Neural Networks learn Representation Theory:
Reverse Engineering how Networks perform Group Operations

Bilal Chughtai, Lawrence Chan, Neel Nanda

PROGRESS MEASURES FOR GROKKING VIA MECHANISTIC INTERPRETABILITY

Neel Nanda
Independent
neelnanda27@gmail.com

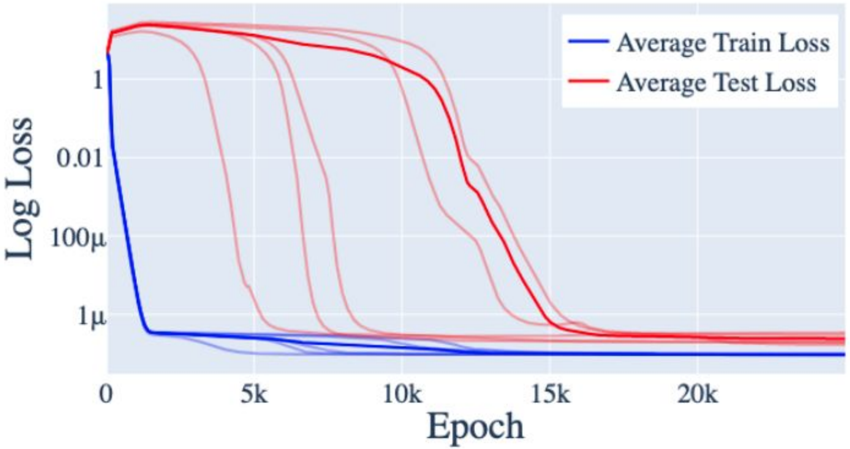
Lawrence Chan
UC Berkeley
chanlaw@berkeley.edu

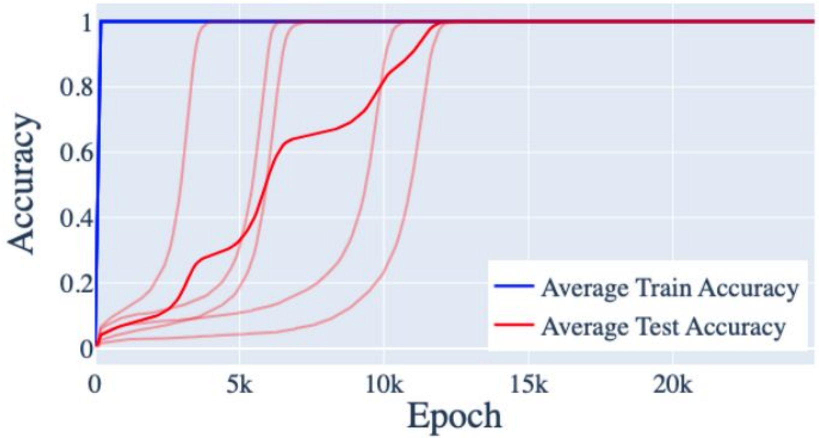
Tom Lieberum
Independent
tlieberum3141@gmail.com

Jess Smith
Independent
smith.jessk@gmail.com

Jacob Steinhardt
UC Berkeley
jsteinhardt@berkeley.edu

Mystery: Why do models grok?





GROKKING: GENERALIZATION BEYOND OVERFITTING ON SMALL ALGORITHMIC DATASETS

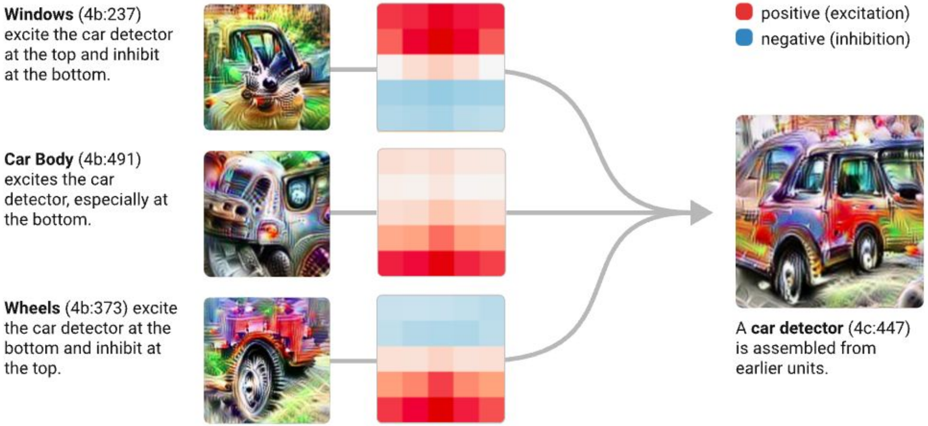
Alethea Power, Yuri Burda, Harri Edwards, Igor Babuschkin
OpenAI

Vedant Misra*
Google

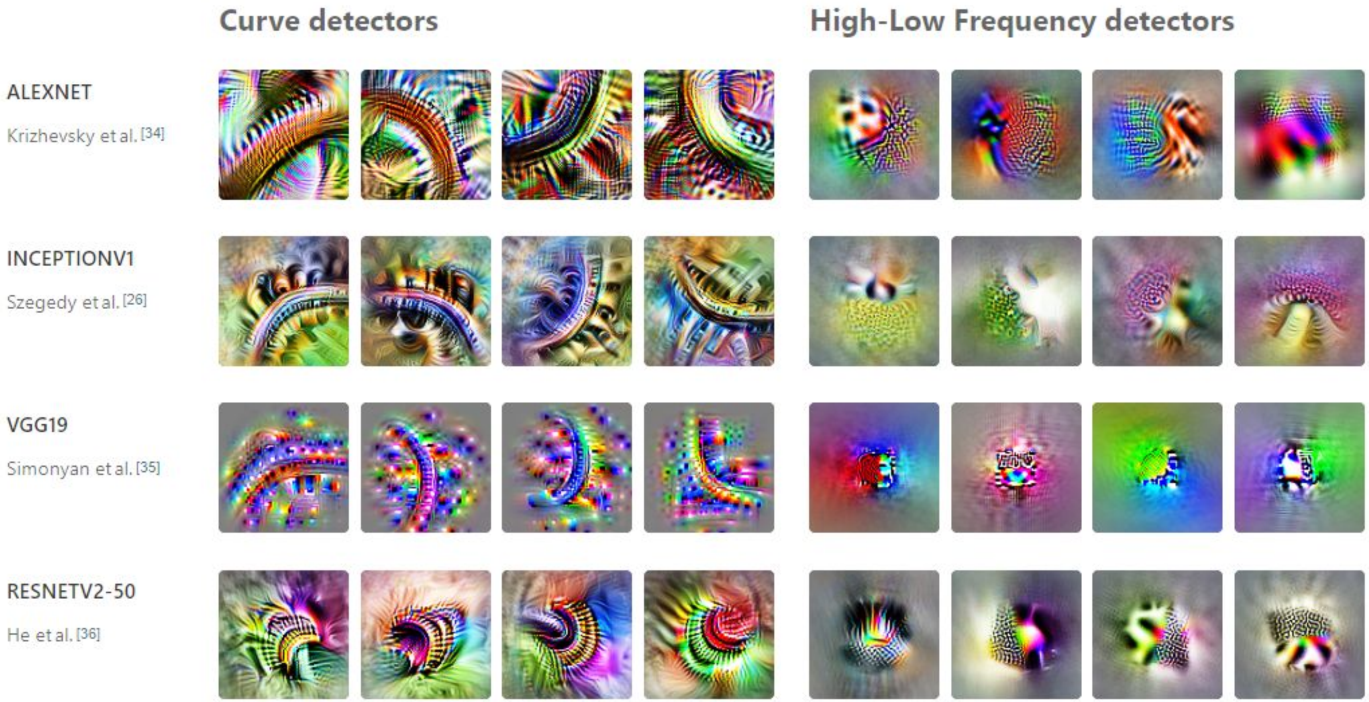
Methodology: Apply mechanistic interpretability

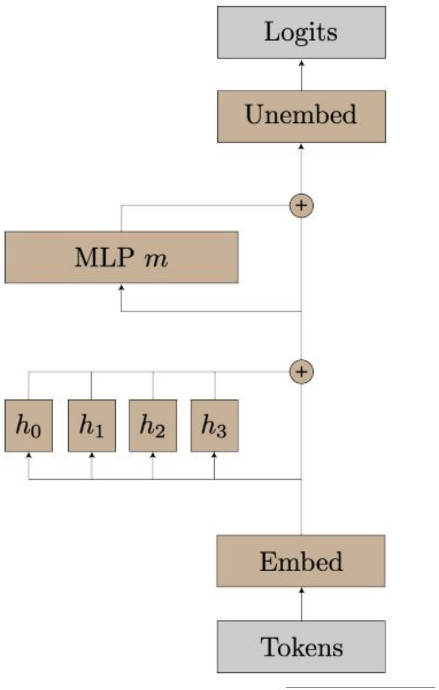
Inspiration: Mechanistic Interpretability

- **Goal:** Reverse engineer neural networks
- **Hypothesis**: Models learn human-comprehensible algorithms and can be understood, if we learn how to make it legible
- Models learn **circuits**, algorithms encoded in the weights
- A deep knowledge of circuits is crucial to understand and predict model behaviour



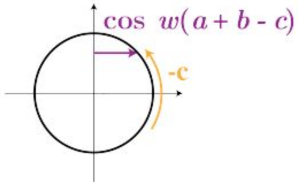
Universality





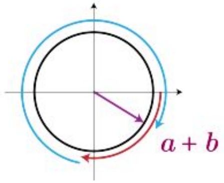
Computes logits using further trig identities:

$$\mathrm{Logit}(c) \propto \cos(w(a+b-c))$$
$$= \cos(w(a+b))\cos(wc) + \sin(w(a+b))\sin(wc)$$



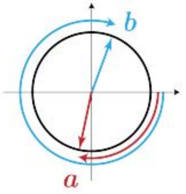
Calculates sine and cosine of $a+b$ using trig identities:

$$\sin(w(a+b)) = \sin(wa)\cos(wb) + \cos(wa)\sin(wb)$$
$$\cos(w(a+b)) = \cos(wa)\cos(wb) - \sin(wa)\sin(wb)$$



Translates one-hot a, b to Fourier basis:

$$a \to \sin(wa), \cos(wa)$$
$$b \to \sin(wb), \cos(wb)$$



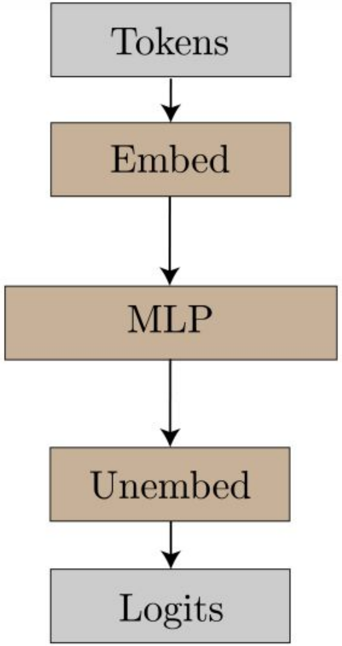
Representation Theory

A (real) **representation** is a homomorphism, i.e. a map preserving the group structure, $\rho : G \to GL(\mathbb{R}^d)$ from the group G to a d-dimensional general linear group, the set of invertible square matrices of dimension d. Representations are in general *reducible*, in a manner we make precise in the Appendix. For each group G, there exist a finite set of fundamental **irreducible representations**. The **character** of a representation is the trace of the representation $\chi_\rho : G \to \mathbb{R}$ given by $\chi_\rho(g) = \mathrm{tr}(\rho(g))$. A key fact our algorithm depends on is that character's are maximal when $\rho(g) = I$, the identity matrix (Theorem C.8). In particular, the character of the identity element, $\chi_\rho(e)$, is maximal.

Example. The cyclic group C_n is generated by a single element r and naturally represents the set of rotational symmetries of an n-gon, where r corresponds to rotation by $2\pi/n$. This motivates a 2 dimensional representation – a set of n 2×2 matrices, one for each group element:

$$\rho(r^k) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

for element r^k corresponding to rotation by $\theta = 2\pi k/n$.



Translates one-hot a,b to representation matrices:

$a, b \mapsto \rho(a), \rho(b)$

Performs matrix multiplication on representations via ReLUs:

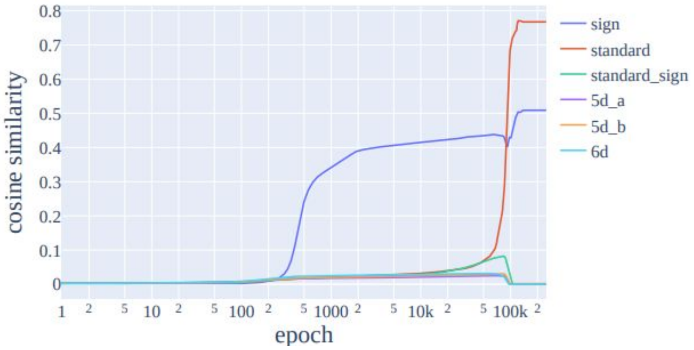
$\rho(a), \rho(b) \mapsto \rho(a)\rho(b) = \rho(ab)$

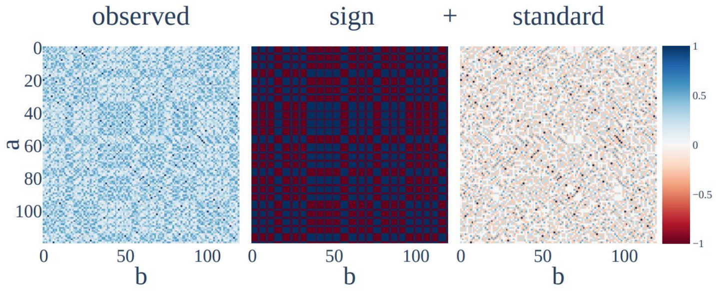
Computes logits by multiplying by $\rho(c^{-1})$ and taking the trace:

$\mathrm{Logit}(c) \propto \chi_\rho(abc^{-1}) = \mathrm{tr}(\rho(abc^{-1}))$

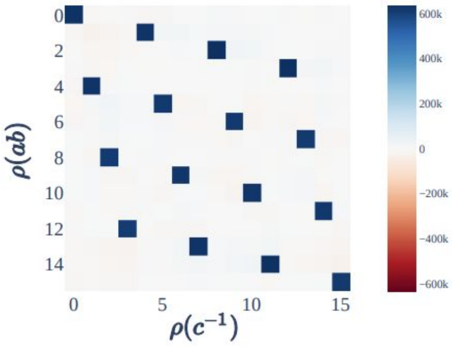
Reverse Engineering S5

1. Logit similarity
2. Embeddings
3. MLP activations & the MLP - Logit map
4. Ablations





	W_a	W_b	W_U
SIGN	6.95%	6.95%	9.58%
STANDARD	93.0%	93.0%	84.5%
RESIDUAL	0.00%	0.00%	5.96%



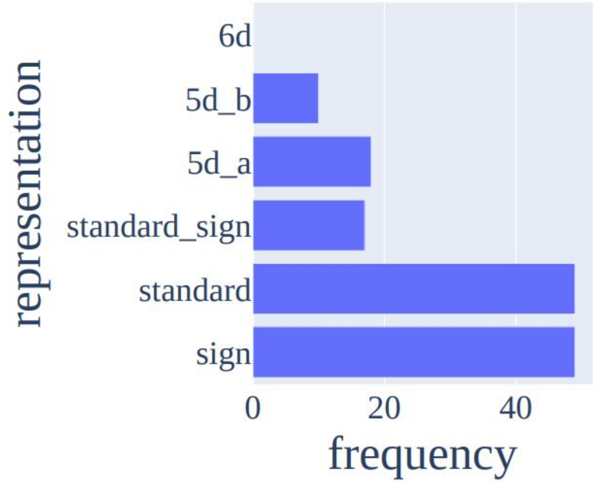
CLUSTER	$\rho(a)$	$\rho(b)$	$\rho(ab)$	RESIDUAL
SIGN	33.3%	33.3%	33.3%	0.00%
STANDARD	39.6%	37.1%	11.3%	12.1%

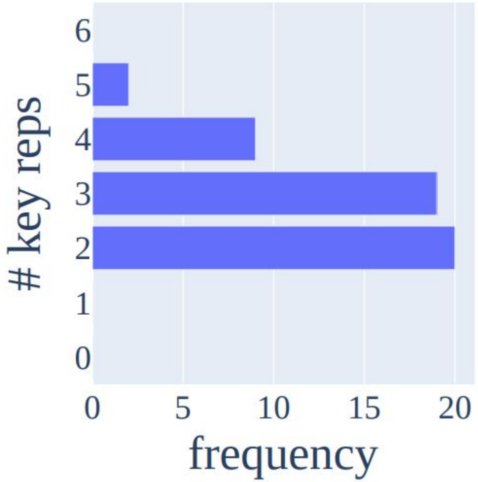
Weak Universality

Table 3. Results from all groups on both MLP and Transformer architectures, averaged over 4 seeds. We find that that features for matrices in the key representations are learned consistently, and explain almost all of the variance of embeddings and unembeddings. We find that terms corresponding to $\rho(ab)$ are consistently present in the MLP neurons, as expected by our algorithm. Excluding and restricting to these terms in the key representations damages performance/does not affect performance respectively.

	MLP								**Transformer**							
	FVE					Loss			FVE				Loss			
Group	W_a	W_b	W_U	*MLP*	$\rho(ab)$	*Test*	*Exc.*	*Res.*	W_E	W_L	*MLP*	$\rho(ab)$	*Test*	*Exc.*	*Res.*
C_{113}	99.53%	99.39%	98.05%	90.25%	12.03%	1.63e-05	5.95	6.88e-03	95.18%	99.52%	92.12%	16.77%	2.67e-07	9.42	2.12e-02
C_{118}	99.75%	99.74%	98.43%	95.84%	13.26%	5.39e-06	8.72	3.60e-03	94.05%	99.64%	94.63%	17.11%	1.73e-07	15.93	2.55e-01
D_{59}	99.71%	99.73%	98.52%	87.68%	12.44%	6.34e-06	12.37	1.60e-06	98.58%	98.53%	85.01%	10.85%	3.20e-06	46.42	2.82e-05
D_{61}	99.26%	99.45%	98.26%	87.61%	12.48%	1.79e-05	12.00	1.69e-06	98.33%	97.40%	85.59%	11.11%	1.63e-02	41.64	9.60e-02
S_5	100.00%	99.99%	94.14%	88.91%	12.13%	1.02e-05	11.72	2.21e-07	99.84%	99.97%	85.28%	10.23%	1.43e-07	17.77	4.44e-09
S_6	99.65%	99.78%	93.67%	86.38%	8.98%	4.95e 05	12.17	2.66e 06	99.94%	99.93%	86.32%	9.35%	2.21e 06	291.67	1.05e 06
A_5	99.04%	99.31%	93.27%	86.69%	10.26%	1.94e-05	9.82	5.28e-07	97.53%	97.40%	83.56%	8.22%	4.88e-02	19.76	7.70e-04

Strong Universality





Implications

- Reverse engineering a single network is insufficient for understanding behaviour in general
- BUT it may be possible to build a periodic table of ‘universal’ features, that in aggregate may be able to explain a given behaviour fully.

Further Work

- Reverse engineering more group theoretic tasks
- Understanding universality better in algorithmic / realistic tasks
- Understanding network inductive biases better

Key Takeaways

- Models naturally learn representation theory
- Only by employing the tools of mechanistic interpretability were we able to figure this out

Future Work

- Further group theoretic tasks
    - Preliminary work has suggested models learn representations in a wider family of group theoretic tasks than simply group composition
- Understanding inductive biases of neural networks better
- Further investigation of universality in algorithmic tasks
- Investigation of universality in realistic tasks and models