

Progress Measures for Grokking via Mechanistic Interpretability

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REFORM reading group

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Emergence behavior

- NNs often exhibit **emergent behavior**, arising from scaling...
 - Amount of parameters
 - Training data
 - Training steps
- **Question:** How can we understand emergence?
 - Find continuous **progress measures**
- In this paper: use **mechanistic interpretability** to find progress measures
 - I.e., reverse-engineer learned behaviors into their individual components, by identifying the **circuits** within a model that implement a behavior
 - Use mech. interp. to discover **progress measures** empirically

Abrupt emergence?

- Usually looks **discontinuous**

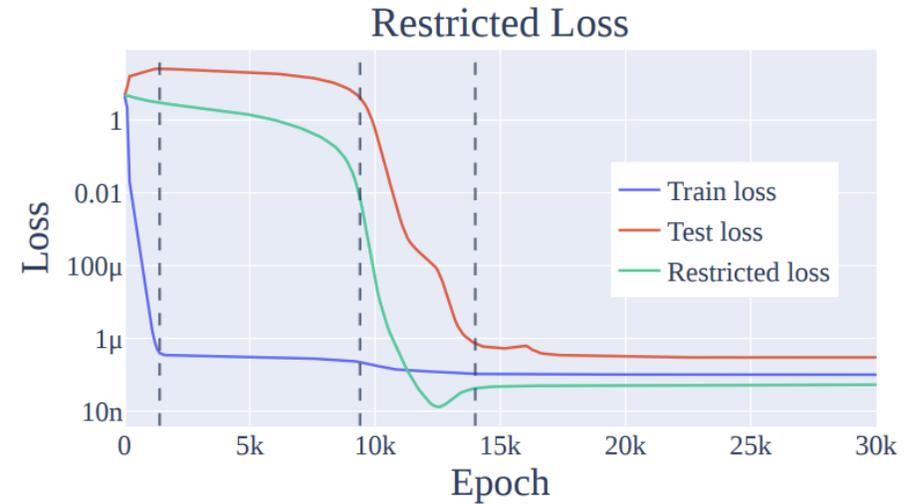
- Abrupt phase transitions
- Task ability
- **Grokking**

- Models first overfit, then abruptly transition to a generalizing solution after a large number of training steps

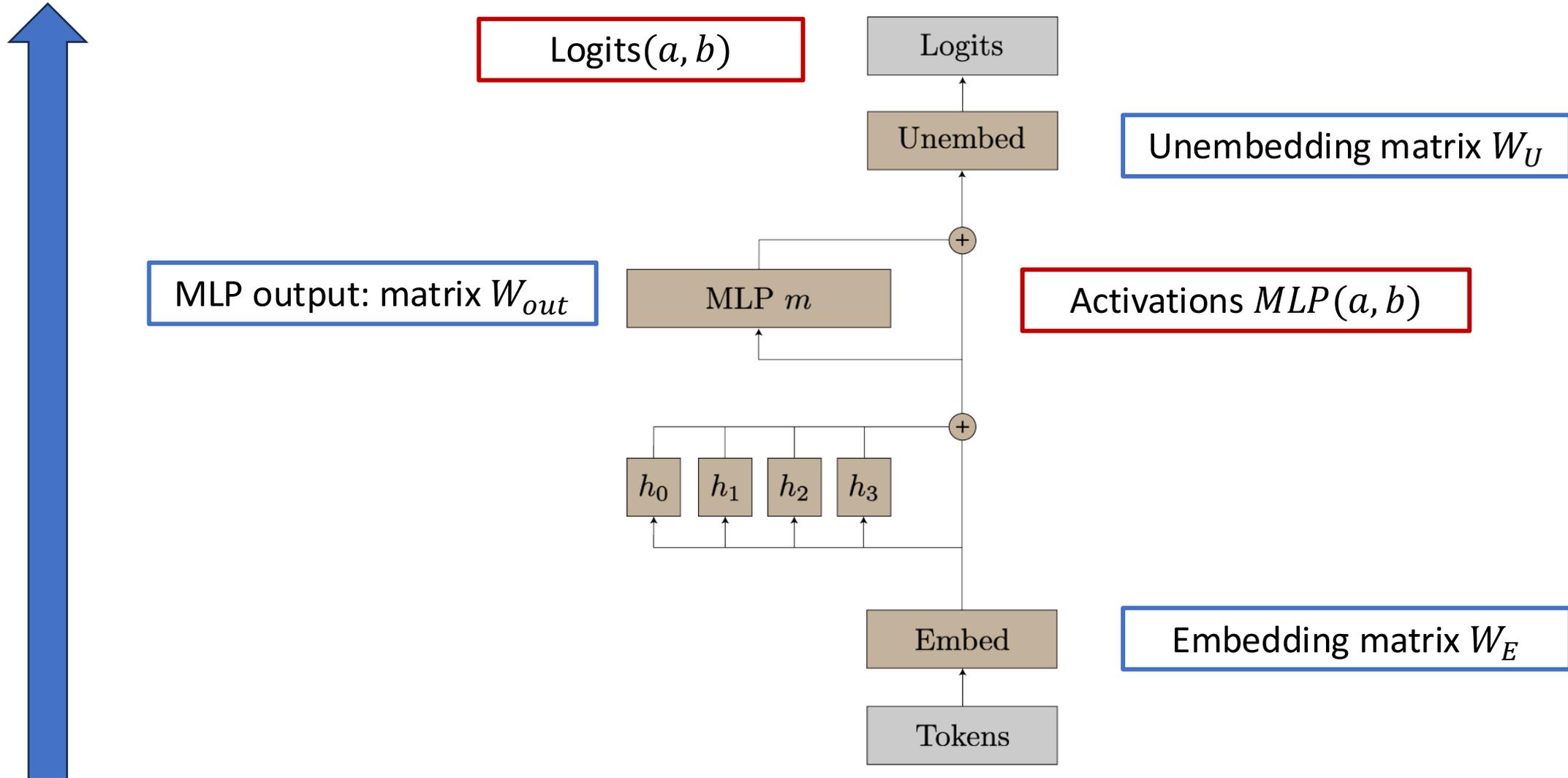
- Cross-entropy loss does not explain the phase changes

- Case study: **modular addition**

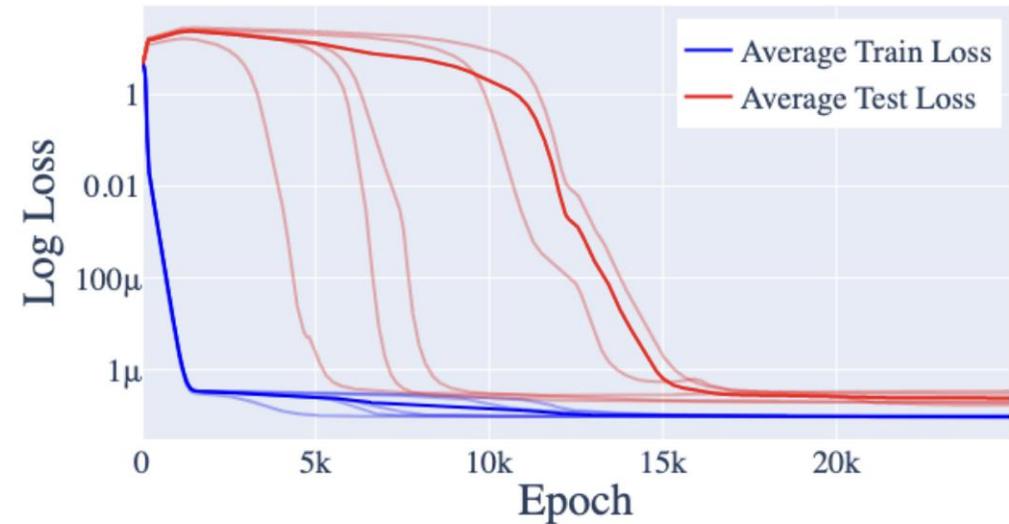
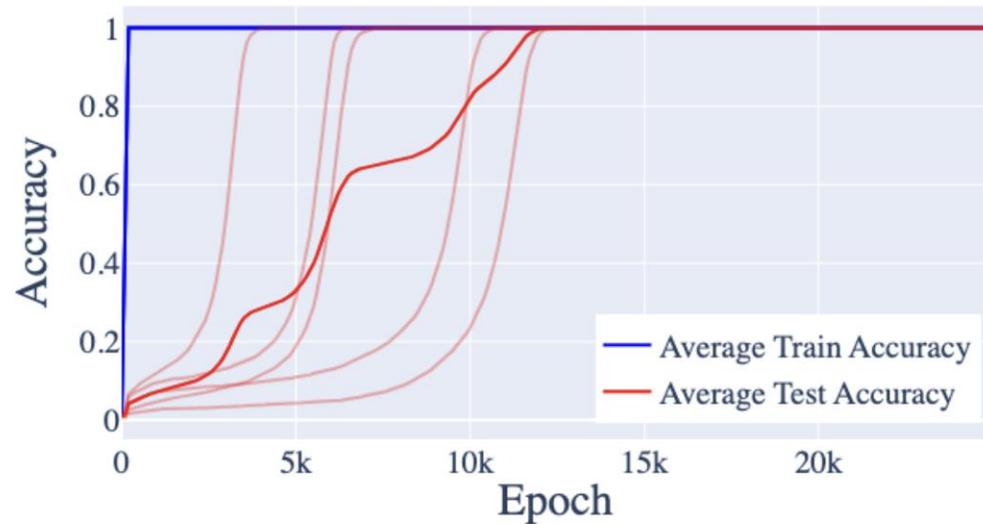
- Input: $a, b \in \{0, \dots, P - 1\}$ for some prime P
- Output: $a + b \bmod P$



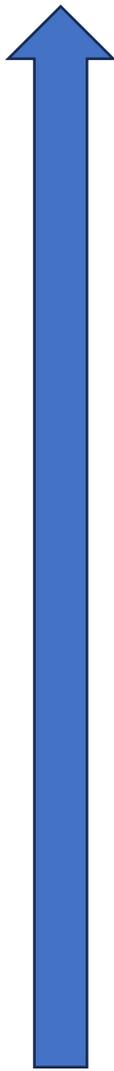
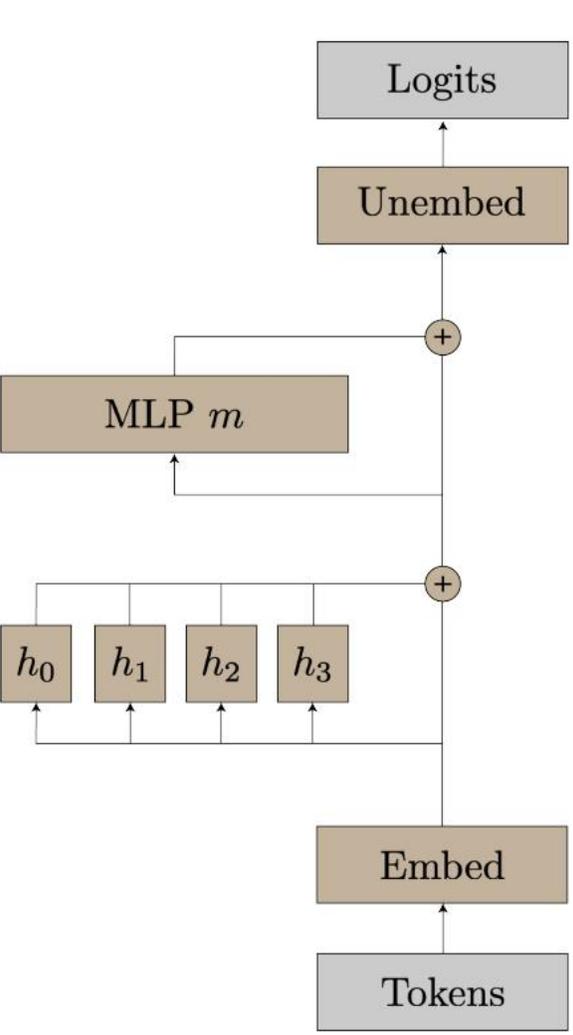
Architecture: a one-layer transformer



1-layer transformers on modular addition exhibit grokking

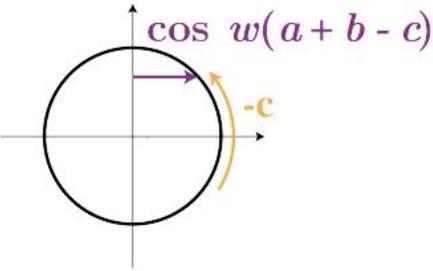


Use $P = 113$; grokking also occurs for other architectures and prime moduli,
but does not occur without regularization

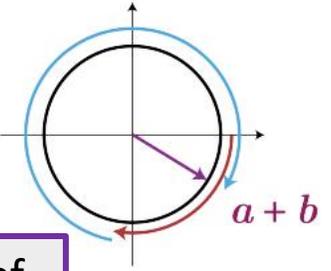


Reads off the logits for each $c \in \{0, 1, \dots, P - 1\}$ by rotating by c to get $\cos(w(a + b - c)) \rightarrow$ maximized when $a + b = c \pmod P$!

Computes logits using further trig identities:
 $\text{Logit}(c) \propto \cos(w(a + b - c))$
 $= \cos(w(a + b)) \cos(wc) + \sin(w(a + b)) \sin(wc)$



Calculates sine and cosine of $a + b$ using trig identities:
 $\sin(w(a + b)) = \sin(wa) \cos(wb) + \cos(wa) \sin(wb)$
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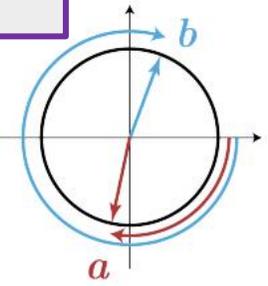


In the attention and MLP layers

Representation of $a + b \pmod P$

Translates one-hot a, b to Fourier basis:
 $a \rightarrow \sin(wa), \cos(wa)$
 $b \rightarrow \sin(wb), \cos(wb)$

Project a, b using w_k



$w_k a, w_k b$ for various frequencies
 $w_k = \frac{2k\pi}{P}, k \in \mathbb{N}$

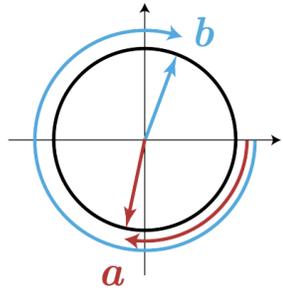
Evidence

Translates one-hot a, b to Fourier basis:

$$a \rightarrow \sin(wa), \cos(wa)$$

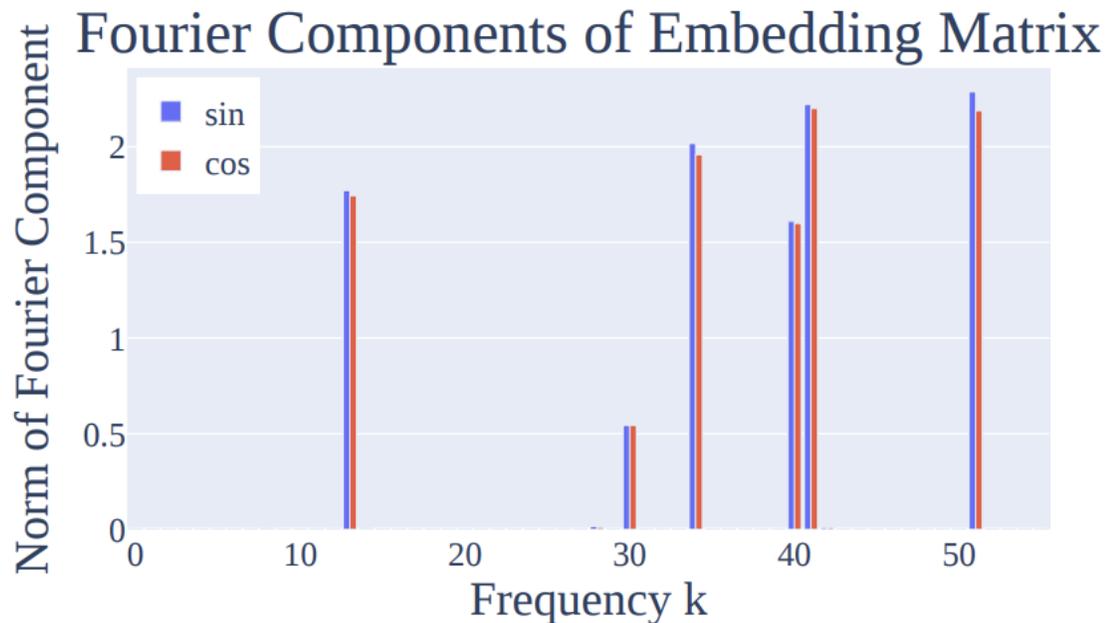
$$b \rightarrow \sin(wb), \cos(wb)$$

Discovering which w_k it uses



1. Periodicity in the embeddings.

- Apply a Fourier transform along the input dimension of W_E
- Compute the ℓ_2 norm along the other dimension

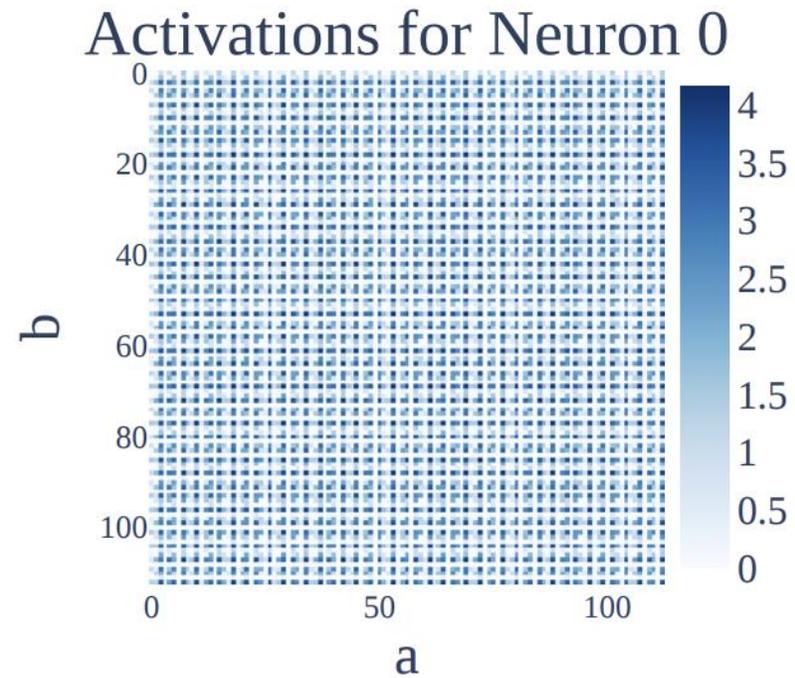
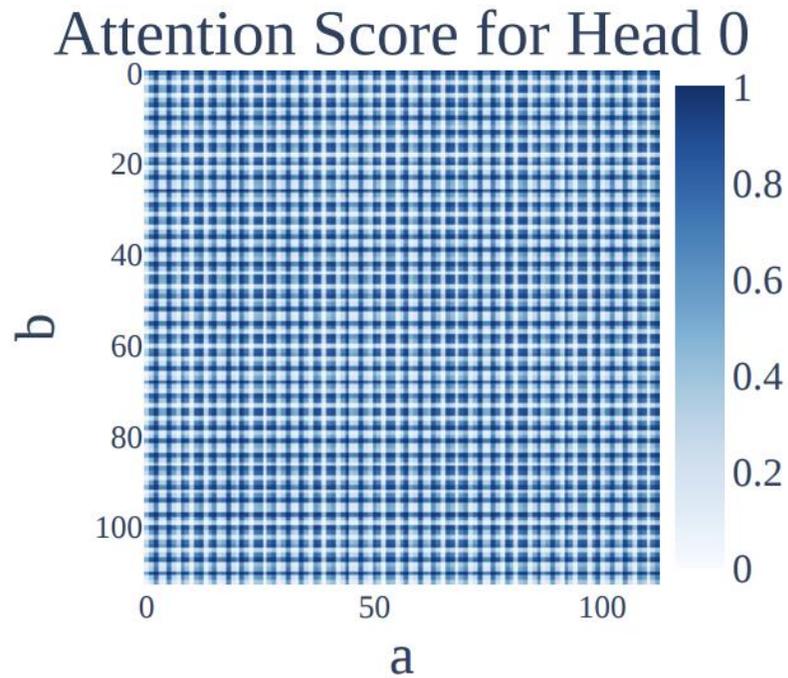


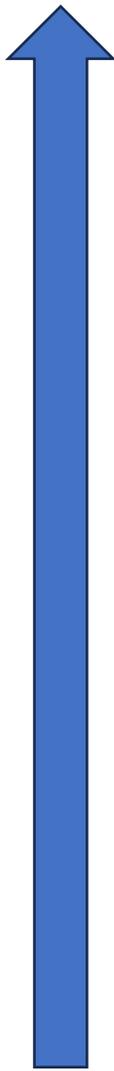
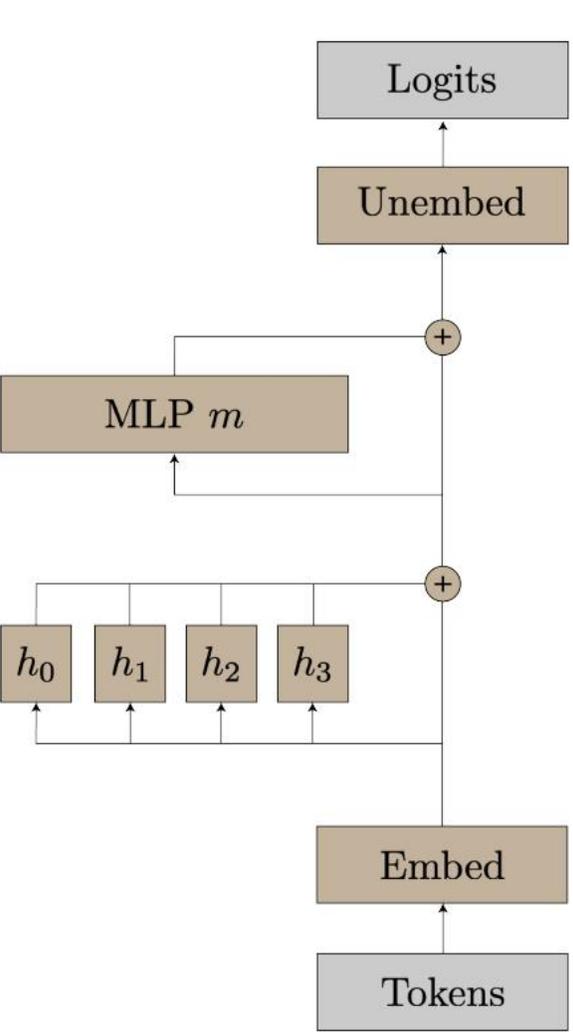
W_E is **very sparse** in the Fourier basis: only 6 frequencies have non-negligible norm \rightarrow **key frequencies**

Evidence

2. Periodicity in the attention heads and MLP neuron activations.

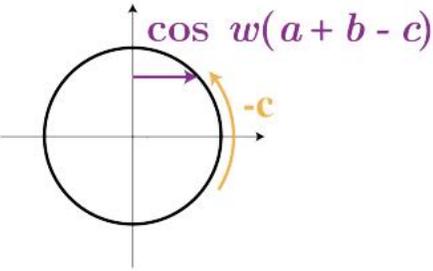
For $k = 35$ and
 $k = 42$



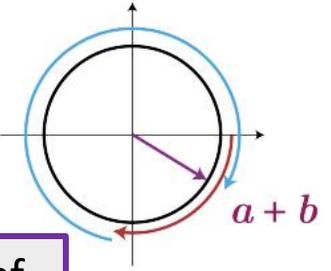


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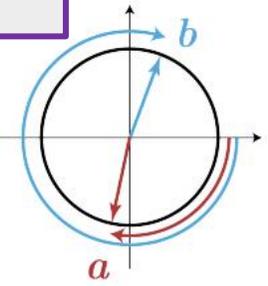


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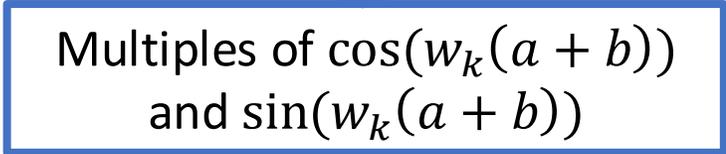
Trigonometric identity

- Matrix W_L : matrix mapping MLP activations to logits
 - It is approximately rank 10 (with the 5 key frequencies)

$$W_L = \sum_{k \in \{14, 35, 41, 42, 52\}} \cos(w_k) u_k^T + \sin(w_k) v_k^T$$

- The model implements the logits for a, b as:

$$\text{Logits}(a, b) = W_L \text{MLP}(a, b) \approx \sum_k \cos(w_k) u_k^T \text{MLP}(a, b) + \sin(w_k) v_k^T \text{MLP}(a, b)$$



Multiples of $\cos(w_k(a + b))$
and $\sin(w_k(a + b))$

Trigonometric identity

Similarly, logits are well approximated by a weighted sum of $\cos(w(a + b - c))$'s

W_L Component	Fourier components of $u_k^T \text{MLP}(a, b)$ or $v_k^T \text{MLP}(a, b)$	FVE
$\cos(w_{14}c)$	$44.6 \cos(w_{14}a) \cos(w_{14}b) - 43.6 \sin(w_{14}a) \sin(w_{14}b) \approx 44.1 \cos(w_{14}(a + b))$	93.2%
$\sin(w_{14}c)$	$44.1 \sin(w_{14}a) \cos(w_{14}b) + 44.1 \cos(w_{14}a) \sin(w_{14}b) \approx 44.1 \sin(w_{14}(a + b))$	93.5%
$\cos(w_{35}c)$	$40.7 \cos(w_{35}a) \cos(w_{35}b) - 43.6 \sin(w_{35}a) \sin(w_{35}b) \approx 42.2 \cos(w_{35}(a + b))$	96.8%
$\sin(w_{35}c)$	$41.8 \sin(w_{35}a) \cos(w_{35}b) + 41.8 \cos(w_{35}a) \sin(w_{35}b) \approx 41.8 \sin(w_{35}(a + b))$	96.5%
$\cos(w_{41}c)$	$44.8 \cos(w_{41}a) \cos(w_{41}b) - 44.8 \sin(w_{41}a) \sin(w_{41}b) \approx 44.8 \cos(w_{41}(a + b))$	97.0%
$\sin(w_{41}c)$	$44.5 \sin(w_{41}a) \cos(w_{41}b) + 44.5 \cos(w_{41}a) \sin(w_{41}b) \approx 44.5 \sin(w_{41}(a + b))$	97.0%
$\cos(w_{42}c)$	$64.6 \cos(w_{42}a) \cos(w_{42}b) - 68.5 \sin(w_{42}a) \sin(w_{42}b) \approx 66.6 \cos(w_{42}(a + b))$	96.4%
$\sin(w_{42}c)$	$67.8 \sin(w_{42}a) \cos(w_{42}b) + 67.8 \cos(w_{42}a) \sin(w_{42}b) \approx 67.8 \sin(w_{42}(a + b))$	96.4%
$\cos(w_{52}c)$	$60.5 \cos(w_{52}a) \cos(w_{52}b) - 65.5 \sin(w_{52}a) \sin(w_{52}b) \approx 63.0 \cos(w_{52}(a + b))$	97.4%
$\sin(w_{52}c)$	$64.5 \sin(w_{52}a) \cos(w_{52}b) + 64.5 \cos(w_{52}a) \sin(w_{52}b) \approx 64.5 \sin(w_{52}(a + b))$	98.2%

Table 1: For each of the directions u_k or v_k (corresponding to the $\cos(w_k)$ and $\sin(w_k)$ components respectively) in the unembedding matrix, we take the dot product of the MLP activations with that direction, then perform a Fourier transform (middle column; only two largest coefficients shown). We then compute the fraction of variance explained (FVE) if we replace the projection with a single term proportional to $\cos(w_k(a + b))$ or $\sin(w_k(a + b))$, and find that it is consistently close to 1.

Final step

Constructive Interference of Cosine Waves of Different Frequencies

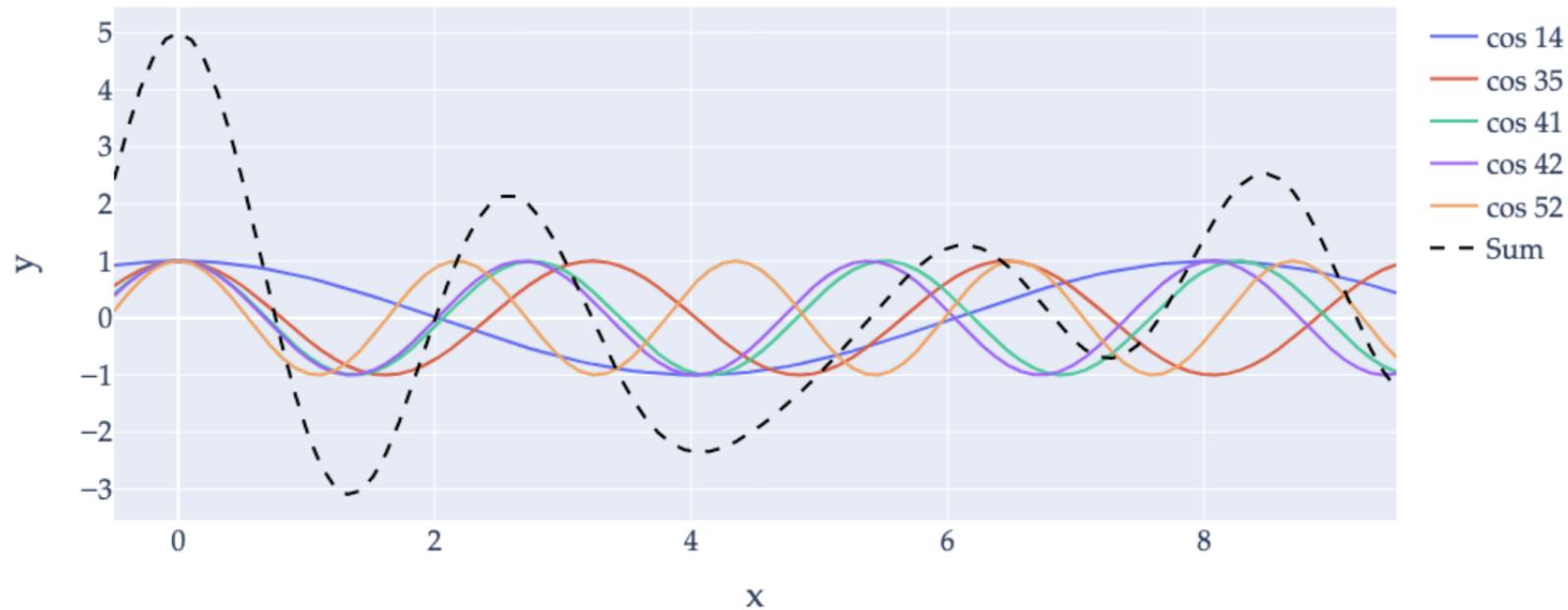
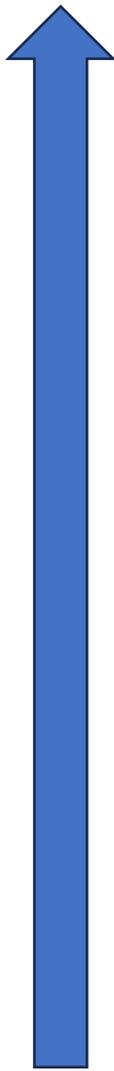
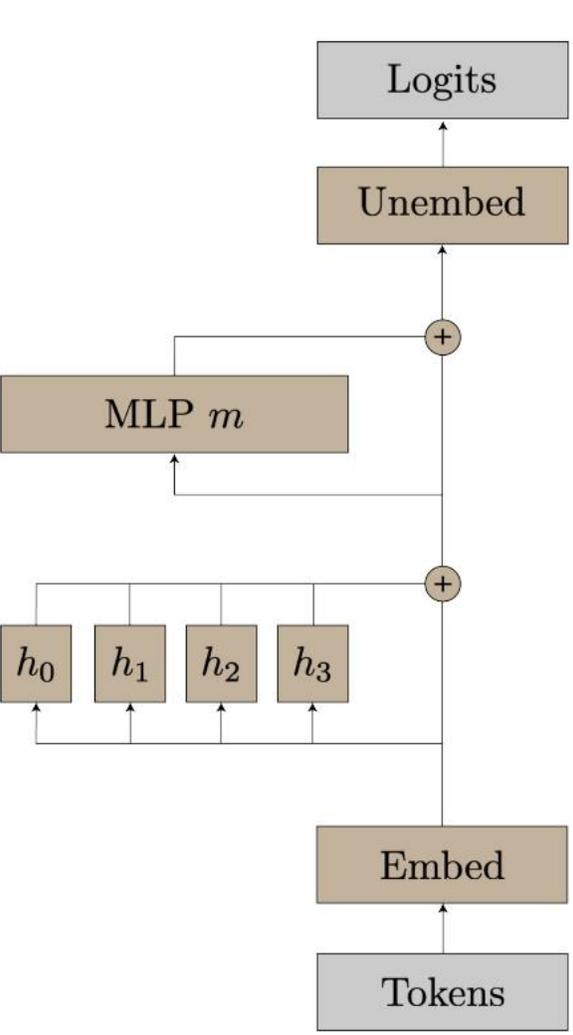
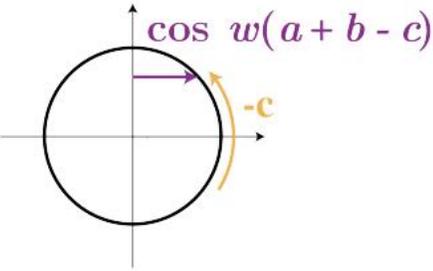


Figure 8: As discussed in Appendix B, while for every $k \in [0, \dots, P - 1]$, $\cos\left(\frac{2k\pi}{P}x\right)$ achieves its maximum value (1) at $x = 0 \pmod{113}$, it still has additional peaks at different values that are close to the maximum value. However, by adding together cosine waves of the 5 keyfrequencies, the model constructs a periodic function where the value at $x = 0 \pmod{113}$ is significantly larger than its value anywhere else.

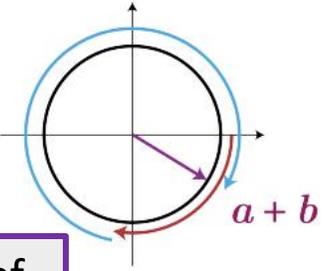


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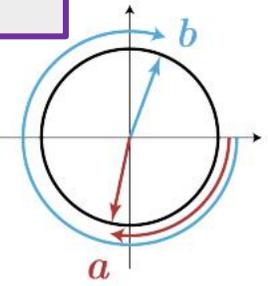


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Progress measures

- Metrics that can be computed during training that track the progress, *including during phase transitions*
- **Restricted loss**: measure how well intermediate versions of the model can do with only the 5 key frequencies
 - Measure the loss of the ablated network
- **Excluded loss**: remove *only* the key frequencies from the logits but keep the rest
 - Measure this on the training data
 - **Memorizing** solution should be spread out in the Fourier domain → ablating a bit doesn't hurt much, but it should hurt the **generalizing** solution

1. Memorization

- Decline of both **excluded** and **train loss**; unused w_k frequencies

2. Circuit formation

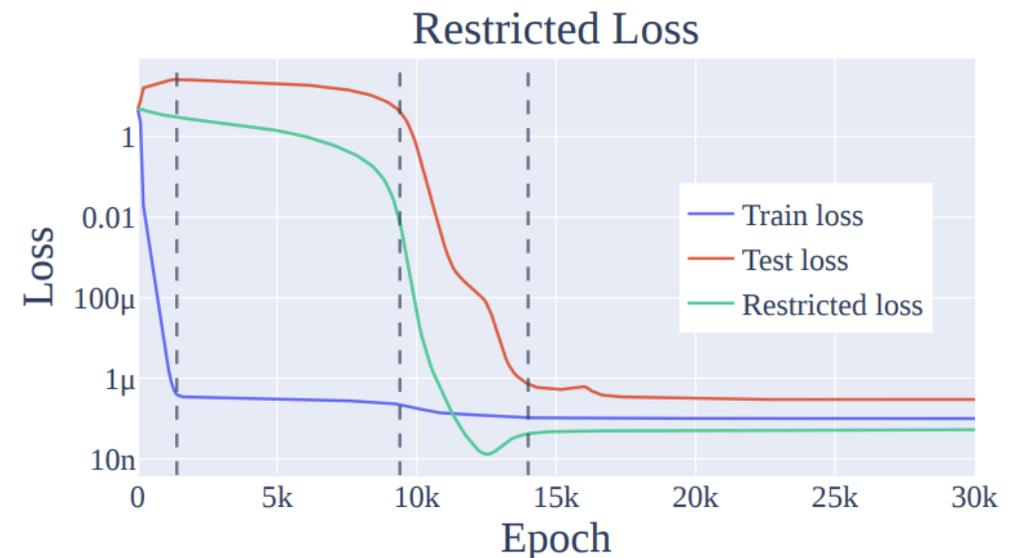
- **Excluded loss** rises, **restricted loss** starts to fall
- Smooth transition from memorizing to Fourier mult. algorithm
- Occurs *well before* the grokking occurs!

Restricted: **only** the key frequencies

Excluded: **without** the key frequencies

3. Cleanup

- **Excluded loss** plateaus, **restricted loss** continues to drop, **test loss** suddenly drops
- Completed Fourier circuit



Grokking, rather than being a sudden shift, arises from the gradual amplification of structured mechanisms encoded in the weights, followed by the later removal of memorizing components