Fourier Circuits in Neural Networks: Unlocking the Potential of Large Language Models in Mathematical Reasoning and Modular Arithmetic

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Background

An individual neuron and one-hidden layer neural network learning

Source "Feature emergence via margin maximization: case studies in algebraic tasks." (arXiv 2023)

Visualizing the mathematical operations learning

Source "Grokking: Generalization Beyond Overfitting on Small Algorithmic Datasets." (arXiv 2022)

The attention and MLP module in the Transformer imbues the neurons with Fourier circuit-like properties

Source "Progress measures for grokking via mechanistic interpretability." (arXiv 2023)

Motivation

Fourier power spectrum for a 1-hidden layer ReLU network and quadratic activation

Source "Feature emergence via margin maximization: case studies in algebraic tasks." (arXiv 2023)

Problem Setup

- The modular dataset
  \[ D_p := \{(a_1, \ldots, a_k), \sum_{i \in [k]} a_i : a_1, \ldots, a_k \in \mathbb{Z}_p\} \]

- One-hidden layer networks
  \[ f(\theta, x) := \sum_{i=1}^{m} \phi(\theta_i, x) \]

- A single neuron
  \[ \phi\{(u_1, \ldots, u_k, w), x_1, \ldots, x_k\} := (u_1 x_1 + \cdots + u_k x_k)^{w} \]

  - For input elements \((u_1, \ldots, u_k)\), a neuron simplifies to
    \[ \phi\{(u_1, \ldots, u_k, w), a_1, \ldots, a_k\} = (u_1 a_1 + \cdots + u_k a_k)^{w} \]

  - With \(\theta = \{u_1, \ldots, u_k, w\}\), the network is denoted as:
    \[ f(\theta, a_1, \ldots, a_k) := \sum_{i=1}^{m} \phi\{u_1, \ldots, u_k, w\}, a_1, \ldots, a_k\] 

Theoretical Results

**Theorem 1**

If \(m \geq 2^{k-1} \cdot \frac{p-1}{2}\), then the max \(L_{2,k+1}\)-margin network satisfies:

- The maximum \(L_{2,k+1}\)-margin for a given dataset \(D_h\) is:
  \[ \gamma^* = \frac{2(k!)}{(2k+2)(k+1)/2(p-1)p^{k-1}/2} \]

- For each neuron \(\phi\{(u_1, \ldots, u_k, w); a_1, \ldots, a_k\}\) there is a constant scalar \(\beta \in \mathbb{R}\) and a frequency \(\zeta \in \{1, \ldots, \frac{p-1}{2}\}\) satisfying
  \[ u_1(a_1) = \beta \cdot \cos(\theta_{u_1} + 2\pi \zeta a_1/p) \]
  \[ u_2(a_2) = \beta \cdot \cos(\theta_{u_2} + 2\pi \zeta a_2/p) \]
  \[ \vdots \]
  \[ u_k(a_k) = \beta \cdot \cos(\theta_{u_k} + 2\pi \zeta a_k/p) \]
  \[ w(c) = \beta \cdot \cos(\theta_{w} + 2\pi \zeta c/p) \]

Take-Home Message

Our research delves into the complexities of neural networks and Transformers, focusing on their strategies for solving modular addition with multiple inputs. We uncover that one-hidden layer networks, with a neuron count of \(m \geq 2^{k-2} \cdot (p-1)\), optimize an \(L_{2,k+1}\)-margin on modular arithmetic datasets, aligning each neuron with a unique Fourier spectrum for problem-solving. Corroborating empirical evidence further illuminates the computational mechanisms, notably in Transformers’ attention matrices, marking a substantial advance in deciphering their algebraic operation sophistication.