Emergence in non-neural models

grokking modular arithmetic via average gradient outer product

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ICML 2025

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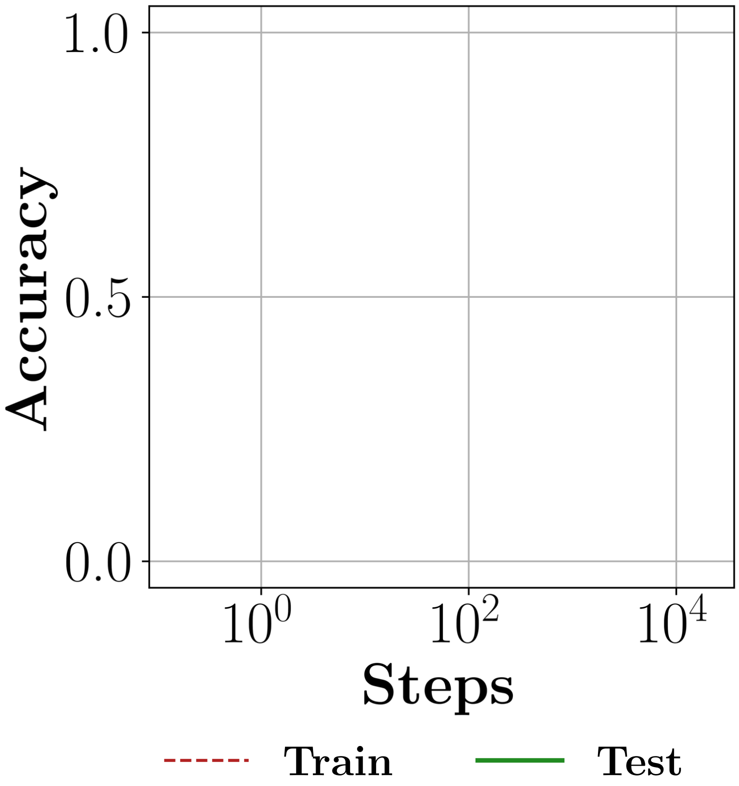
Classical approaches to tracking progress



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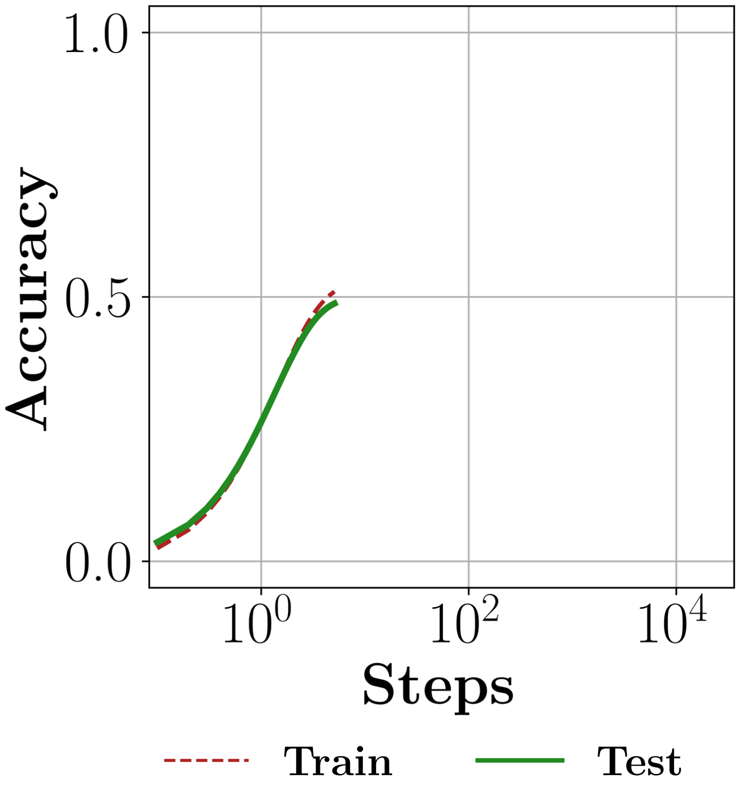

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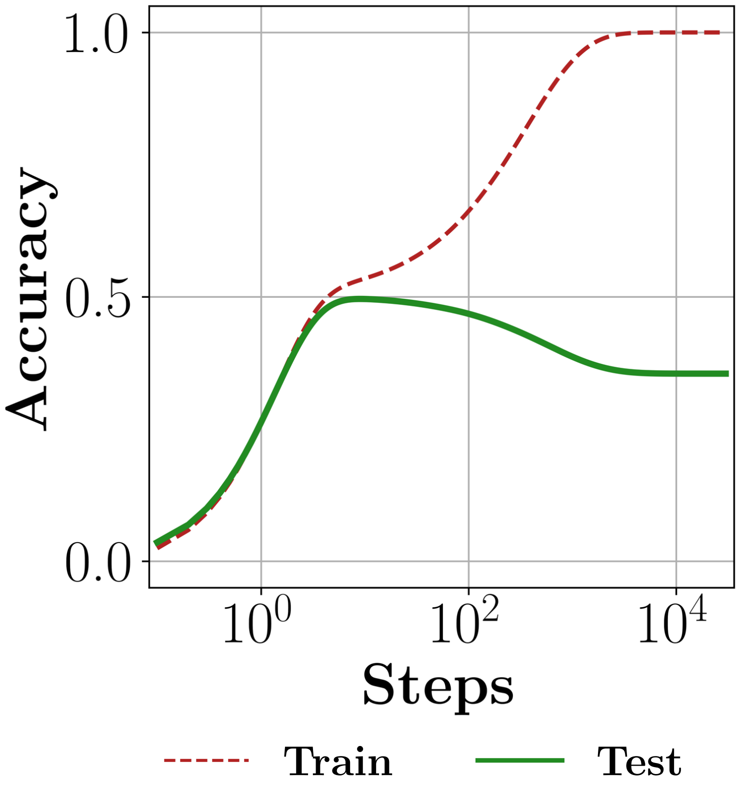

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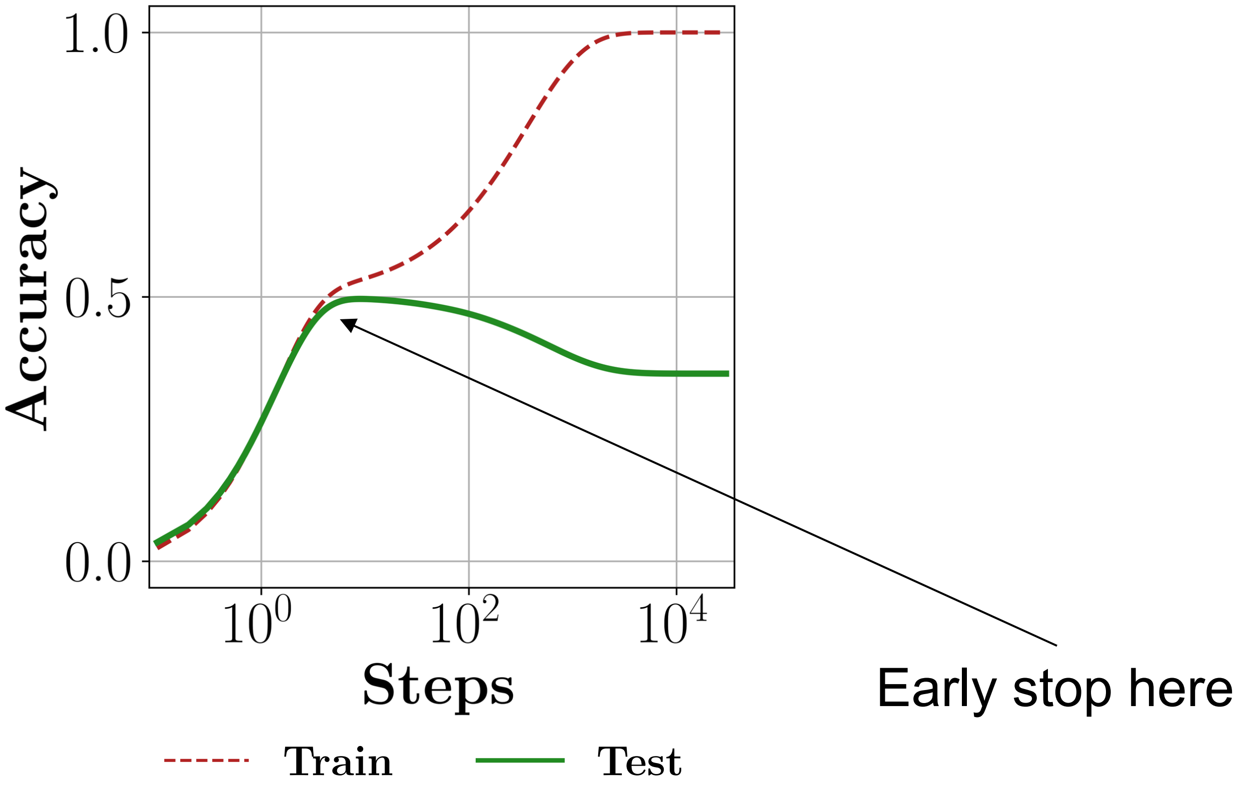
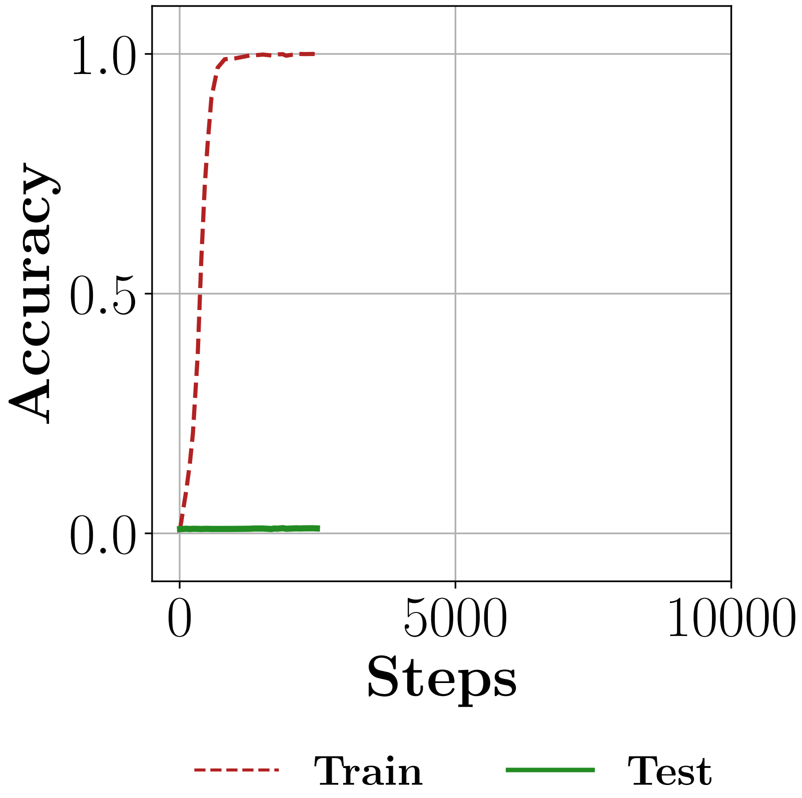


Test accuracy does not track progress!

Emergent setting:



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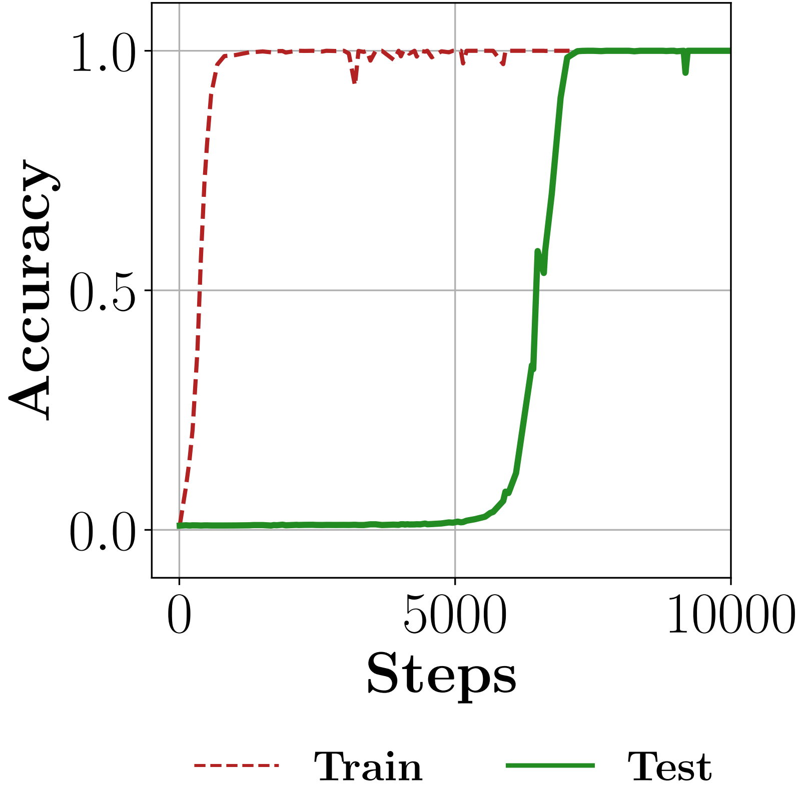

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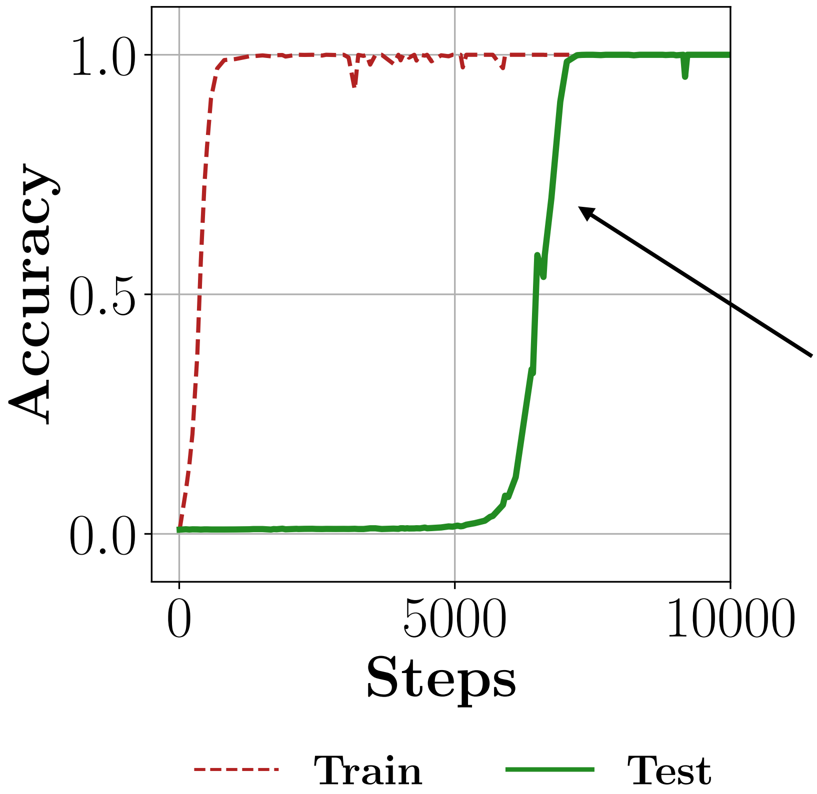

"Grokking" in modular arithmetic, originally shown by (Power, Burda, Edwards, Babuschkin & Misra, *preprint* 2022)

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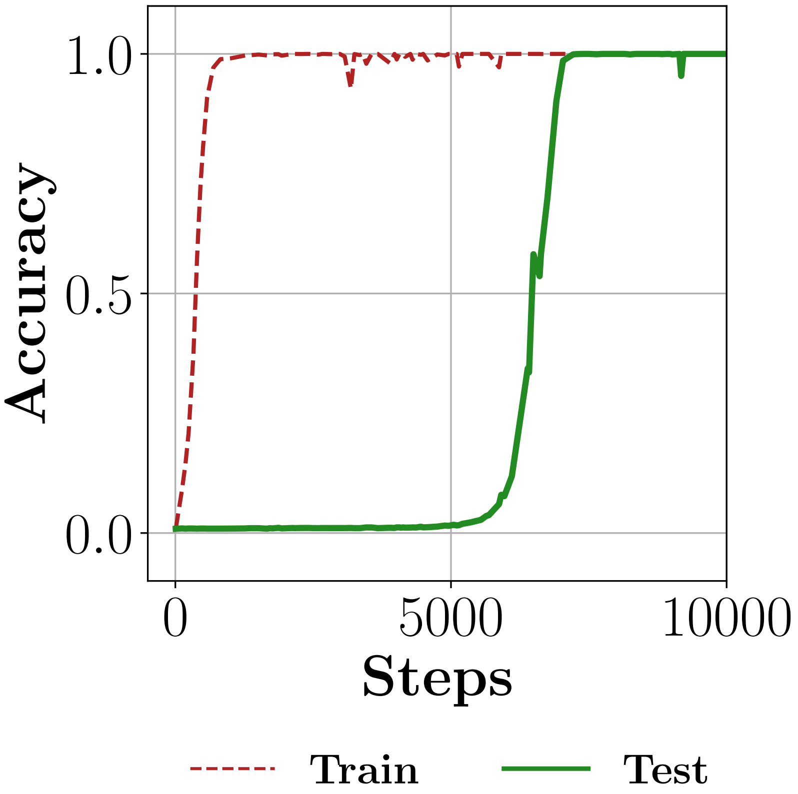

Key Questions:

- Is this phenomenon unique to neural networks?
- If not, is there a unified way to understand this behavior in neural and non-neural models?
- Is there an alterative to test accuracy?

How to set up a model to learn modular arithmetic

Given: digits a, b and prime p
Learn: a + b mod p

Example: p = 3, a = 1, b = 2

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(Cayley table)

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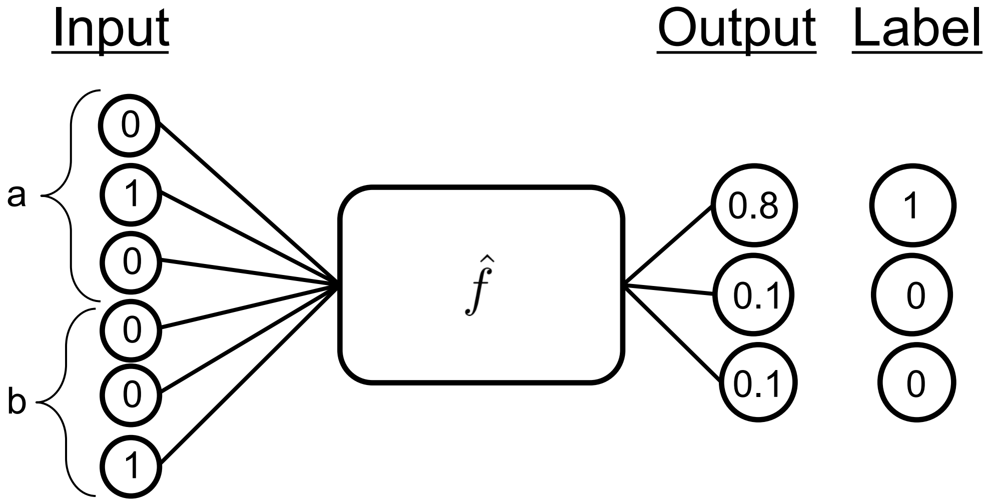
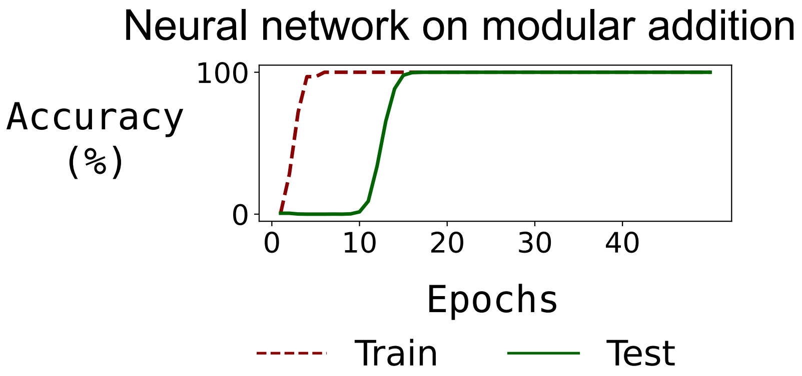
$$\text{Input: } (\underbrace{0\ 1\ 0}_{a=1}\ \ \underbrace{0\ 0\ 1}_{b=2})\ ;\ \text{Label: } \underbrace{(1\ 0\ 0)}_{a+b \mod 3=0}$$



Modular arithmetic and feature learning

- Neural networks can “grok” this task



- Non-feature learning methods (e.g. standard kernels) do not generalize (no grokking!)

A general mechanism for feature learning

- Understand features through Average Gradient Outer Product (AGOP) (Härdle & Stoker, *JASA* 1989)

Given a predictor, f, and training data $x_i \in \mathbb{R}^d$, define:

$$\mathbf{AGOP}(f, \{x_i\}_{i=1}^n) = \frac{1}{n}\sum_{i=1}^n \nabla_x f(x_i)\ \nabla_x f(x_i)^\top \in \mathbb{R}^{d\times d}$$

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- AGOP captures neural network features (Radhakrishnan*, Beaglehole*, Pandit & Belkin, *Science* 2024)

Intuition for AGOP

Given a predictor, f, and training data $x_i \in \mathbb{R}^d$, define:

$$\mathbf{AGOP}(f, \{x_i\}_{i=1}^n) = \frac{1}{n} \sum_{i=1}^n \nabla_x f(x_i) \ \nabla_x f(x_i)^\top \in \mathbb{R}^{d \times d}$$

- Input perturbations on certain features affect the output predictor most
- Intuitively AGOP = supervised PCA
- AGOP decouples features from predictors

Recursive Feature Machines (RFM)

- AGOP enables feature learning for general models
- RFM gives an algorithm for this (Radhakrishnan*, Beaglehole*, Pandit & Belkin, *Science* 2024)

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RFM Algorithm:

Given: Training data (X, y), initial features M_0, total iterations T

For $t \in [T]$ *iterations*:

Step 1: Fit an estimator $f^{(t)}$ to (filtered) training data XM_t and labels y

Step 2: Update features as $M_{t+1} = \mathbf{AGOP}(f^{(t)}, X)$

Repeat Step 1 & Step 2

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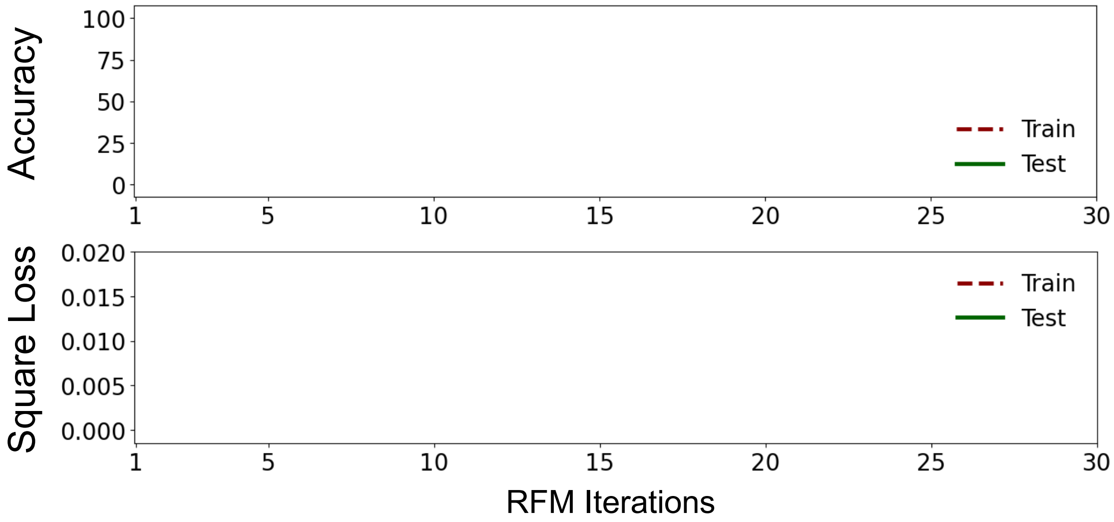
Kernel RFM groks modular addition



Initialize: $M_1 = I_{2p}$

Iteration (t): 1

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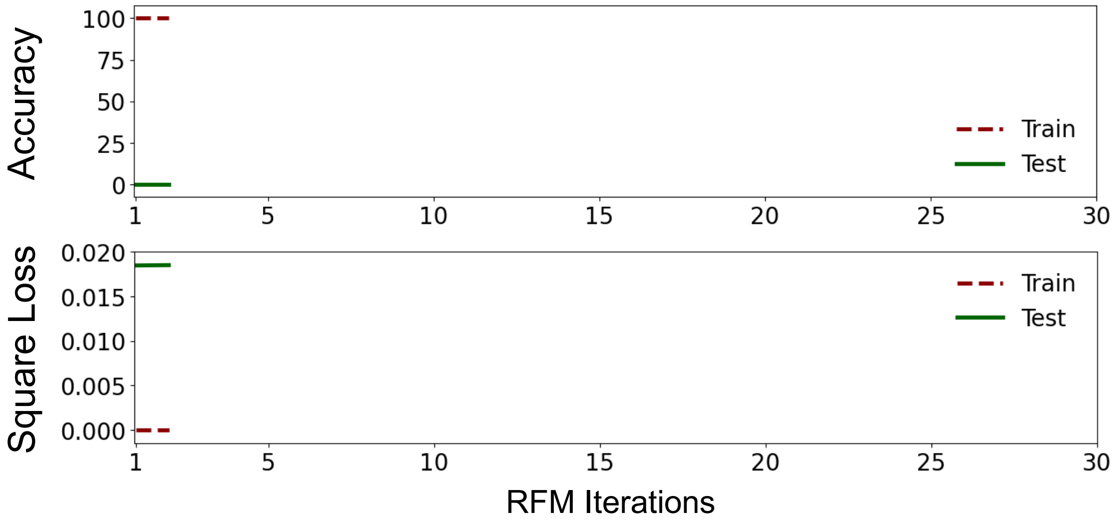

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<u>(1) Solve kernel regression:</u>

$K_{tr} = k(X_{tr}, X_{tr}; M_1)$

$\alpha = K_{tr}^{-1} y_{tr}$

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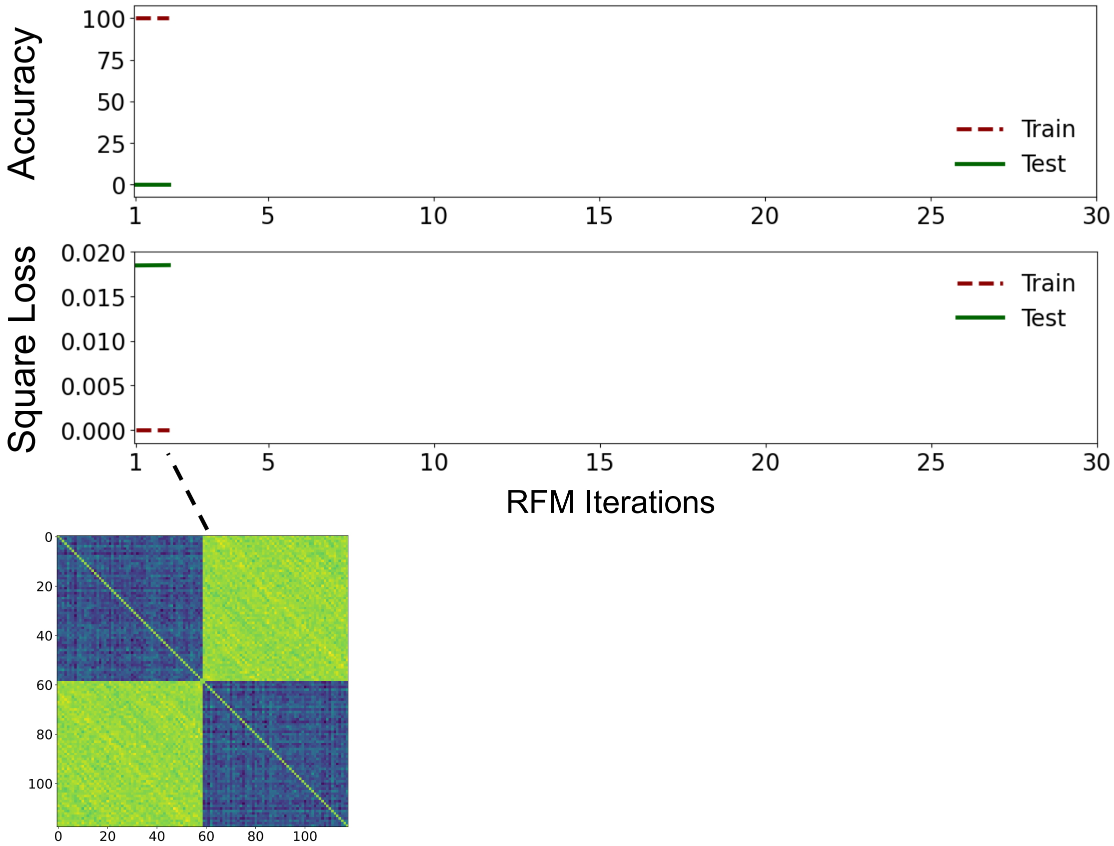

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(1) Solve kernel regression:

$$K_{tr} = k(X_{tr}, X_{tr}; M_1)$$
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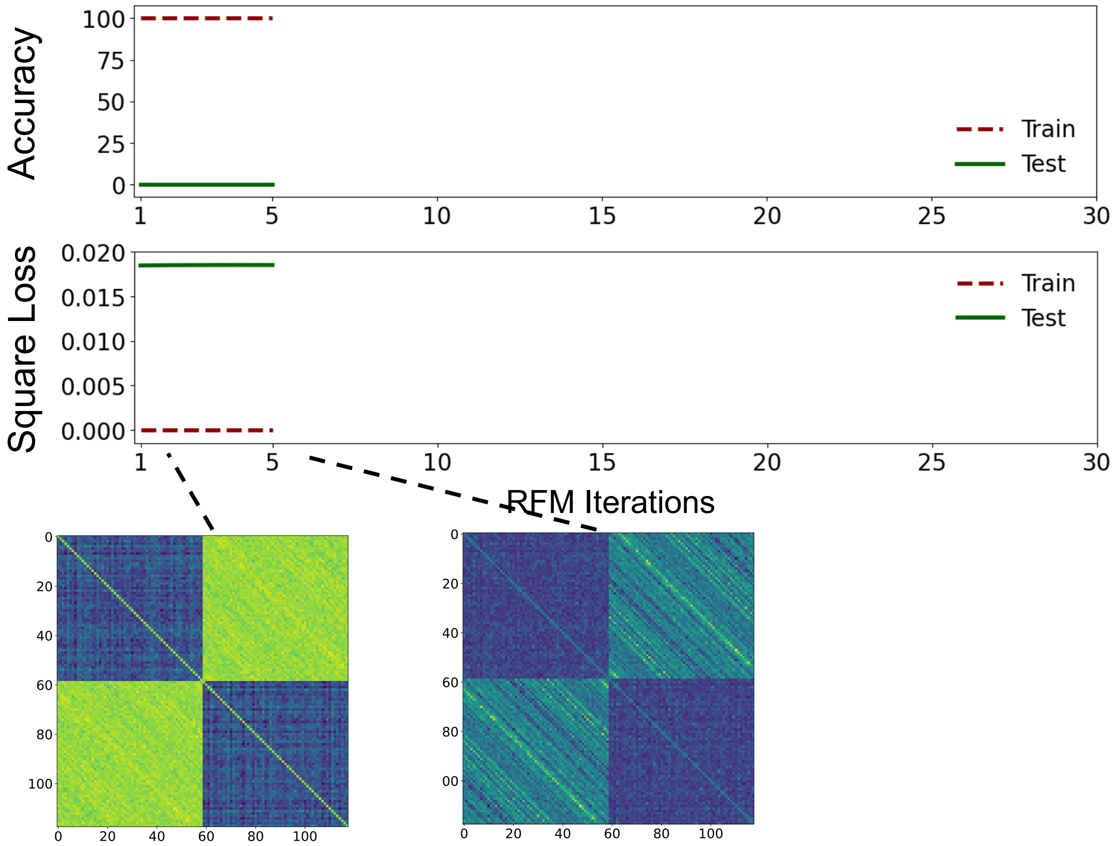
(2) Update features:

$$f(x) = \sum_{i=1}^{n} \alpha_i \, k(x, X_{tr}^{(i)}; M_1)$$
$$M_2 = AGOP(f, X_{tr})$$

Kernel RFM groks modular addition



Iteration (t): 5

(1) Solve kernel regression:

$$K_{tr} = k(X_{tr}, X_{tr}; M_5)$$
$$\alpha = K_{tr}^{-1} y_{tr}$$

(2) Update features:

$$f(x) = \sum_{i=1}^{n} \alpha_i \, k(x, X_{tr}^{(i)}; M_5)$$
$$M_6 = AGOP(f, X_{tr})$$

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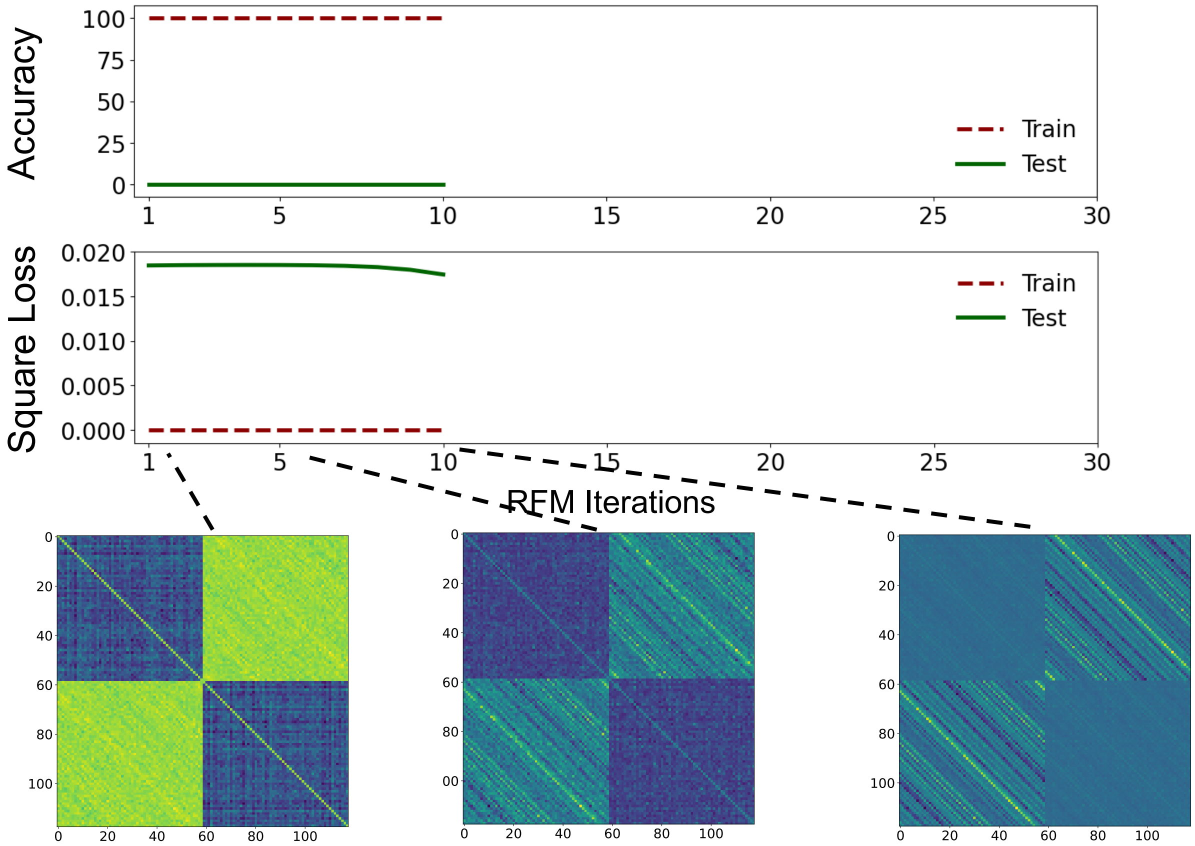

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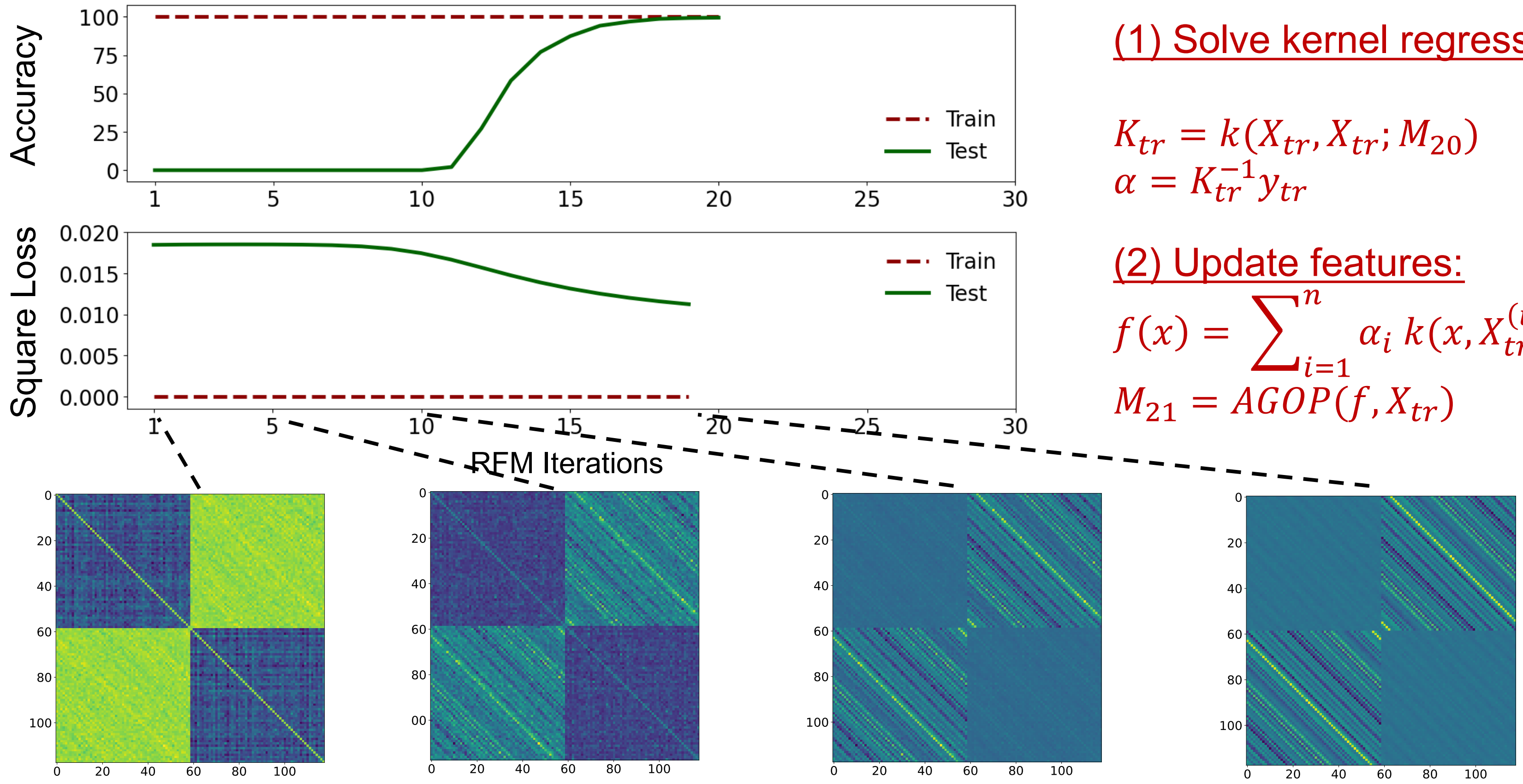


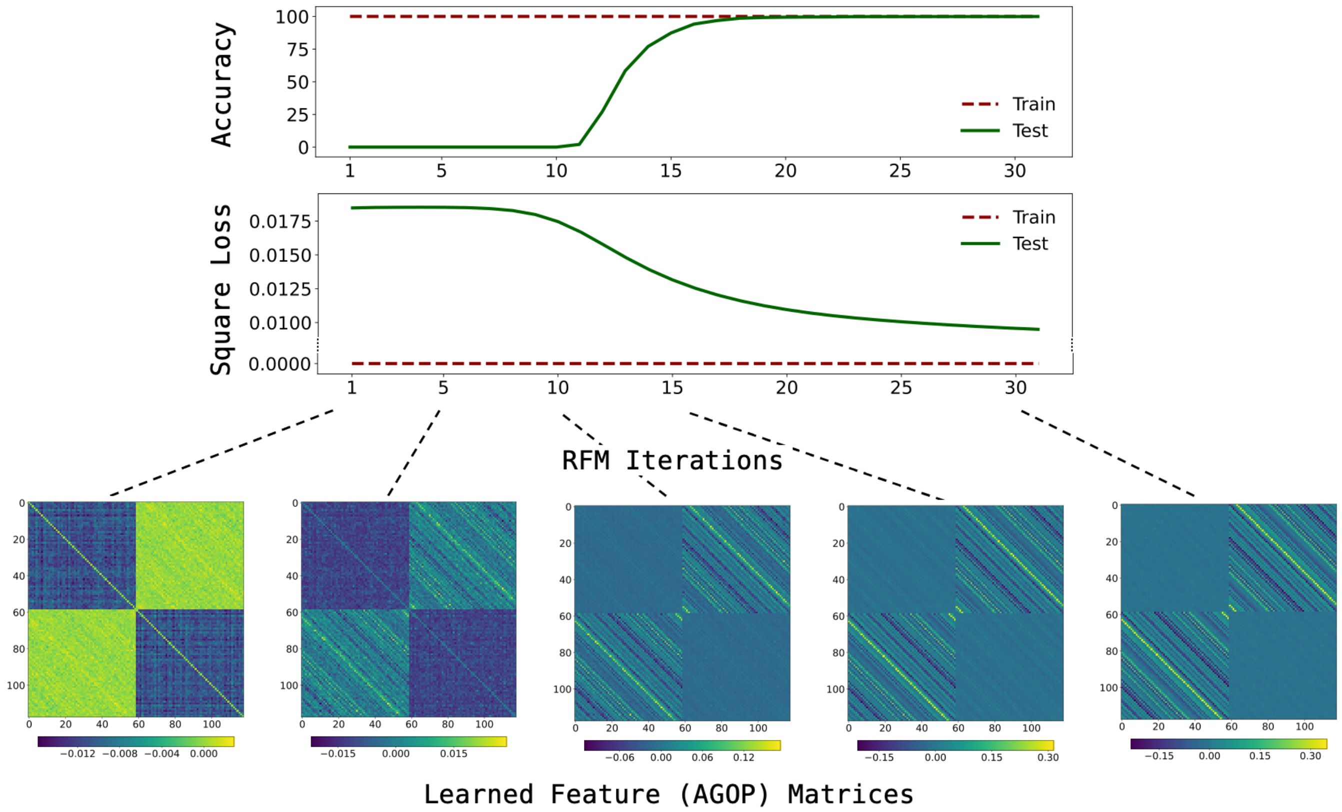
(1) Solve kernel regression:

$$K_{tr} = k(X_{tr}, X_{tr}; M_{20})$$
$$\alpha = K_{tr}^{-1} y_{tr}$$

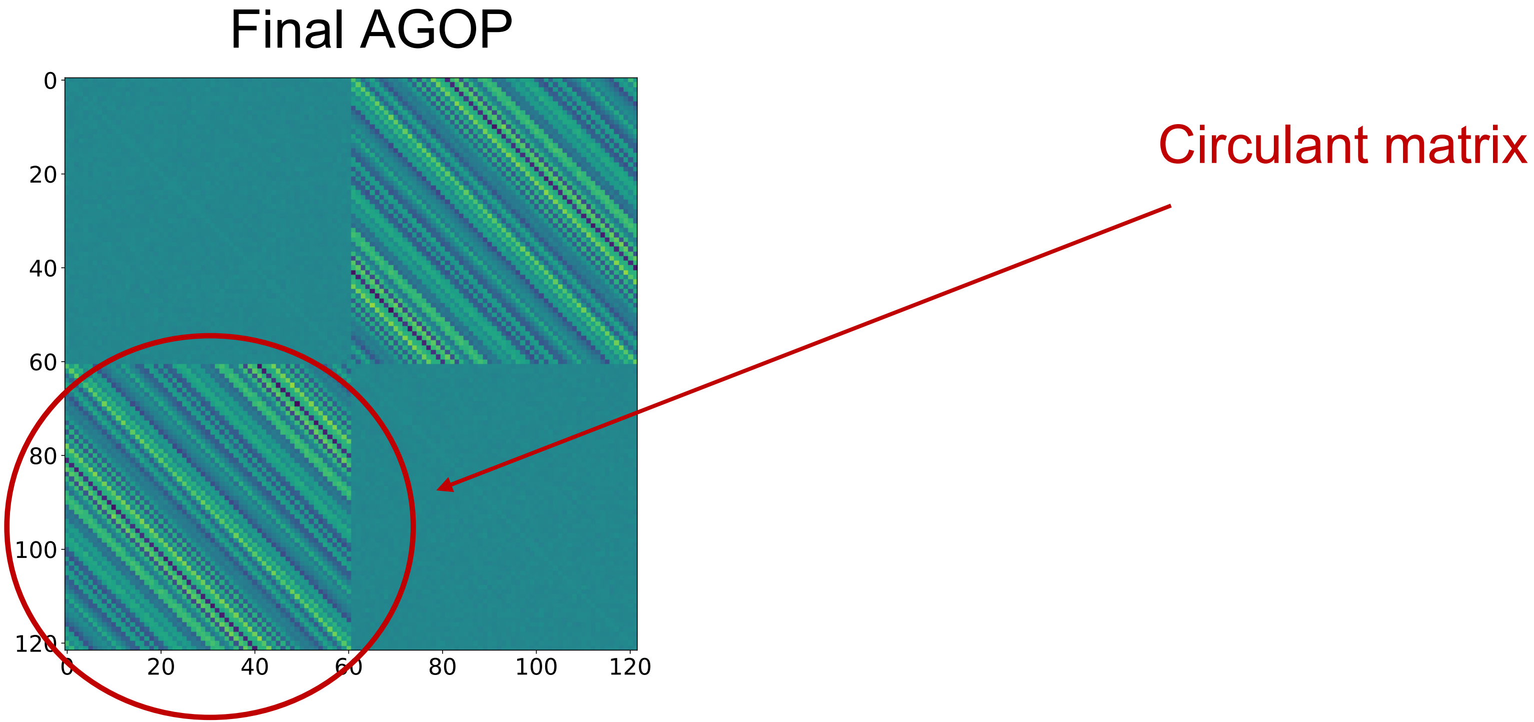
(2) Update features:

$$f(x) = \sum_{i=1}^{n} \alpha_i \, k(x, X_{tr}^{(i)}; M_{20})$$
$$M_{21} = AGOP(f, X_{tr})$$

Kernel RFM groks modular addition



What is happening under the hood for addition?



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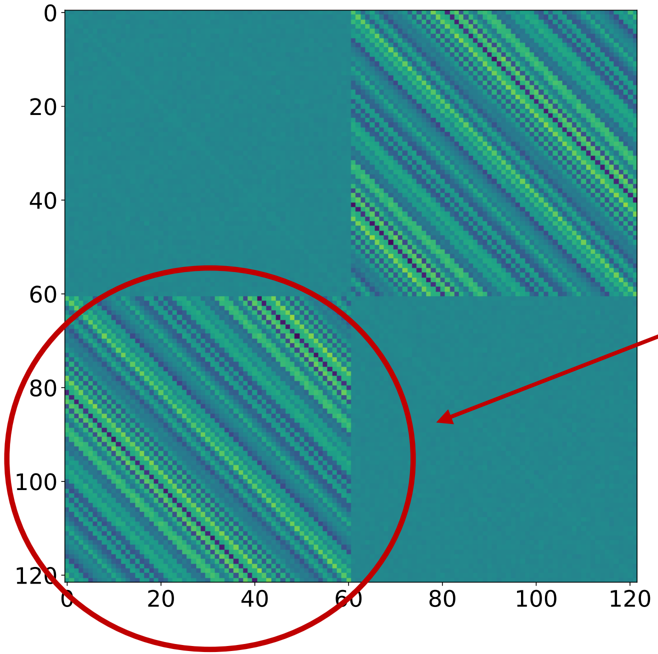
Final AGOP

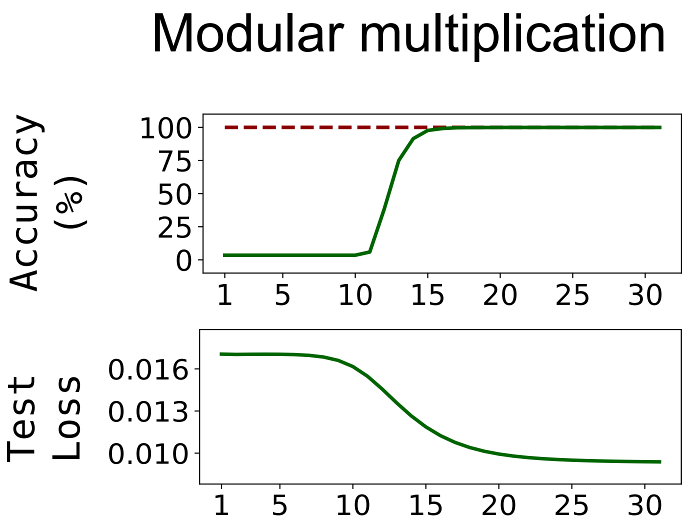


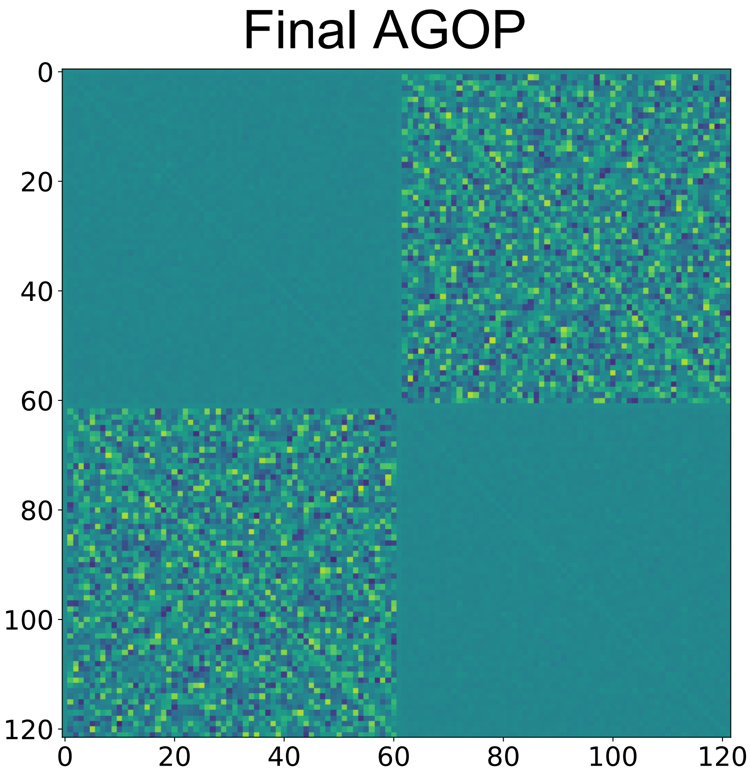
Circulant matrix

Fourier Multiplication Algorithm:

$$\arg\max(F^{-1}(Fe_a \odot Fe_b)) = (a+b) \mod p$$

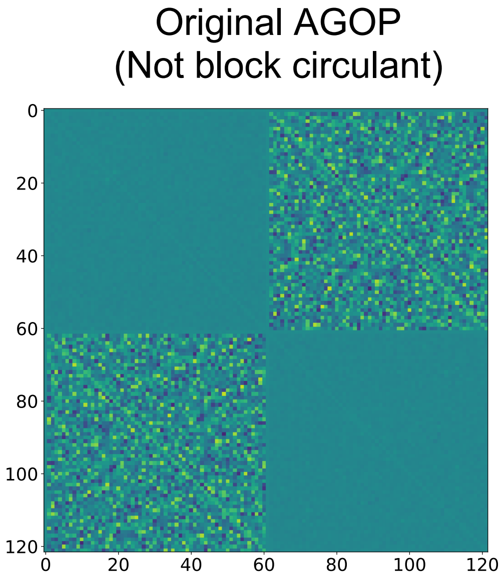
Kernel RFM groks multiplication mod p





Kernel RFM groks multiplication mod p

- Log turns multiplication into addition: log(ab) = log(a) + log(b)
- There is a notion of discrete logarithm for modular arithmetic



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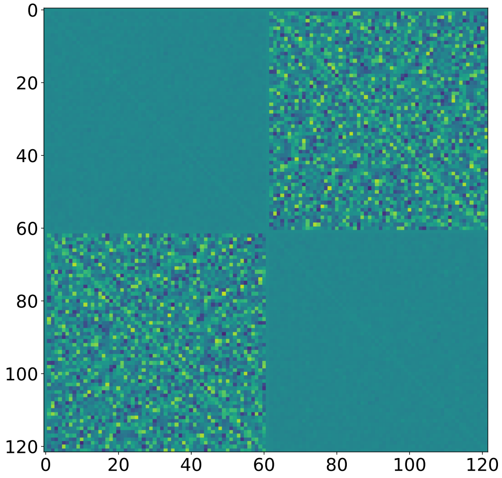
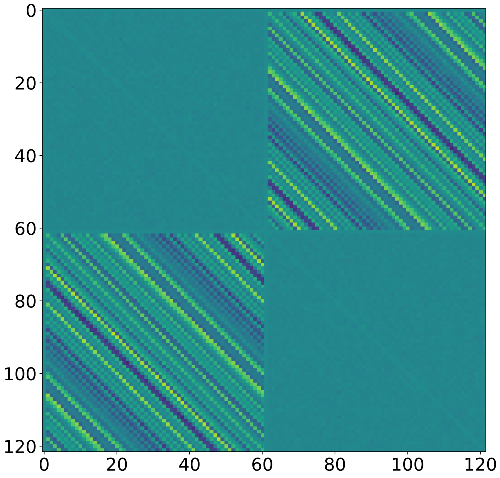
Original AGOP
(Not block circulant)

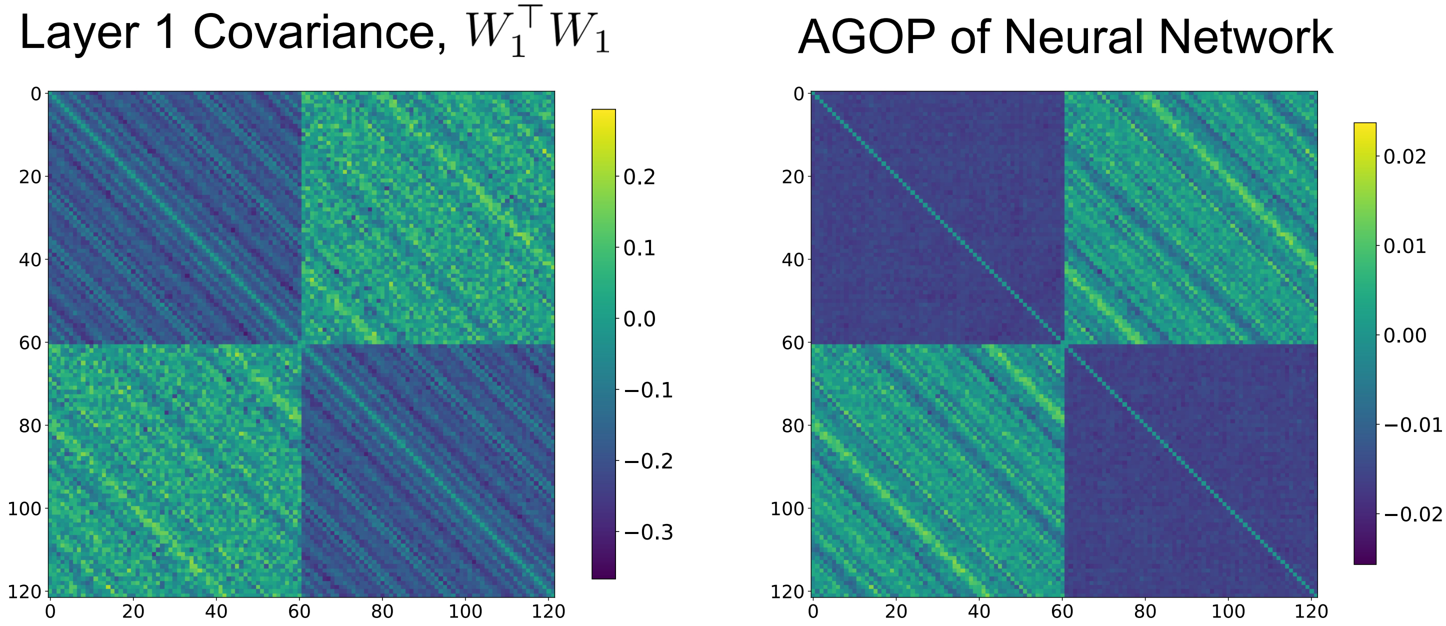


Reorder by discrete log mod p

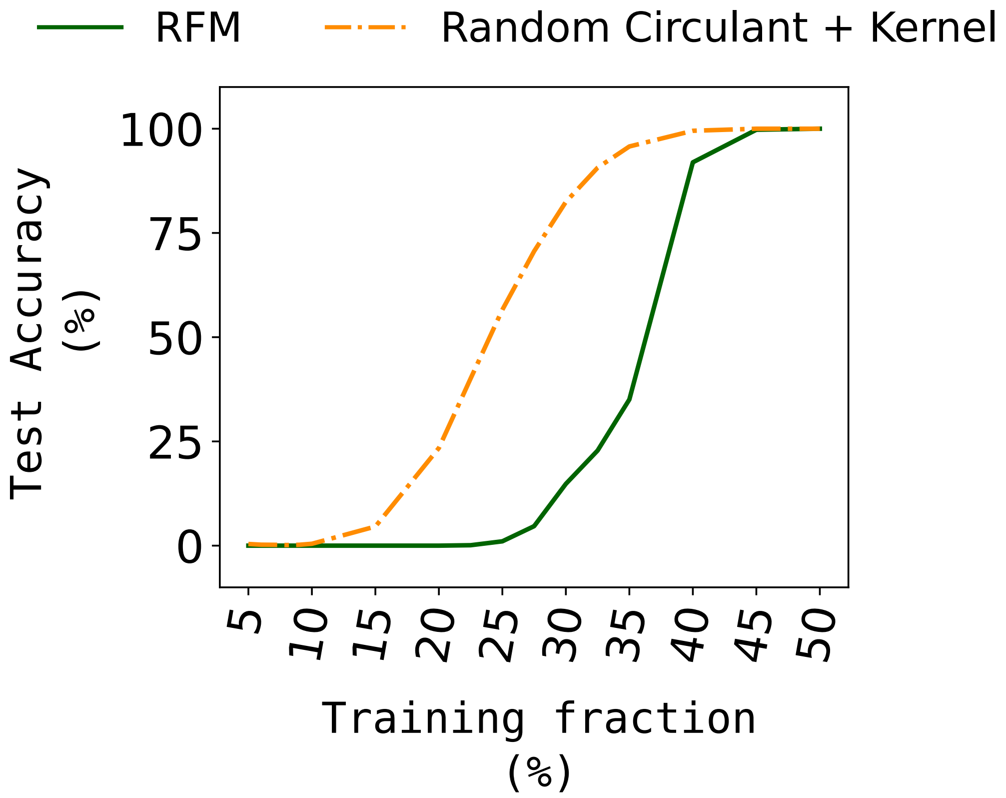
Reordered AGOP
(Block circulant)



Neural networks also learn block circulant features



Random circulant features are sufficient to generalize



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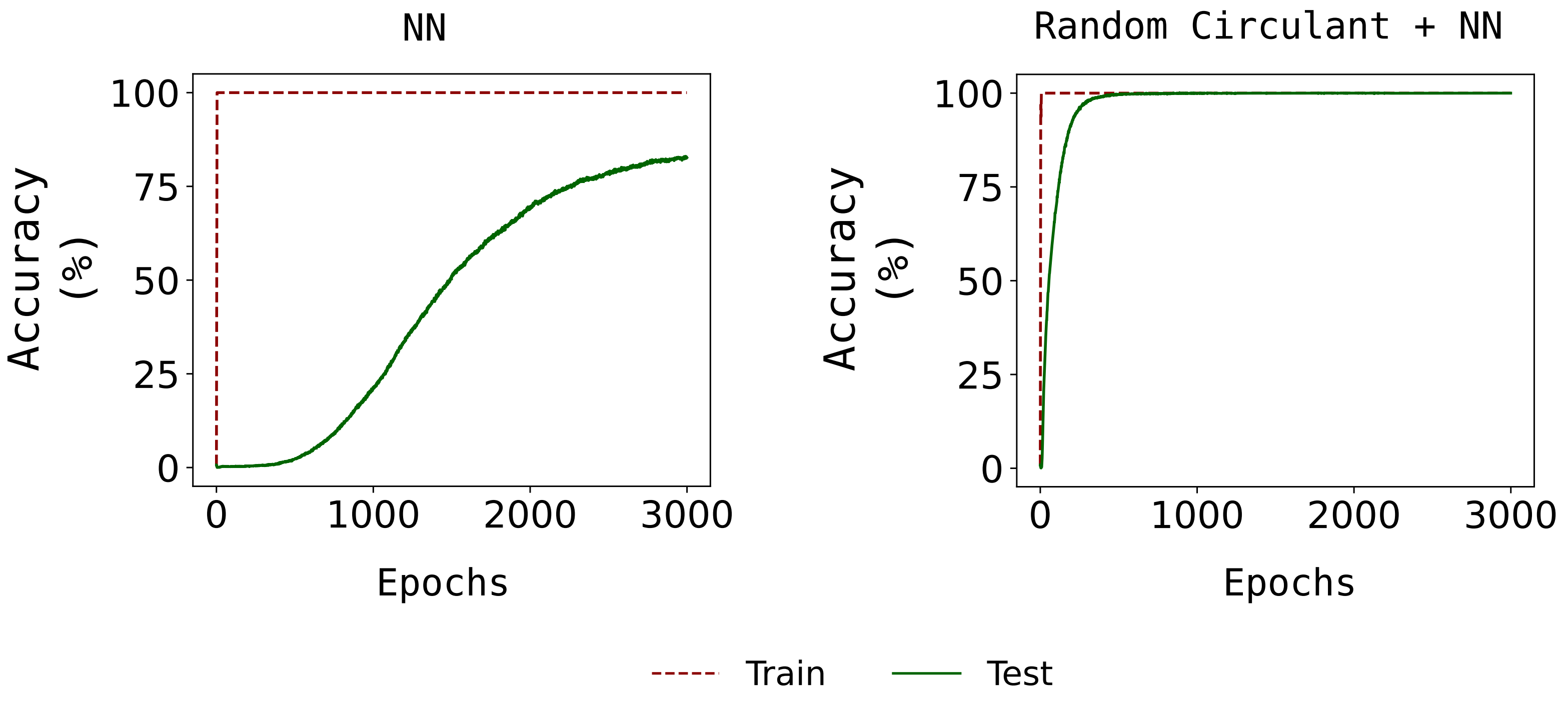
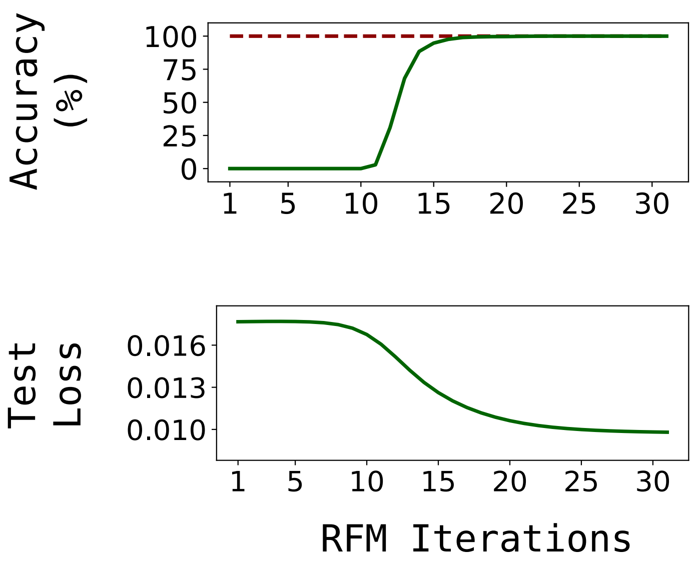


Progress measures

Back to our original question: **how do we track progress?**

“A priori” measures



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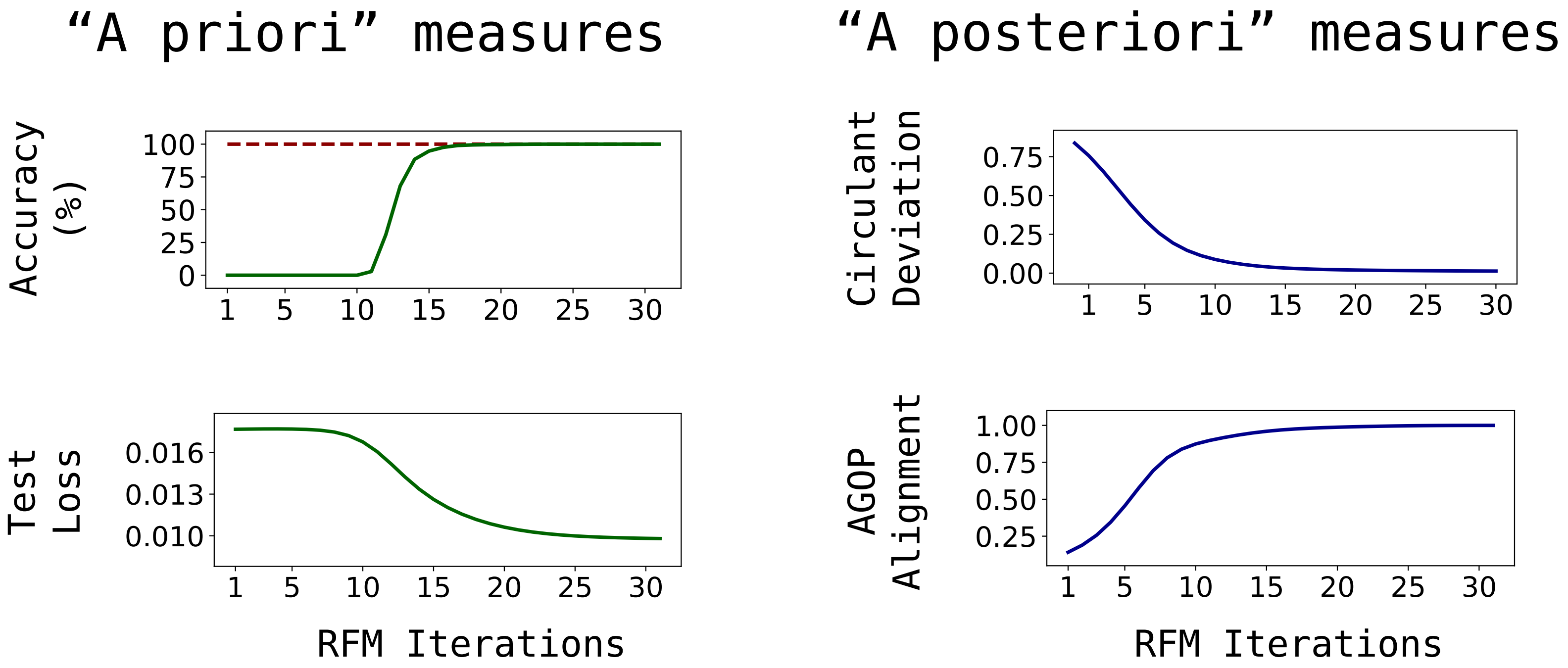

Non-neural models can grok modular arithmetic from data

1. We show for the first time that non-neural models can grok modular arithmetic from data
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2. AGOP is key to understanding feature learning
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3. Grokking modular arithmetic is NOT:
   a) tied to gradient descent based optimization methods
   b) predicted by training nor testing loss, let alone accuracy

In close collaboration with:

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The Broad Institute of MIT and Harvard

Parthe Pandit
IIT Bombay

Misha Belkin
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Thank you!

Poster session is tomorrow (Wed, July 16th) from 11am - 1:30pm!

Paper:

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P.S. I am on the job market!