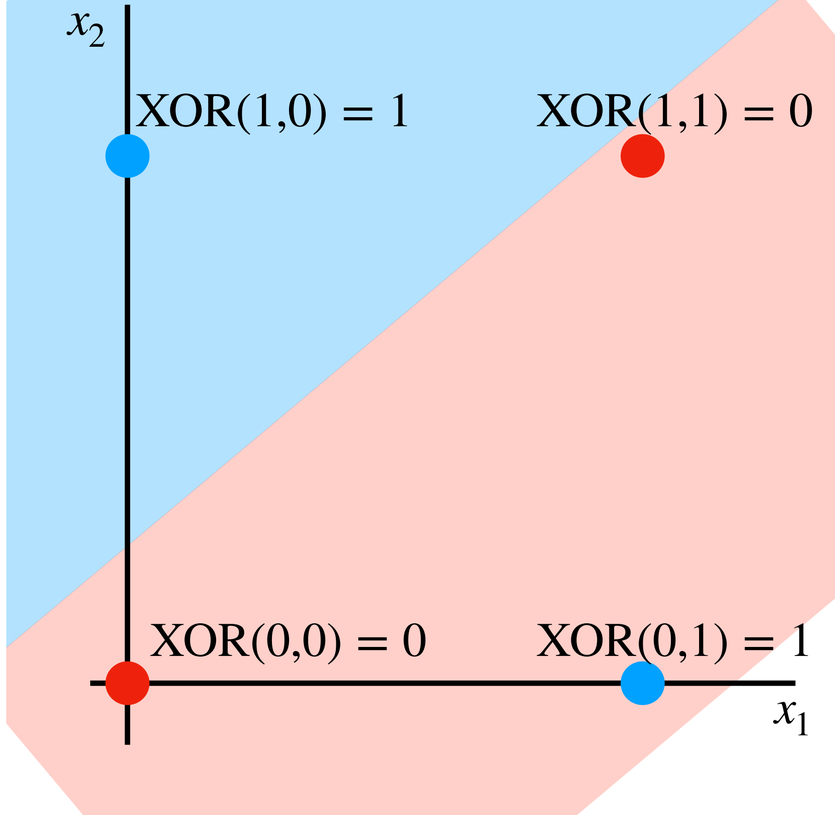

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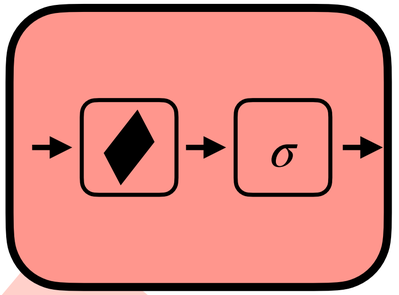

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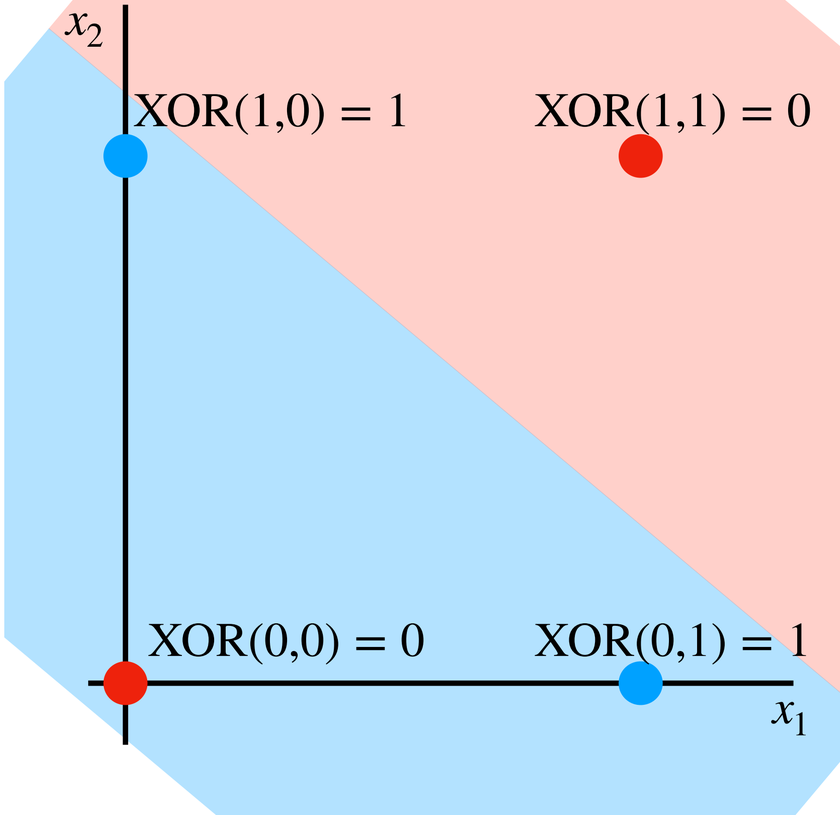
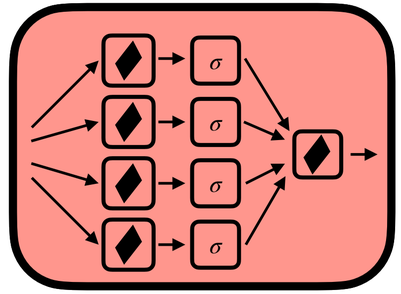
➡Fundamental limitation of Perceptron.



Universal Approximation Theorem

Funahashi et al; Hornik et al; Cybenko, ’89



Two-layer NN: $f(x) = \sum_{i=1}^{m} u_i \sigma(w_i^\top x + b_i)$

Positive result: For continuous $h : \mathbb{R}^d \to \mathbb{R}$, accuracy $\epsilon > 0$, and compact $\mathcal{X} \subset \mathbb{R}^d$, there exists a 2-layer network f with

$$\max_{x \in \mathcal{X}} |f(x) - h(x)| \leq \epsilon \,.$$

[+] Rules out impossible XOR-like targets for neural networks of depth at least 2.

[-] No optimization guarantees—how do you find it?

[-] No size guarantees—how large is the width m?

Thesis questions

Positive results:
Which tasks can an architecture **efficiently** solve?

Negative results:
Which tasks **cannot** be efficiently solved by an architecture?

Contrasts:
Which tasks distinguish the powers of two architectures?

Dissertation chapters

1. 2-layer random feature NNs
   [Hsu, **S**, Servedio, Vlatakis-Gkaragkounis ‘21]

2. Shallow vs deep NNs
   [**S**, Chatziafratis ’22]

3. 2-layer regularized NNs
   [Ardeshir, Hsu, **S** ’23]

4. Single-layer transformers
   [**S**, Hsu, Telgarsky ’23]

5. Multi-layer transformers
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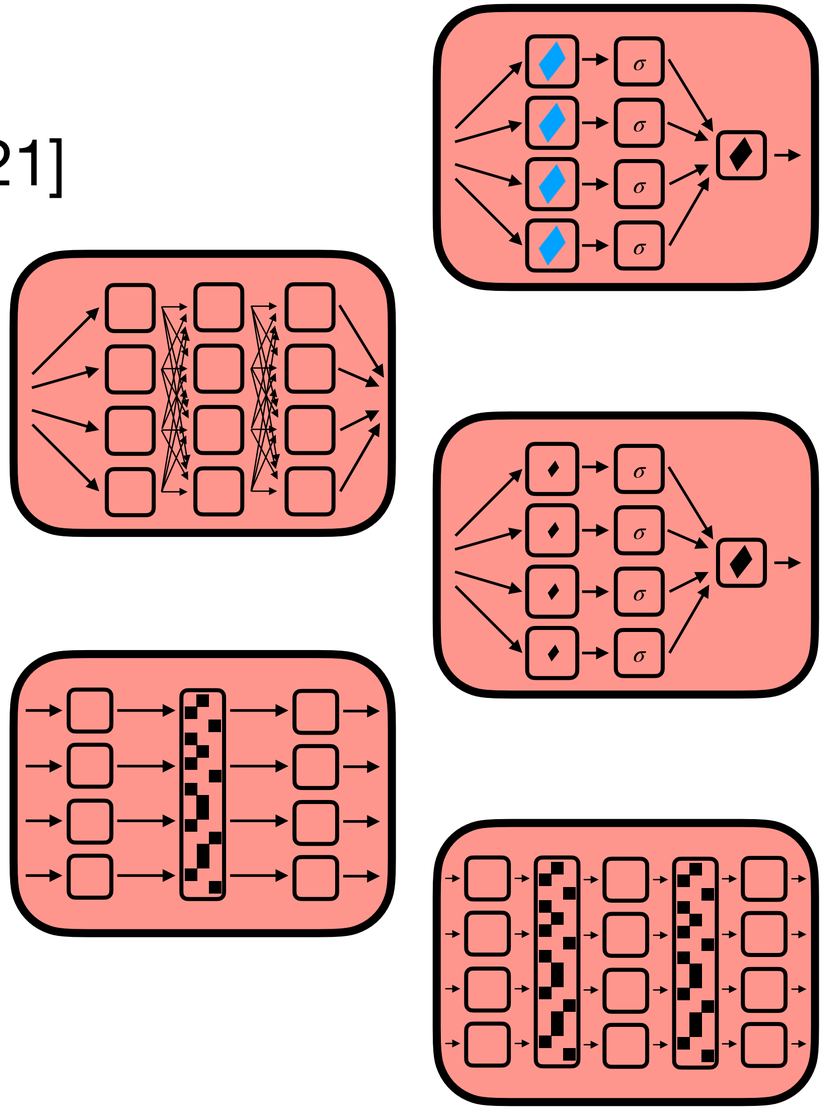

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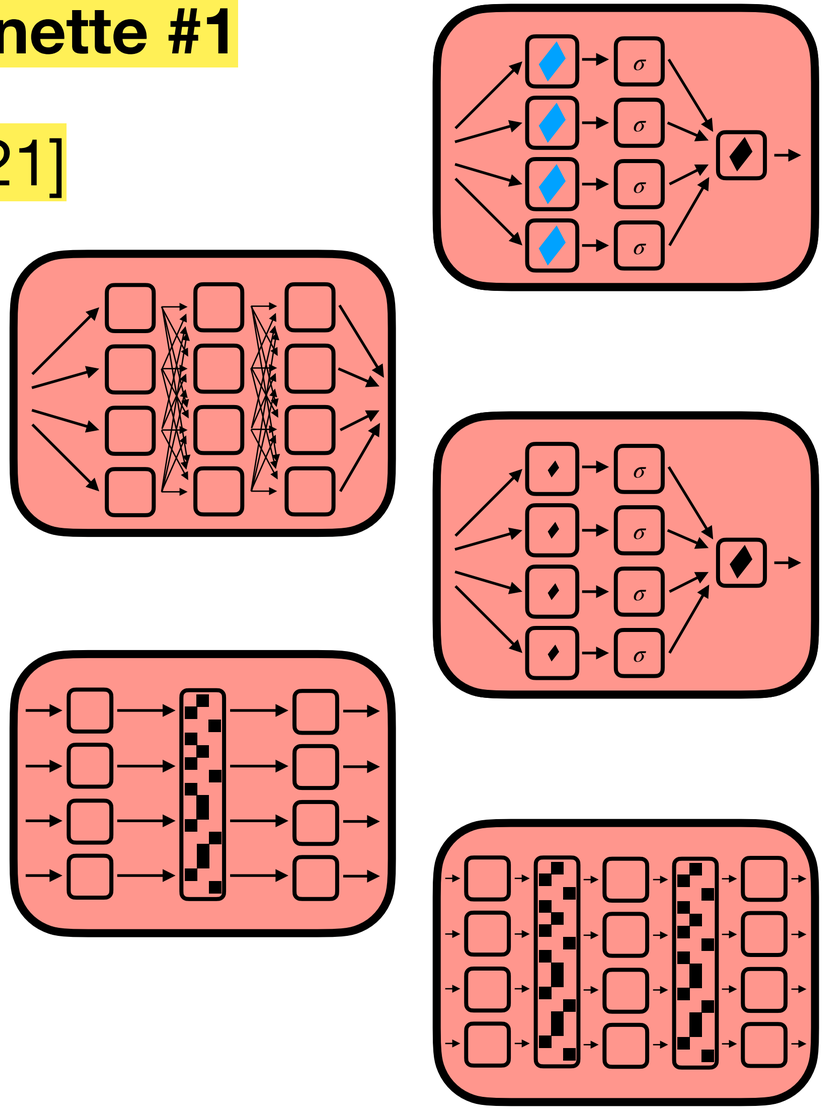

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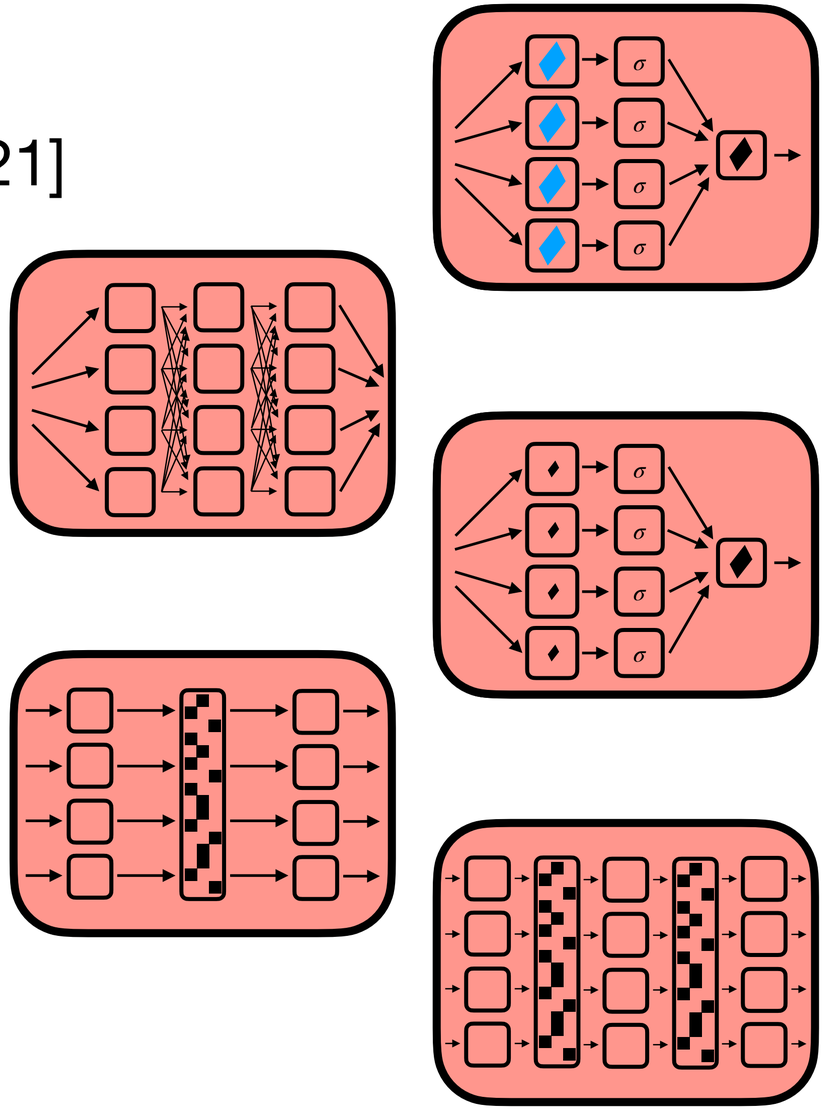
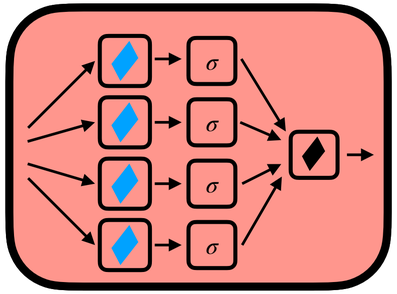
Vignette #2

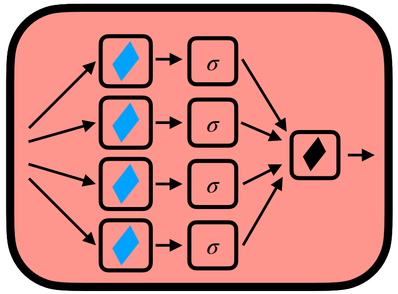




Vignette #1:
Random Feature Models

Two-layer random feature models (RFMs)

Architecture: $f(x) = \sum_{i=1}^{m} u_i \sigma(\mathbf{w}_i^\top x + \mathbf{b}_i).$



- Bottom-layer weights fixed, sampled at random: $(\mathbf{w}_i, \mathbf{b}_i) \sim \mathscr{P}$.
- Top-layer weights $u = (u_1, \ldots, u_m)$ chosen based on $(\mathbf{w}, \mathbf{b})$.

Questions:

- Representational capabilities and limitations of RFMs?
- Comparison with standard 2-layer NNs?

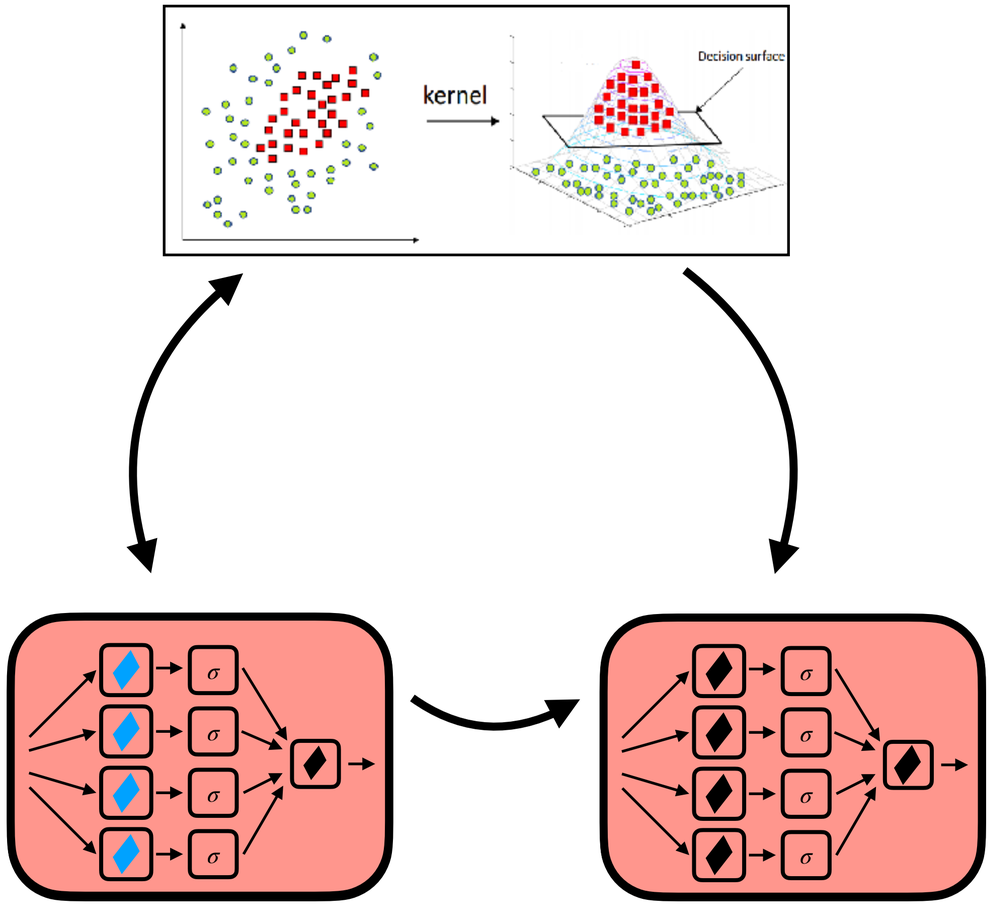
RFMs, kernels, and neural networks

Motivating question: Can neural networks be accurately analyzed as kernel machines?

- Wish: Obtain NN optimization and generalization guarantees from kernels.

Connections:

- RFMs are NNs.
- Kernel machines are approximable by RFMs [Rahimi, Recht ’07].
- Certain NN initializations train like kernels (NTK) [Jacot, et al ’19].



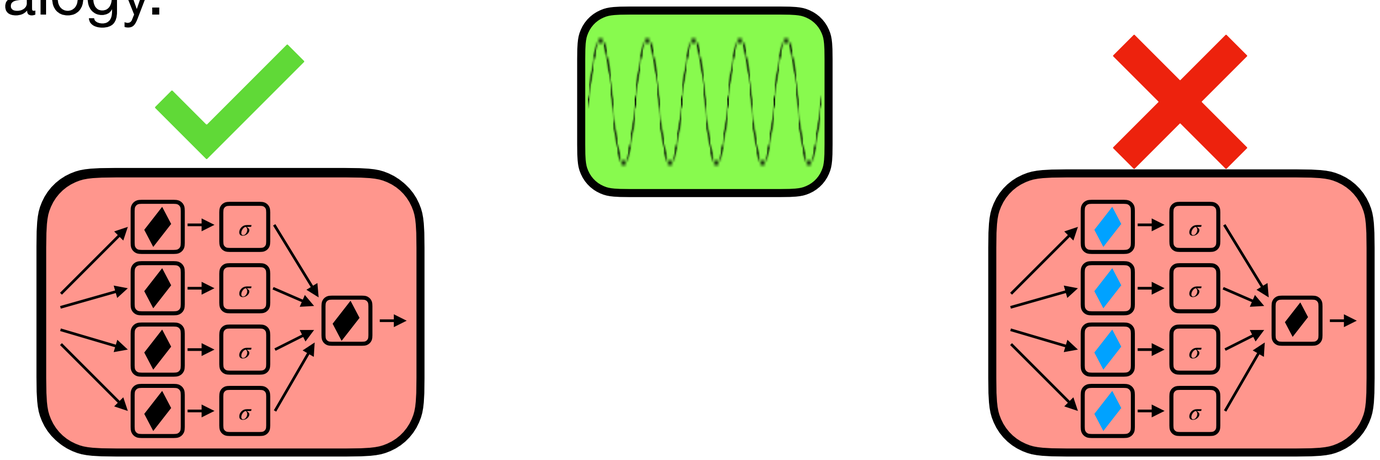
Contributions

1. **Positive result:**
   RFMs (and two-layer NNs) can approximate low-dimensional or smooth targets.

2. **Negative result:**
   RFMs cannot approximate high-dimensional “jagged” targets.

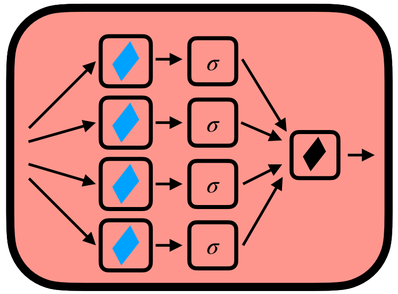
3. **Contrast:**
   Sinusoidal targets are efficiently approximable by NNs, but not by RFMs.

   ➡Flaw in NN-kernel analogy.



Theoretical results

Two-layer RFM: $f(x) = \sum_{i=1}^{m} u_i \sigma(\mathbf{w}_i^\top x + \mathbf{b}_i)$.



- h is L-**Lipschitz** if $|h(x) - h(x')| \leq L\|x - x'\|_2$.

Theorem: The minimum width m of an RFM f needed to approximate any d-dimensional L-Lipschitz target satisfies:

$$m = \min\{d^{\Theta(L^2)}, L^{\Theta(d)}\}$$

- **Theoretical significance**: First nearly-tight results for all choices of L and d.

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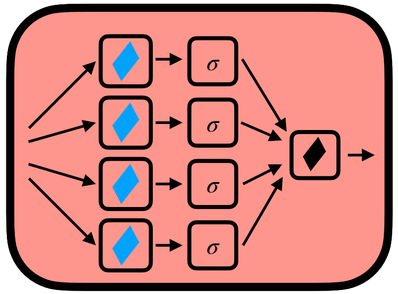
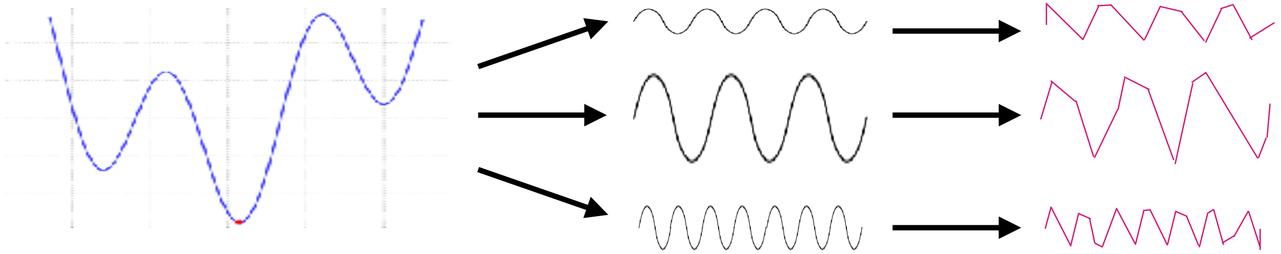


- h is L-**Lipschitz** if $|h(x) - h(x')| \leq L\|x - x'\|_2$.

Theorem [positive]: There exists a width-m RFM f that approximates any d-dimensional L-Lipschitz target h when:

$$m \leq \min\{d^{O(L^2)}, L^{O(d)}\}$$

Proof idea: Approx. h with sinusoids, approx. sinusoids with random neurons.



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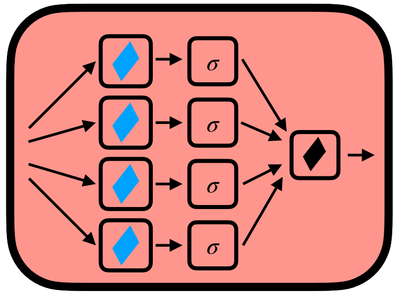


- h is L-**Lipschitz** if $|h(x) - h(x')| \leq L\|x - x'\|_2$.

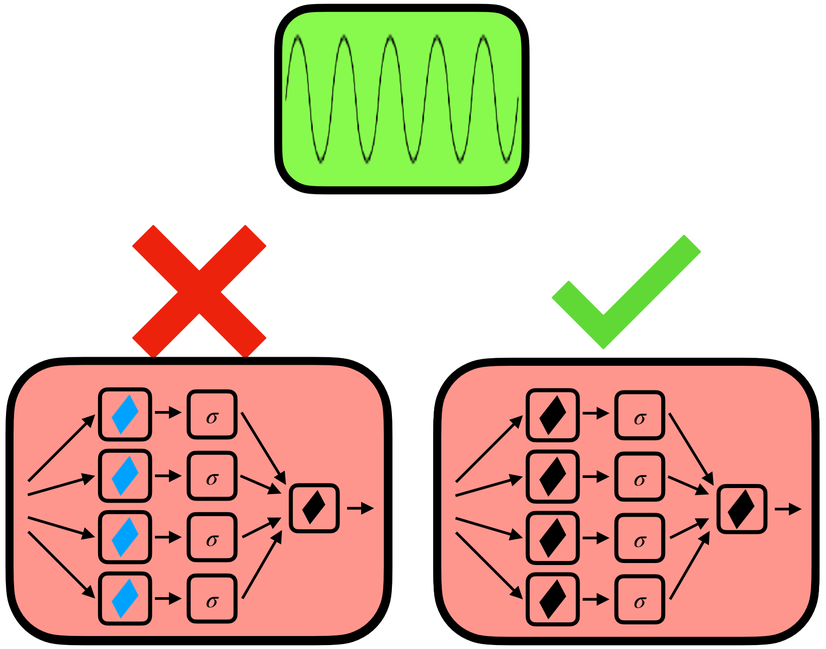
Theorem [negative]: For d-dimensional L-Lipschitz target h, every width-m RFM f that approximates it has:

$$m \geq \min\{d^{\Omega(L^2)}, L^{\Omega(d)}\}$$

Proof idea: Kernel-based dimensionality argument.

Separation with 2-layer NNs

Contrast: Sinusoidal target $h(x) = \sin(\sqrt{d} v^\top x)$.



- All RFMs that approximate h have large width: $m = \exp(d)$].
- But, 2-layer NN can approximate h with small width: $m = \mathrm{poly}(d)$.

Implication: NNs can represent “simple” targets; RFMs cannot.

- Similar optimization conclusions [e.g. Damian, Lee, Soltanolkotabi ’22].

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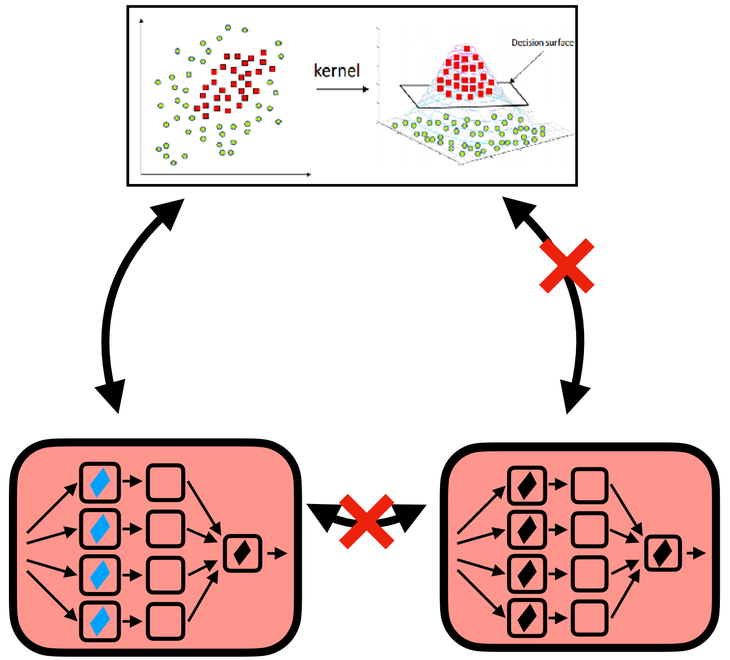

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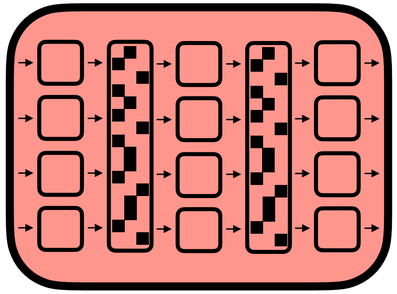
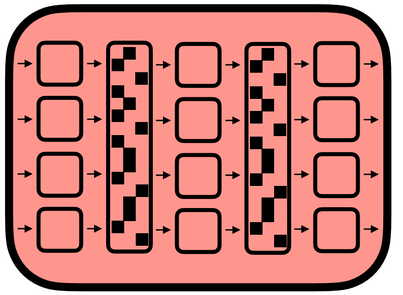
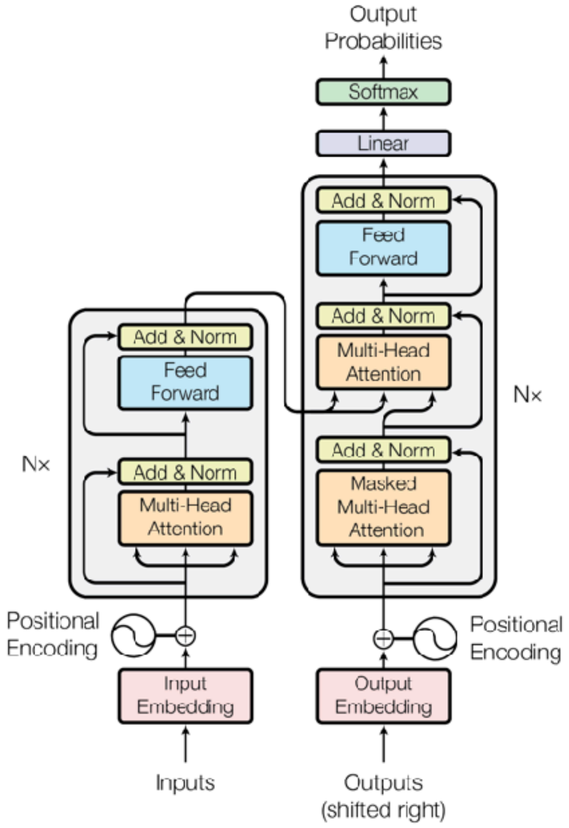


Vignette #2: Transformers and Sequential Architectures

Transformer architecture

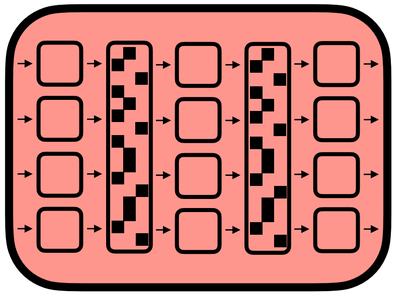


- Backbone of modern large language models.
- **Sequence-to-sequence** architecture.
  - Sequence length $N \gg$ embedding dim m.
  - Large sequence length N in practice:
    32K GPT-4, 100K Claude, 1M Gemini.



Vaswani et al ‘17

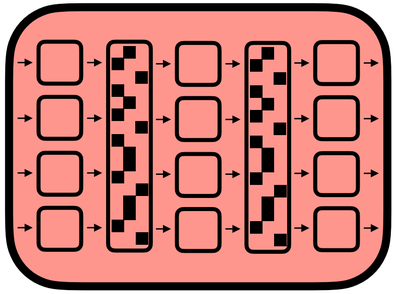
Motivating questions

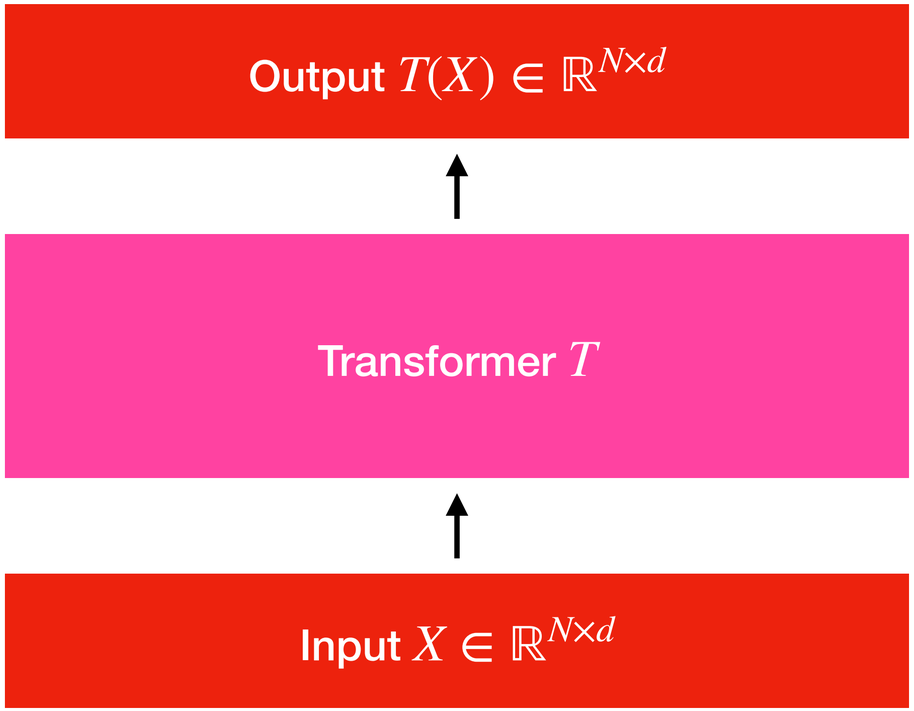


1. Are RNNs and “shortcut transformers” as powerful as standard transformers?

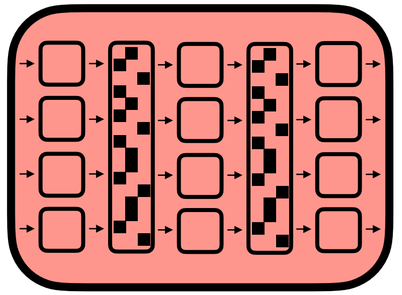
2. How to scale transformers (width and depth)?

Transformer architecture





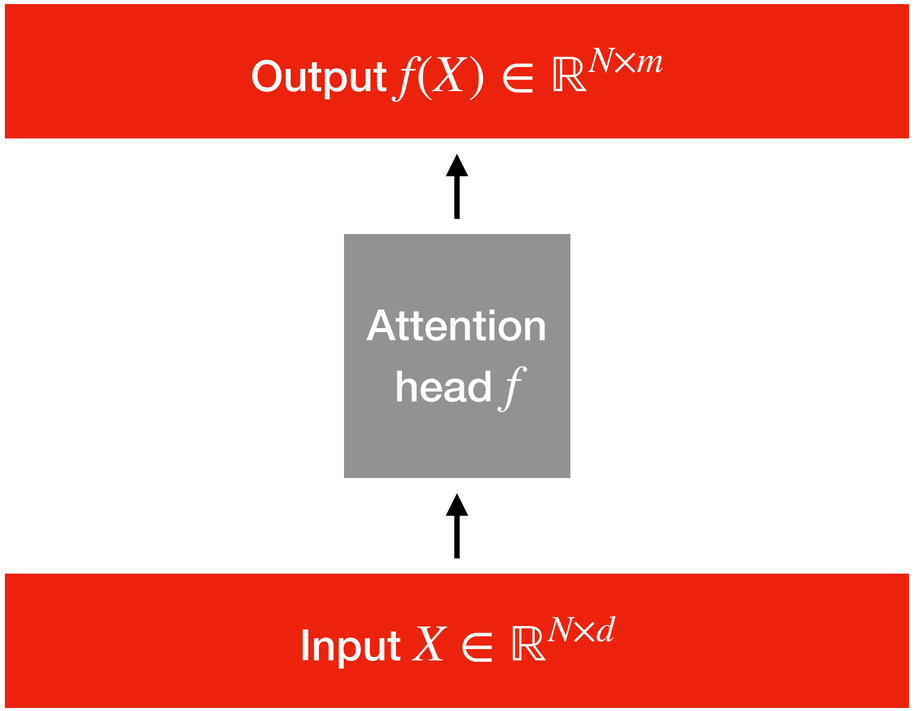
Transformer architecture



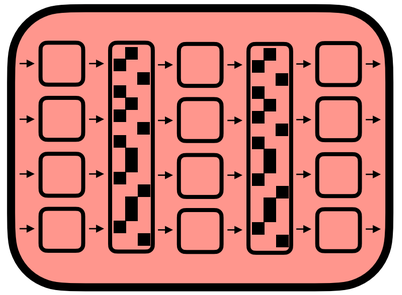
Attention head:

$f(X) = \text{softmax}(XQK^TX^T)XV.$

Parameters: $Q, K, V \in \mathbb{R}^{d \times m}$.



Transformer architecture



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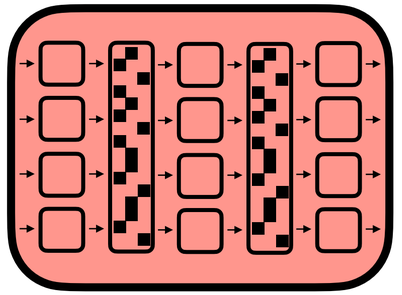
$$f(X) = \underbrace{\text{softmax}\left(\underbrace{XQ}_{\mathbb{R}^{N\times m}} \times \underbrace{K^TX^T}_{\mathbb{R}^{N\times m}} \right)}_{=} \times \underbrace{XV}_{\mathbb{R}^{N\times m}}$$

$$= \underbrace{\text{softmax}(XQK^TX^T)}_{\mathbb{R}^{N\times N}} \times \underbrace{XV}_{\mathbb{R}^{N\times m}}$$

N^2 time!

Transformer architecture



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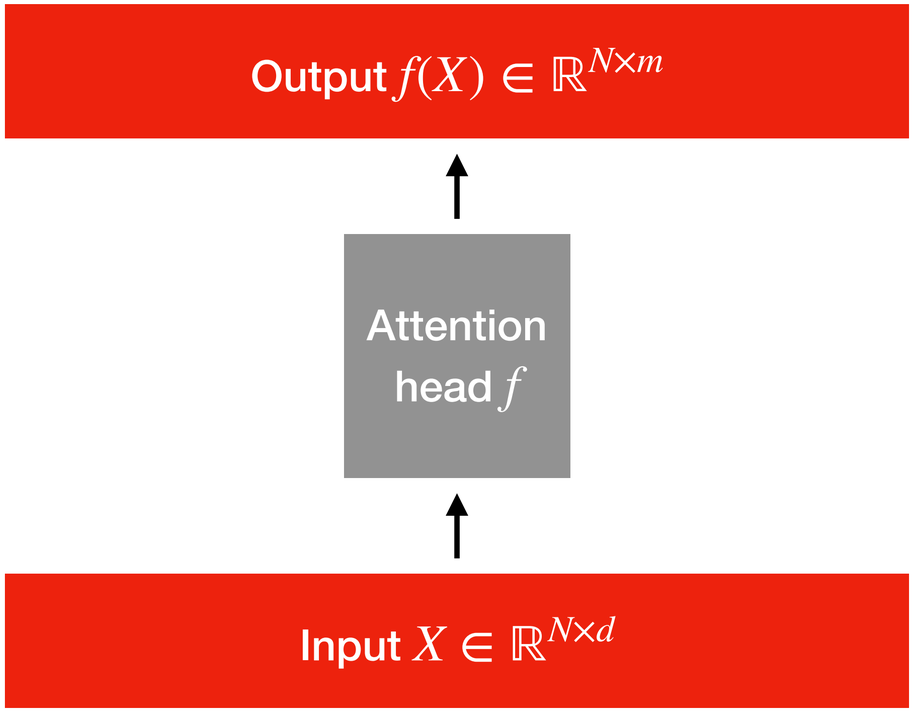
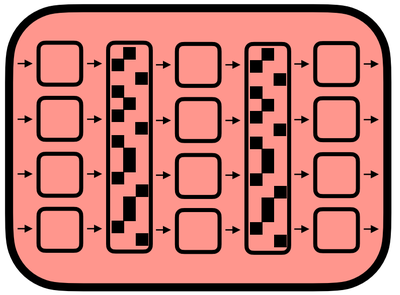


Transformer architecture



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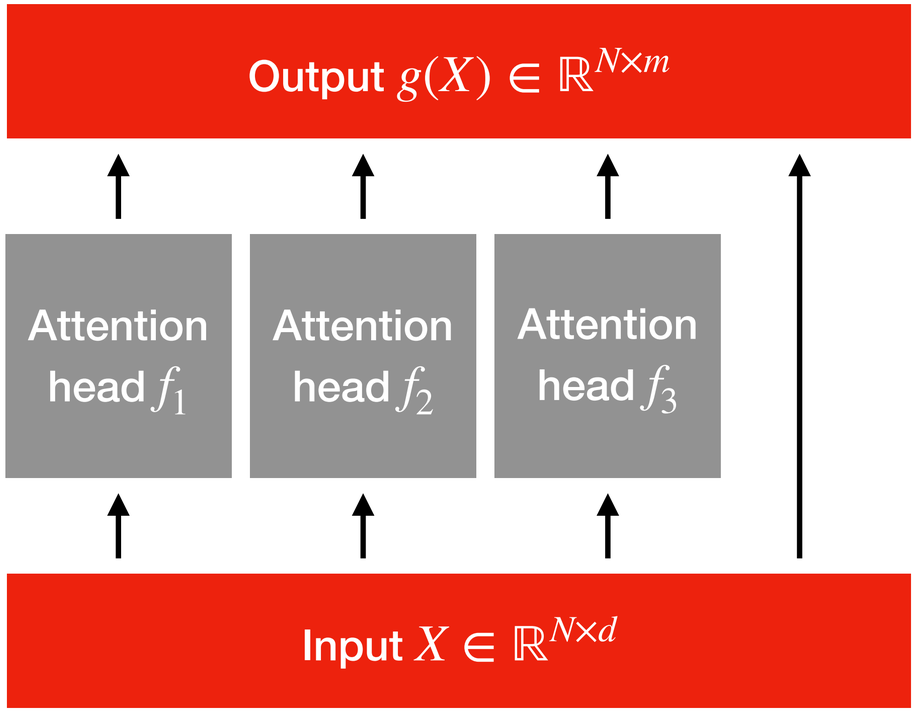
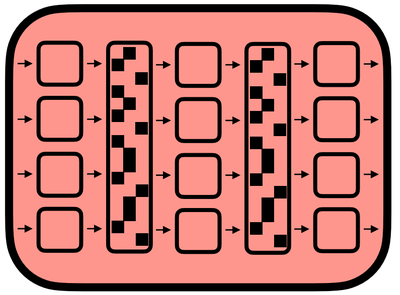
Multi-headed attention:

$$g(X) = X + \sum_{h=1}^{H} f_h(X).$$



Transformer architecture



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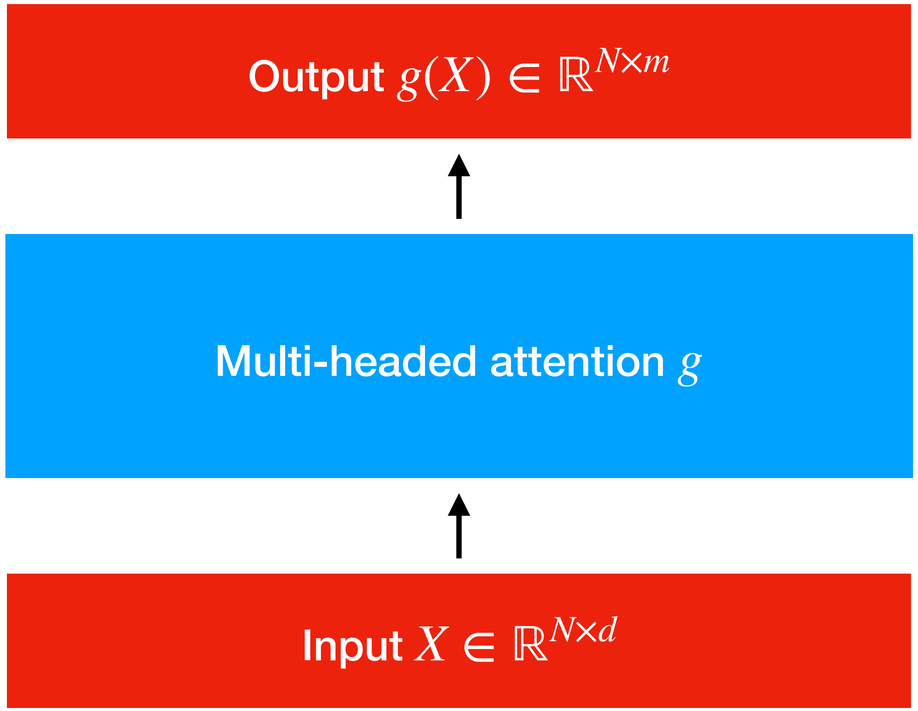
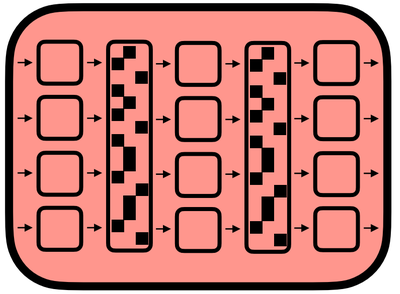
Element-wise multi-layer perceptron (MLP):

$\phi(X) = (\phi(x_1), \ldots, \phi(x_N))$.



Transformer architecture



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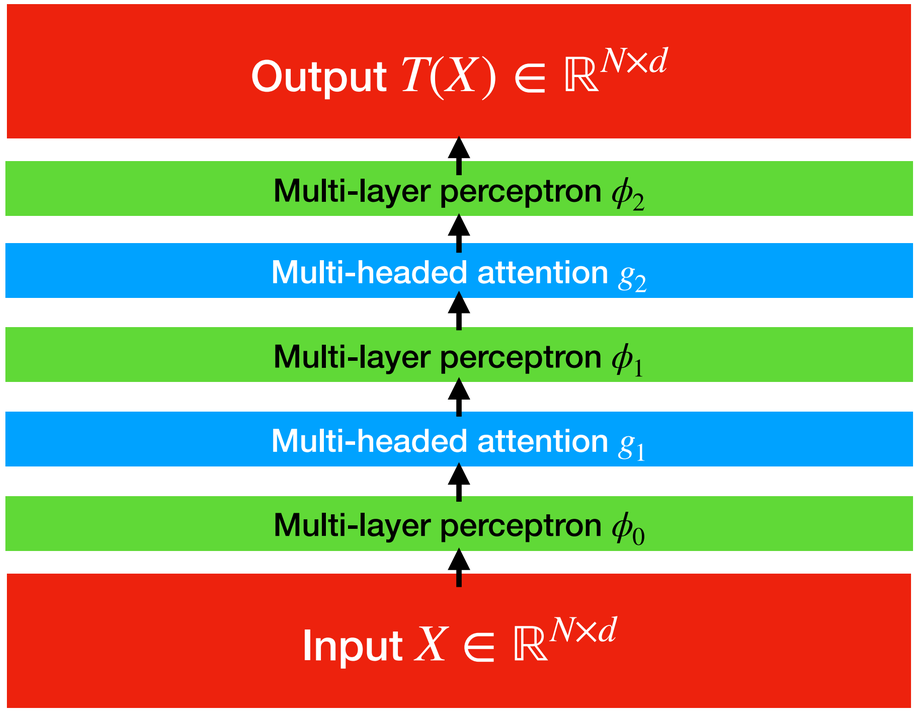
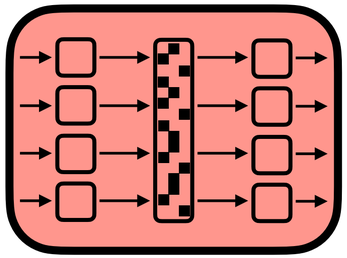
Full transformer:

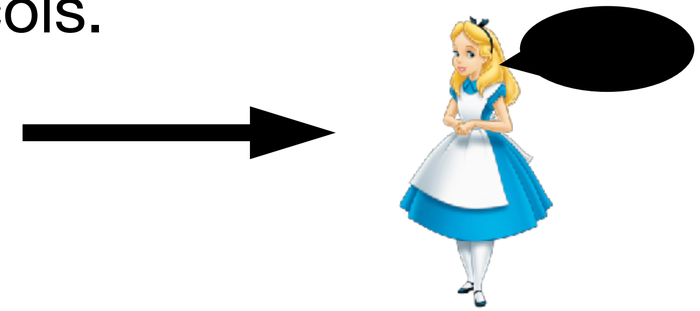
$T(X) = (\phi_L \circ g_L \circ \ldots \circ g_1 \circ \phi_0)(X).$

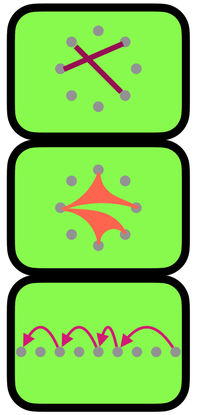


Transformers and communication

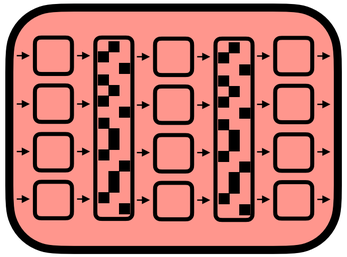
Relationship #1: 1-layer m-width transformers are m-bit Alice-Bob communication protocols.

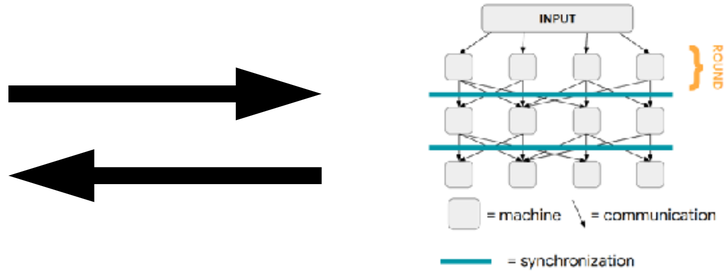


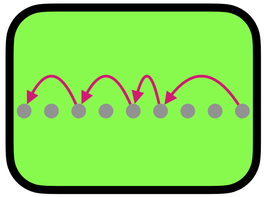




Relationship #2: L-layer m-width transformers are L-round Massively Parallel Computation (MPC) protocols with m local memory,



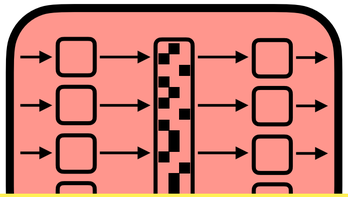


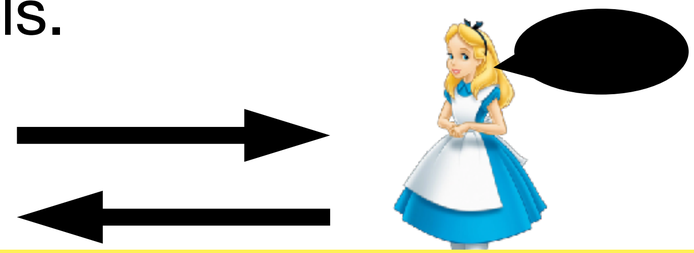


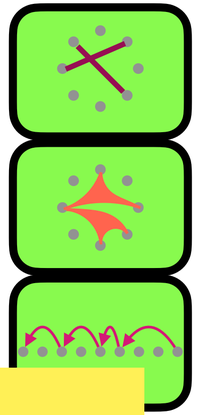
Contributions

Connections between transformers and distributed computational models.

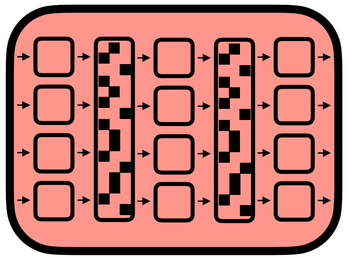
Relationship #1: 1-layer m-width transformers are m-bit Alice-Bob communication protocols.

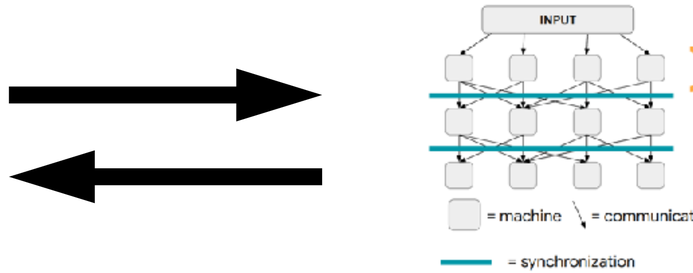


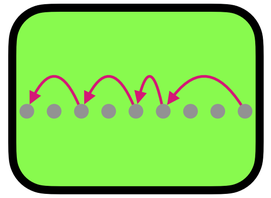




Relationship #2: L-layer m-width transformers are L-round Massively Parallel Computation (MPC) protocols with m local memory,



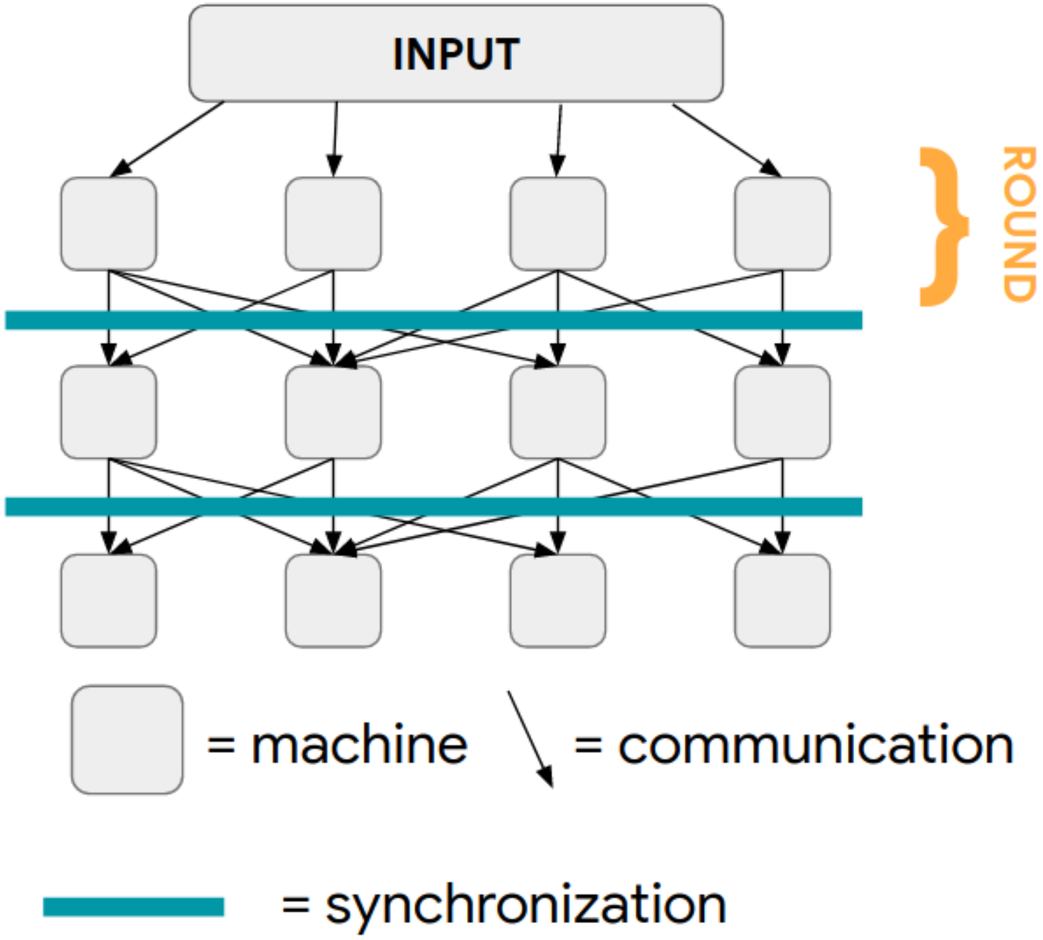




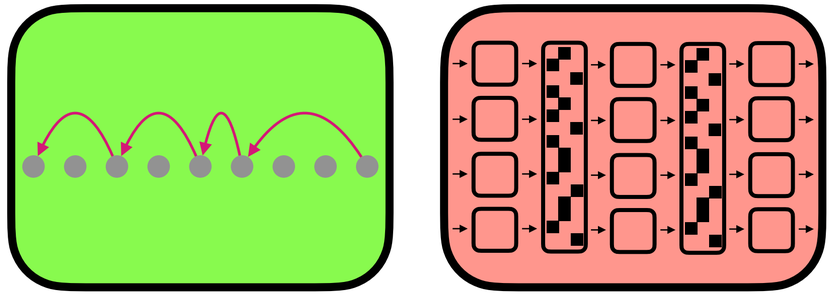
Massively Parallel Computation model (MPC)

Computational model of MapReduce

- Input divided among q machines with local memory s.
- Round $r = 1, \ldots, R$:
  - Each machine performs computations on local memory.
  - Each machine sends and receives $\leq s$ bits of information.



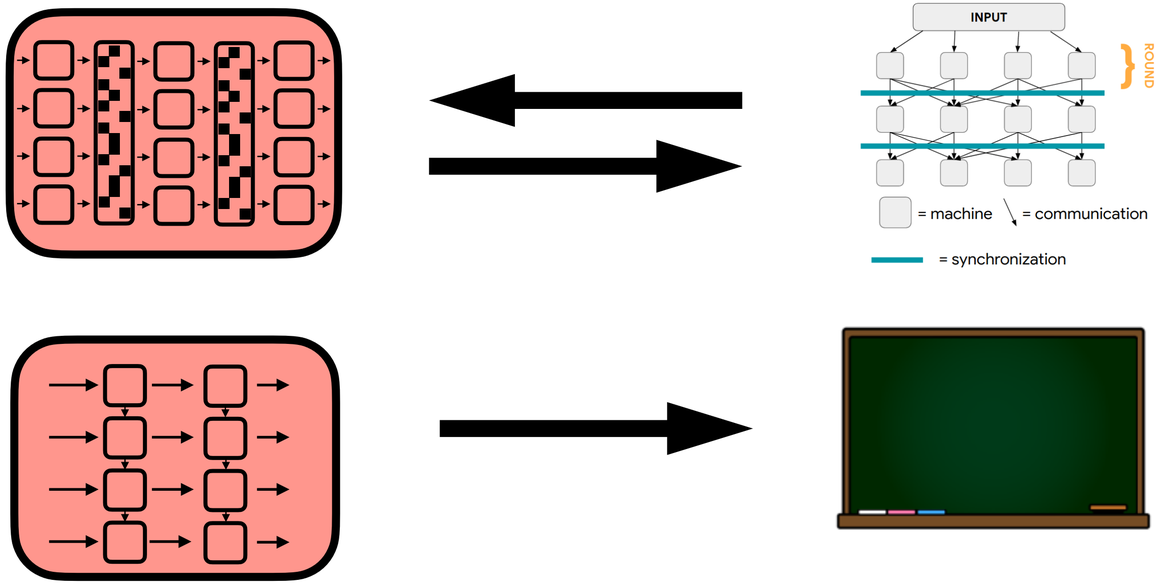
Transformers and distributed computing



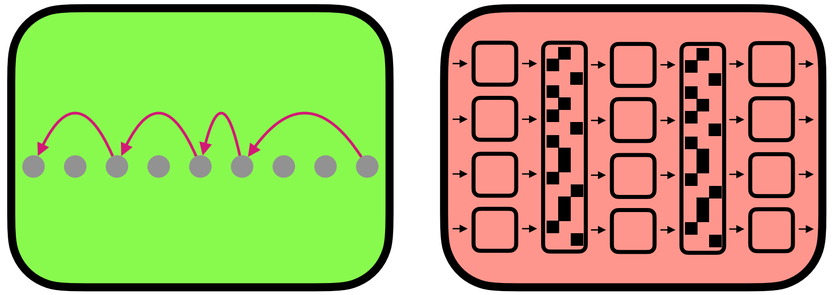
Broader equivalences

- Transformers can simulate MPC algorithms.
- MPC algorithms can simulate transformers.
- Serial blackboard model can simulate alternative models (RNNs, sub-quadratic transformers).

➡Alternatives are not parallelizable!



Depth separation (1 vs 2)



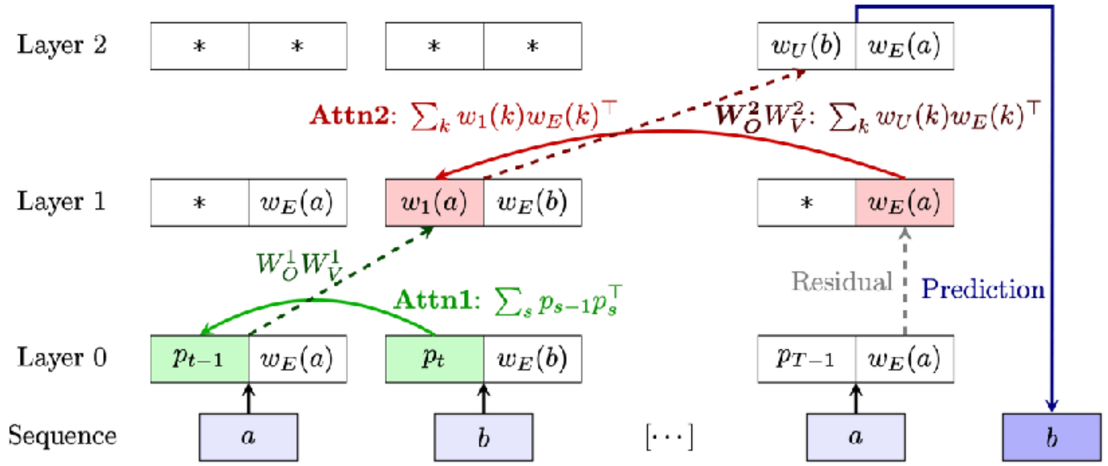
Induction Heads: Most recent bigram match.

$$\mathrm{IH}(\ldots ab \ldots a)_N = b$$

Positive result [Bietti, et al ’23]:
A 2-layer transformer efficiently solves IH.

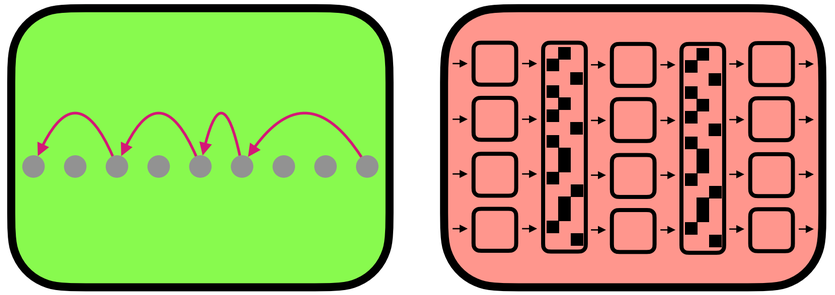
Negative result:
1-layer transformers that solve IH
have width $m \geq N^{\Omega(1)}$.

- Proof idea: Communication complexity



[Bietti, et al ’23]

Depth separation ($\log k$)

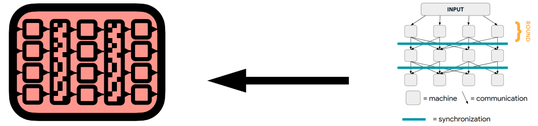


k-**Induction Heads**: Composition of IH.

$$k\text{-IH}(\ldots a_k a_{k+1} \ldots a_{k-1} a_k \ldots\ldots a_2 a_3 \ldots a_1 a_2 \ldots a_1) = a_{k+1}$$

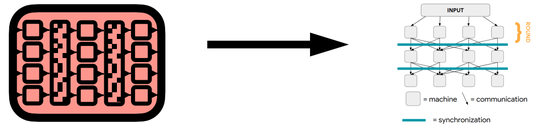
Positive result: A transformer efficiently solves k-IH and has depth $L \leq O(\log k)$.

- Proof idea: MPC algorithm that combines partial solutions.



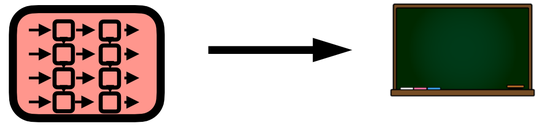
Negative result: Transformers that efficiently solve k-IH have depth $L \geq \Omega(\log k)$.

- Proof idea: MPC cycle identification lower bound conjecture.

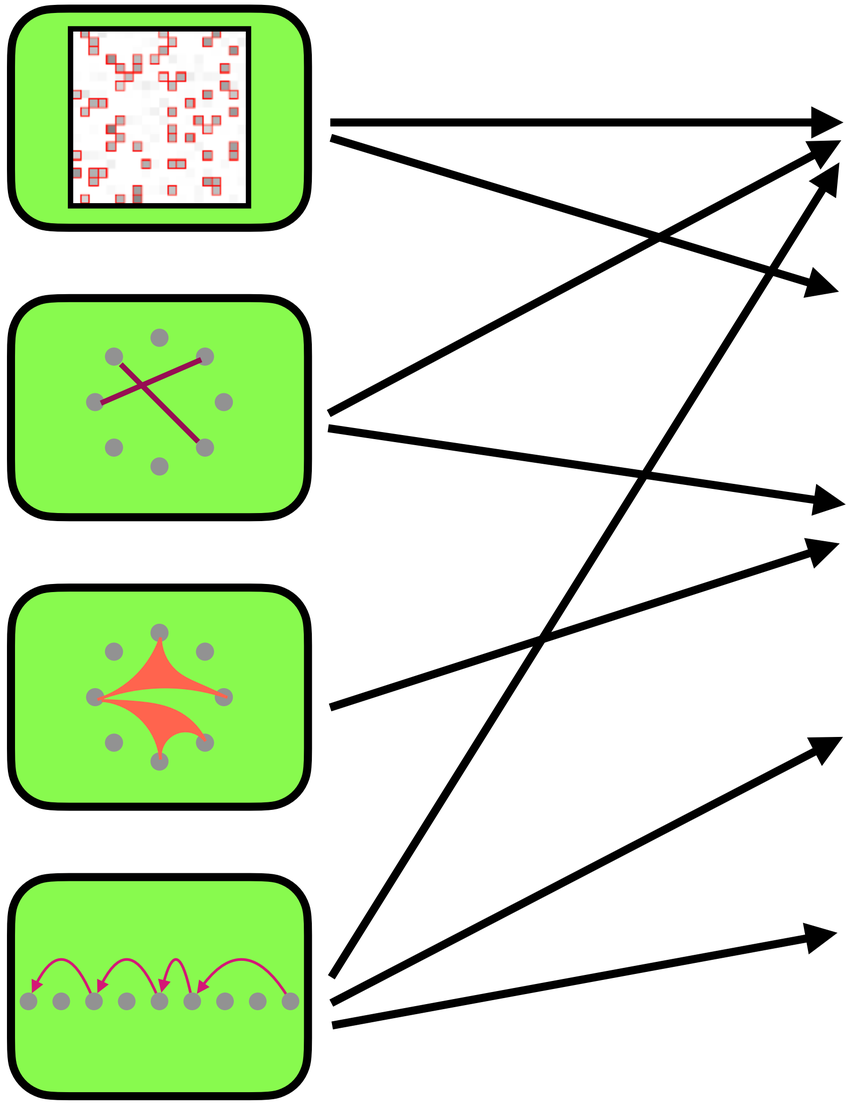


Contrast: RNNs and sub-quad. transformers that efficiently solve k-IH have depth $L \geq k$.

- Proof idea: Pointer chasing communication lower bounds.



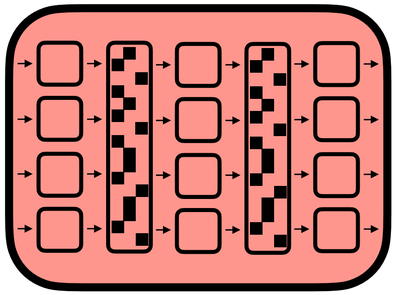
Tasks



Takeaways

Transformers vs RNNs/ sub-quadratic separations	Contrast
Expressivity of embedding dimension m	Positive result Negative result
Transformer layers are inherently pairwise	Negative result Contrast
Expressivity of depth L	Positive result Negative result
Efficient computation of compositional tasks	Positive result

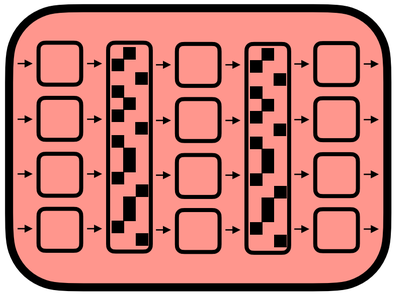
Implications



1. Are RNNs and sub-quadratic models as powerful as standard transformers?

2. How to scale transformers (width and depth)?

Implications



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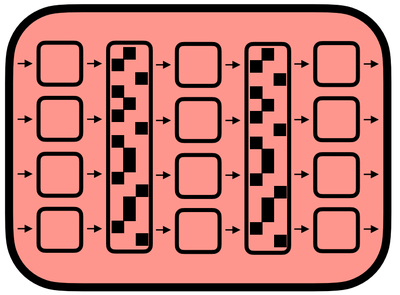

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   No, evidenced by parallel and pointer chasing (k-IH) algorithms.

2. How to scale transformers (width and depth)?
   Communication/distributed computing bounds on both.

Recap

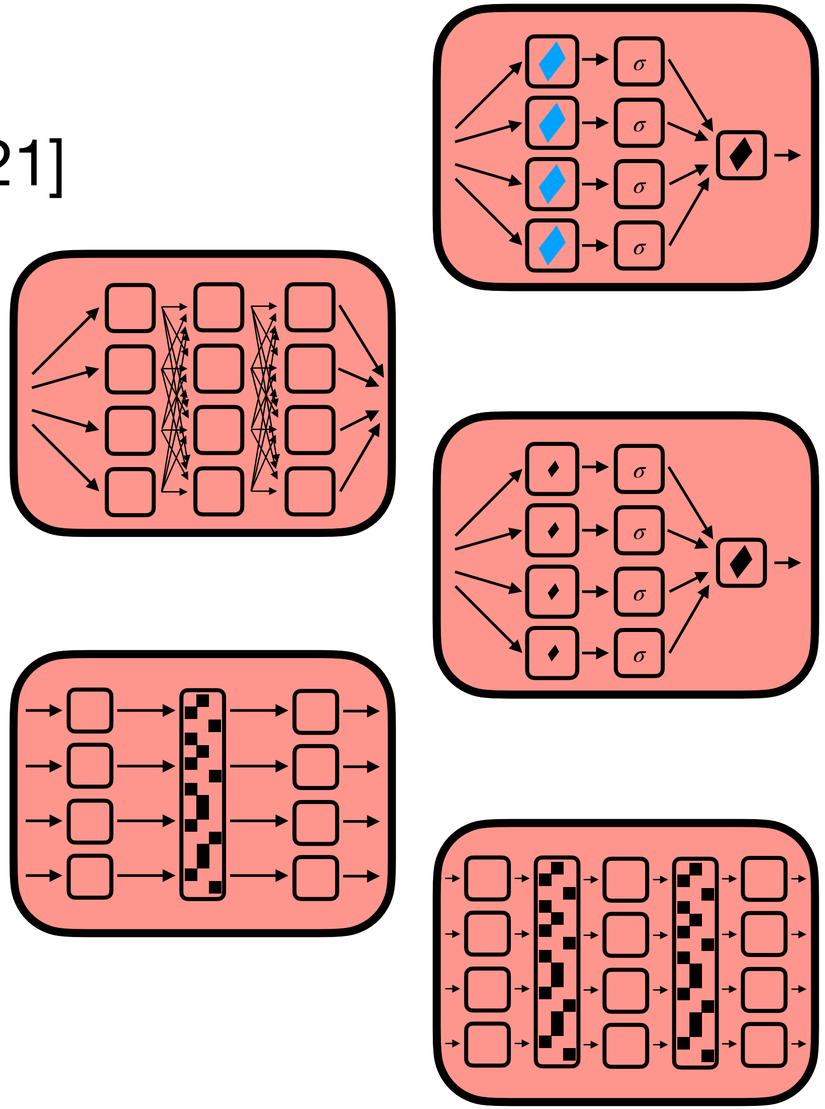
1. 2-layer random feature NNs
   [Hsu, **S**, Servedio, Vlatakis-Gkaragkounis ‘21]

2. Shallow vs deep NNs
   [**S**, Chatziafratis ’22]

3. 2-layer regularized NNs
   [Ardeshir, Hsu, **S** ’23]

4. Single-layer transformers
   [**S**, Hsu, Telgarsky ’23]

5. Multi-layer transformers
   [**S**, Hsu, Telgarsky ’24]



Final notes

Primary contributions: Fundamental trade-offs between architectures.

Technical contributions: Novel connections between NNs and rich theoretical CS subfields.

- Dynamical systems, communication complexity, distributed computing, …

Beyond representation:

- Other work about generalization and optimization.
- Future work: Optimization and generalization of transformers.

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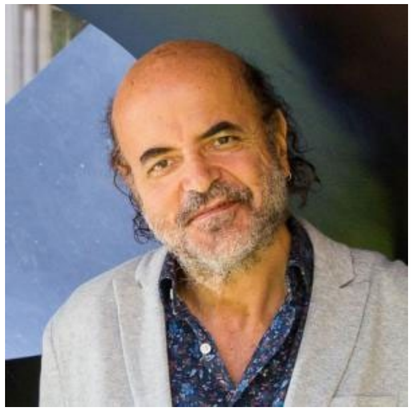
Photo: Manolis Vlatakis-Gkaragkounis

Committee members

Joan Bruna, Daniel Hsu, Christos Papadimitriou, Rocco Servedio, Matus Telgarsky





Research collaborators























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Dr. Barbara Hugus (1927 - 2021)

Mom and Barbara

Thank you.