ReLU Can Compute Numerical Integration
Mechanistic Interpretation of a Non-linear Activation

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Abstract

We hypothesize that the key challenge to mechanistically interpreting MLP layers is the difficulty of compressing non-linear behavior. In this work, we extend the analysis from Nanda et al. (2023) and Zhong et al. (2023), to develop an end-to-end interpretation of the 1 layer ReLU-only modular addition transformer model. We present a new interpretation of the ReLU: that it implement quadrature schemes to carry out numerical integration, and we provide anecdotal and mathematical evidence in support.

1. Introduction

A key open problem in interpreting toy models is interpreting densely connected non-linear activations (Elhage et al., 2021; 2022). The difficulty seems tied to the expressiveness of nested nonlinearities. While deep linear networks are not any more expressive than shallow linear networks of the same width, the same is not true for nonlinear networks. As a toy model, consider simply adding or multiplying k matrices of shape $m \times m$: a complete description of input-output behavior requires only m^2 parameters, independent of k. Deep non-linear networks are not similarly compressible: inserting nonlinearities such as ReLU around binary matrix operations in our toy example blows up the effective parameter count to km^2, and complexity of the resulting function is exponential in k (Raghu et al., 2017).

In practice, we can easily compress nonlinear components that are well-approximated as linear (Nanda et al., 2023; Akyürek et al., 2023). Sparsely connected nonlinear components can also be compressed by treating activations as detecting binary ("on-off") features with scaling (Bricken et al., 2023; Olah et al., 2020; Marks et al., 2024; Elhage et al., 2022; Cunningham et al., 2023). However, per the toy model, we do not expect these conditions to be the default.

Nanda et al. (2023) and Zhong et al. (2023) provide excellent

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mechanistic interpretations of 1-layer ReLU transformers trained on modular addition. However, the MLPs of these models are neither sparse nor approximately linear. As a result, only the black-box input-output behavior of the ReLUs is described. In this work, we compress the nonlinear function using an infinite sum lens.

Briefly, we think of dense linear layers as finite approximations to an infinite-MLP-width limit. This permits us to turn summations into approximate integrals and analyze the remaining operations of the network – including the nonlinear operations – analytically. Similar to linear approximations, we validate that our approximation is sound by bounding error terms.

As an example, consider the linear layer output L_x given by

$$0.1f_x(.2)+0.11f_x(.4)+0.09f_x(.6)+0.12f_x(.8)+0.08f_x(1)$$

Taking the limit as the number of terms in the sum goes to infinity while fixing the overall total of the coefficients, we might say that this expression is roughly

$$\frac{1}{2}\sum_{i=1}^{n} f_x\left(\frac{i}{n}\right)\frac{1}{n} \quad \underset{n\to\infty}{\Longrightarrow} \quad \frac{1}{2}\int_0^1 f_x(\xi)\,\mathrm{d}\xi$$

If we can non-vacuously lower-bound the error term $E_x := |L_x - \frac{1}{2}\int_0^1 f_x(\xi)\,\mathrm{d}\xi|$ in time linear in n but *independent* of the number of input function values f_x considered, we can be assured that this approximation allows us to compress the work the linear layer is doing.

We describe the model architecture in section 2, following Nanda et al. (2023) and Zhong et al. (2023) in analysing the model by way of Fourier transform; here we present the input-output behavior specification of the MLP following Zhong et al. (2023). In section 3, we describe how using the amplitude-phase form of the Fourier series rather than the sine-cosine allows us to describe the MLP as implementing a quadrature scheme to carry out numerical integration to double the frequency of trigonometric functions, and present suggestive evidence in support. In section 4, we demonstrate how understanding of numerical integration allows us to compute and verify a non-vacuous worst-case bound on the error of the model in time linear in the parameter count. We close with a discussion in section 5 on how

our infinite-width integration approach might be extended to other models with dense nonlinearities.

2. Setup

We work with the 'pizza' model from Zhong et al. (2023): a one-layer ReLU transformer with constant attention $= \frac{1}{2}$ for all tokens, trained to compute $M : (x, y) \mapsto (x + y) \bmod p$. The model takes input (x, y) encoded as one-hot vectors, and outputs $\mathrm{logit}(x, y, z)$ for all possible values $(\bmod \, p)$, with the largest logit representing its predicted answer. Ignoring the skip connection and the biases, which are small in our model, we represent the model computation of logits as

$$\mathrm{logit}(x, y, z) \approx \sum_i \mathrm{ReLU}(\underbrace{\mathrm{OV}(x)_i + \mathrm{OV}(y)_i}_{F(x,y)_i}) \cdot (W_{\mathrm{out}})_{zi}$$

See Appendix A for a more precise equation of the model and details of the derviation whose main results are presented in this section. Here, the W_{out} matrix combines the unembed layer and final linear layer, the notation $\mathrm{OV}(x)$ represents the OVE circuit applied to the one-hot vector for x, and we have used underbraces to define the function F.

As explained in (Nanda et al., 2023), we carry out Fourier transform on the OV vectors in the token dimension and on W_{out} in the output dimension. In our model, each neuron is "single-frequency" both pre-ReLU and in the output dimension, and these frequencies match:

$$\mathrm{OV}(x)_i \approx a_i \cos(k_i x) + b_i \sin(k_i x) = c_i \cos(k_i x + \phi_i)$$
$$(W_{\mathrm{out}})_{zi} \approx e_i \cos(k_i z + \psi_i)$$

Note that, unlike Zhong et al. (2023) and Nanda et al. (2023), we use the amplitude-phase form of the Fourier series rather than the sine-cosine form; this will prove crucial to finding a relationship between W_{out} and OV that we can analyze analytically.

Using the cosine addition formula we get

$$F(x, y)_i \approx d_i \cos(k_i(x - y)/2) \cos(k_i(x + y)/2 + \phi_i)$$

and manipulating the expression for logits gives

$$\mathrm{logit}(x, y, z)$$
$$\approx \sum_i \mathrm{ReLU}((F(x, y))_i)(W_{\mathrm{out}})_{zi}$$
$$\approx \sum_k |\cos(k(x - y)/2)| \Big(\tag{1}$$
$$\{\sum_i r_i \mathrm{ReLU}[\cos(k(x + y)/2 + \phi_i)] \cos(\psi_i)\} \cos(kz)$$
$$- \{\sum_i r_i \mathrm{ReLU}[\cos(k(x + y)/2 + \phi_i)] \sin(\psi_i)\} \sin(kz) \Big)$$

with $r_i = |d_i| e_i$. Hence, after slight manipulation and factoring out the dependence on z and $x - y$, we have that the inputs to the ReLU are $\cos(k(x + y)/2) \cos(\phi_i) - \sin(k(x + y)/2) \sin(\phi_i)$, and the outputs are multiplied by $r_i \cos(\psi_i)$ and $-r_i \sin(\psi_i)$ and summed.

Letting $G_k(t) := \sum_i r_i \mathrm{ReLU}[\cos(kt/2 + \phi_i)] \cos(\psi_i)$ and $H_k(t) := \sum_i r_i \mathrm{ReLU}[\cos(kt/2 + \phi_i)] \sin(\psi_i)$, we could plot $G_k(t)$ and $H_k(t)$ for a fixed k as Zhong et al. (2023) do in their Appendices A & L, and find that they are proportional to $\cos(kt)$ and $\sin(kt)$ respectively. This gives us a black-box input-output specification for the ReLU computation, which require doing d_{mlp} computations for each of the p points.

Figure 1. A diagram showing our model architecture and existing interpretations. The question marks indicate that the explanation there is incomplete: a brute force algorithm was used to plot the graph to ensure that the result was valid over $[-\pi, \pi]$.

3. Numerical integration: infinite-width limit

We note from Figure 2 that in Equation 1, $\psi_i \approx -2\phi_i$.

Furthermore, noting that the weighted sum by r_i resembles a quadrature scheme, suppose we replaced

$$\sum_i r_i \mathrm{ReLU}[\cos(k(x + y)/2 + \phi_i)] \cos(-2\phi_i)$$

with

$$R_k \int_{-\pi}^{\pi} \mathrm{ReLU}[\cos(k(x + y)/2 + \phi)] \cos(-2\phi) \, \mathrm{d}\phi$$

and similarly for the second term. Computing the integrals:

$$\int_{-\pi}^{\pi} \cos(-2\phi) ReLU \cos(\tfrac{k}{2} + \phi) \, \mathrm{d}\phi = \tfrac{2}{3} \cos(k)$$

Figure 2. Angles for frequency $k = 12$. $\psi_i \approx -2\phi_i$ for the primary frequency of each neuron but not in general.

Figure 3. Converting the weighted sum into rectangles to estimate an integral (for frequency $k = 12$).

$$\int_{-\pi}^{\pi} \sin(-2\phi) ReLU \cos(\tfrac{k}{2} + \phi) \, d\phi = \tfrac{2}{3} \sin(k)$$

We would then recover

$$\text{logit}(x, y, z)$$
$$\approx \sum_k \frac{2}{3} R_k (\cos(k(x+y)) \cos(kz) + \sin(k(x+y)) \sin(kz))$$
$$= \sum_k \frac{2}{3} R_k \cos(k(x+y-z))$$

which matches the derivation of the final unembed layer shown in Nanda et al. (2023).

One way to make sense of the quadrature scheme is to interpret the RHS as rectangles with width r_i sampled at the point ϕ_i gives the visualization of Figure 3, as follows:

First normalise the widths r_i such that $\sum_i r_i = 2\pi$, the range of integration. Then, sort the angles and line up the

rectangles with width r_i correspondingly to form end-points $a_0 = -\pi, a_1 = -\pi + r_1, a_2 = -\pi + r_1 + r_2, \ldots, a_n = -\pi + r_1 + \ldots + r_n = \pi$.

4. Computing numerical integration error

The question then becomes a mathematical one of evaluating the efficiency of the quadrature scheme

$$\int_{-\pi}^{\pi} f(\phi) \, d\phi \approx \sum_i \frac{r_i}{R_k} f(\phi_i)$$

We first provide empirical evidence. For ease of further investigation, we split the ReLU function as

$$\text{ReLU}(x) = \frac{x}{2} + \frac{|x|}{2}$$

(i.e. respectively the 'id' component and the 'abs' component)

The maximum empirical error (obtained by evaluating the expression for each value of $x + y \pmod{p}$) is shown below:

Error Bound Type \ Freq.	12	18	21	22
Normalised abs error	0.04	0.03	0.04	0.03
Normalised id error	0.06	0.05	0.04	0.04
Numerical abs $\int$ bound	0.60	0.41	0.46	0.41
Naive abs bound	0.74	0.74	0.74	0.74

The naive bound is given by the average value of

$$\left| \int_{-\pi}^{\pi} f(\phi) \, d\phi \right|$$

and the error is given by

$$\left| \int_{-\pi}^{\pi} f(\phi) \, d\phi - \sum_i \frac{r_i}{R_k} f(\phi_i) \right|$$

We compute the error both by brute force exactly (the first two rows) and by mathematical analysis (the third row). The exact error is much smaller than the size of the integral, and the mathematical error bound is also smaller than the size of the integral. This gives convincing evidence that the model is indeed performing numerical integration.

Below we show how the mathematical error bound is produced.

Note that since the function is 2π-periodic, we can shift the intervals formed above by any constant. In what follows, when bounding approximation error, we use the shift that gives the lowest bound.

Additionally, by utilising the fact that the function $f(x)$ is actually π-periodic rather than 2π-periodic, we can overlap

Figure 4. Error bound is the red area (for frequency $k = 12$). Note how the red area includes both the actual curve and the numerical integration approximation.

the two halves of sampled points to try and reduce the error of integration. (In this way, the rectangles in the approximation are narrower and so the error would be smaller.)

The discrepancy is: $\left| \int_{-\pi}^{\pi} f(x) - f(\phi_i) \, \mathrm{d}x \right|$ where ϕ_i is the angle s.t. $x \in [a_{i-1}, a_i]$. A crude bound is:

$$\leq \int_{-\pi}^{\pi} |f(x) - f(\phi_i)| \, \mathrm{d}x$$
$$\leq \int_{-\pi}^{\pi} |x - \phi_i| \cdot \sup_x |f'(x)| \, \mathrm{d}x$$
$$\leq \sup_x |f'(x)| \sum_i \left(\int_{a_{i-1} - \phi_i}^{a_i - \phi_i} |x| \, \mathrm{d}x \right)$$

We must also include approximation error from $\psi_i \approx 2\phi_i$: we have $\sum_i r_i |\cos(k_i(x+y)/2 - \phi_i)| \cdot (\cos \psi_i - \cos 2\phi_i) \leq \sum_i r_i |\cos(k_i(x+y)/2 - \phi_i)| \cdot |\psi_i - 2\phi_i| \leq \sum_i r_i |\psi_i - 2\phi_i|$.

Using the specific frequency $k = 12$, the angle discrepancy gives us a bound of 0.15. The code for the analysis is linked here.

We can bound (analytically)

$$\sup_x |f'(x)| \leq 2$$

and the integral within the sum can be evaluated easily in $O(d_{mlp})$ time. This gives us a way of bounding the error in integration in time linear in the number of sample points (p). This bound is represented visually in Figure 4.

Using this method on our data gives a bound of 0.45, so combined with above, this gives a bound of 0.60. We can compare this bound with the brute force bound and the naive bound as shown in the table above. We also include results for the other frequencies.

Note that our bounding argument is $O(n_{\text{freq}} d_{mlp})$, while the procedure to check the maximum error is $O(p d_{mlp})$. Since there are $p d_{mlp}$ effective parameters in the MLP layer, our argument is of order square root in the number of parameters (assuming $p \approx d_{mlp}$ and $n_{\text{freq}} \ll p$). This showcases the tradeoff between computational complexity and bound accuracy as set out in Gross et al. (2024). The fact that we get a valid bound (better than the naive estimate) in sublinear time shows that our guess is very likely on the right track. However, our large bound shows that there is more to understand about how the quadrature scheme works, such as how do we align the intervals, what do the values of the ϕ_i and r_i play here, etc.

5. Discussion, interpretation, and further work

First, note the correspondence between the complexity of the argument and mechanistic understanding of the model. In the first stage, restricting each node to a single frequency (using mechanistic insight) means we only need $\mathcal{O}(p \cdot d_{mlp})$ time complexity to compute the neuron activations (the $x - y$ term can be grouped together and considered later since it is the same factor for all neurons of the same frequency). In the second stage, there is a lack of explanation of how the ReLU layer works in Zhong et al. (2023, Appendix L), where they just evaluated all the combinations in the simplified expression, to check that we indeed get $\cos(k(x+y))$ terms. Our numerical integration argument can infer about the accuracy of the scheme just by looking at the angle samples ϕ_i and ψ_i, which is $\mathcal{O}(p + d_{mlp})$ complexity. This corresponds to a better explanation of how the ReLU layer works. In particular, this argument should allow us to produce a large family of hand-coded, parameterised models which we know will perform the task well, and this family of models approximates what happens when they are trained empirically. Producing this family of models is future work.

Second, the argument presented here is not fully rigorous. We have not obtained a proof that the network as a whole indeed well-approximates numerical integration. (In fact, it is difficult even to obtain good error bounds for the 'single frequency' approximation of the neurons.) This reflects a general problem of mechanistic interpretability – a lot of the evidence is merely demonstrative or anecdotal, and something which looks 'obvious' to some human eyes may actually be impossible to prove. Thus, to have truly convincing interpretability work, we should put more effort into rigorous proofs or guarantees about the correctness of our observations and approximations.

Finally, although we have only considered one model, we hope our analysis might inspire further work on other models. It might be possible, for example, to find a scheme for using gradient descent to find denser and denser approximations to the infinite-MLP-width limit in cases where linear

layers are already dense. In such cases, we might be able to understand

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Author Contributions

Chun Hei Yip was the primary contributor to the project, running the experiments and developing the interpretation that ReLU implements quadrature. Rajashree Agrawal worked on distillation, developing the toy model and providing significant editorial feedback. Jason Gross advised the project, steering the research direction and writing of the paper.

Impact Statement

This paper presents work with the goal to advance the field of Mechanistic Interpretability. There are many potential societal consequences of our work, none which we feel must be specifically highlighted here.

References

Akyürek, E., Schuurmans, D., Andreas, J., Ma, T., and Zhou, D. What learning algorithm is in-context learning? investigations with linear models, 2023. URL https://arxiv.org/abs/2211.15661.

Bricken, T., Templeton, A., Batson, J., Chen, B., Jermyn, A., Conerly, T., Turner, N., Anil, C., Denison, C., Askell, A., Lasenby, R., Wu, Y., Kravec, S., Schiefer, N., Maxwell, T., Joseph, N., Hatfield-Dodds, Z., Tamkin, A., Nguyen, K., McLean, B., Burke, J. E., Hume, T., Carter, S., Henighan, T., and Olah, C. Towards monosemanticity: Decomposing language models with dictionary learning. *Transformer Circuits Thread*, 2023. URL https://transformer-circuits.pub/2023/monosemantic-features/index.html.

Cunningham, H., Ewart, A., Riggs, L., Huben, R., and Sharkey, L. Sparse autoencoders find highly interpretable features in language models, 2023. URL https://arxiv.org/abs/2309.08600.

Elhage, N., Nanda, N., Olsson, C., Henighan, T., Joseph, N., Mann, B., Askell, A., Bai, Y., Chen, A., Conerly, T., DasSarma, N., Drain, D., Ganguli, D., Hatfield-Dodds, Z., Hernandez, D., Jones, A., Kernion, J., Lovitt, L., Ndousse, K., Amodei, D., Brown, T., Clark, J., Kaplan, J., McCandlish, S., and Olah, C. A mathematical framework for transformer circuits. *Transformer Circuits Thread*, 2021. URL https://transformer-circuits.pub/2021/framework/index.html.

Elhage, N., Hume, T., Olsson, C., Schiefer, N., Henighan, T., Kravec, S., Hatfield-Dodds, Z., Lasenby, R., Drain, D., Chen, C., Grosse, R., McCandlish, S., Kaplan, J., Amodei, D., Wattenberg, M., and Olah, C. Toy models of superposition. *Transformer Circuits Thread*, 2022. URL https://transformer-circuits.pub/2022/toy_model/index.html.

Gross, J., Agrawal, R., Kwa, T., Ong, E., Yip, C. H., Gibson, A., Noubir, S., and Chan, L. Compact proofs of model performance via mechanistic intepretability, June 2024. URL https://arxiv.org/abs/2406.11779.

Marks, S., Rager, C., Michaud, E. J., Belinkov, Y., Bau, D., and Mueller, A. Sparse feature circuits: Discovering and editing interpretable causal graphs in language models, 2024. URL https://arxiv.org/abs/2403.19647.

Nanda, N., Chan, L., Lieberum, T., Smith, J., and Steinhardt, J. Progress measures for grokking via mechanistic interpretability. *arXiv preprint*, 2023. doi: 10.48550/arXiv.2301.05217.

Olah, C., Cammarata, N., Schubert, L., Goh, G., Petrov, M., and Carter, S. Zoom in: An introduction to circuits. *Distill*, 2020. doi: 10.23915/distill.00024.001. URL https://distill.pub/2020/circuits/zoom-in.

Raghu, M., Poole, B., Kleinberg, J., Ganguli, S., and Sohl-Dickstein, J. On the expressive power of deep neural networks, 2017. URL https://arxiv.org/abs/1606.05336.

Zhong, Z., Liu, Z., Tegmark, M., and Andreas, J. The clock and the pizza: Two stories in mechanistic explanation of neural networks, 2023.

A. Derivation of the logit expression

A more precise equation of the model is

$$\text{logit}(x, y, z) = \sum_i \text{ReLU}(\text{OV}(x)_i + \text{OV}(y)_i + \text{embed}(y)_i)$$
$$\cdot (W_{\text{out}})_{zi} + \text{residual terms} \qquad (2)$$

A more precise version of the breakdown from section 2 is

$$F_1(x, y) = \text{OV}(x) + \text{OV}(y) + \text{Embed}(y)$$
$$F_2(x, y) = W_{\text{in}} F_1(x, y) + b_{\text{in}}$$
$$\text{logits}(x, y) = W_{\text{out}} \text{ReLU}(F_2(x, y)) + b_{\text{out}} + W_U F_1(x, y)$$

where W_{in}, W_{out}, W_U, b_{in}, b_{out}, are parameters of the model.

We start with

$$\text{OV}(x)_i \approx a_i \cos(k_i x) + b_i \sin(k_i x) = a_i \cos(k_i x + \phi_i)$$

Then

$$F_1(x, y) = \text{OV}(x) + \text{OV}(y) + \text{Embed}(y)$$
$$\approx a_i(\cos(k_i x) + \cos(k_i y)) + b_i(\sin(k_i x) + \sin(k_i y))$$
$$+ \text{Embed}(y)$$
$$= c_i(\cos(k_i x + \phi_i) + \cos(k_i y + \phi_i)) + \text{Embed}(y)$$

where we use the reverse direction of the cosine addition formula

$$\cos(k_i x + \phi_i) = \cos(k_i x)\cos(\phi_i) - \sin(k_i x)\sin(\phi_i)$$

We ignore the Embed term (which is the residual stream), and use the trigonometric identity

$$\cos(x) + \cos(y) = 2\cos((x+y)/2)\cos((x-y)/2)$$

to get

$$F_2(x, y) = W_{\text{in}} F_1(x, y) + b_{\text{in}}$$
$$\approx W_{\text{in}} c_i(\cos(k_i x + \phi_i) + \cos(k_i y + \phi_i)) + b_{\text{in}}$$
$$\approx d_i \cos(k_i(x-y)/2)\cos(k_i(x+y)/2 + \phi_i)$$

where $d_i = 2(W_{\text{in}} c)_i$.

Finally, for the logit expression, using

$$(W_{\text{out}})_{zi} \approx e_i \cos(k_i z + \psi_i)$$

we have

$$\text{logits}(x, y) = W_{\text{out}} \text{ReLU}(F_2(x, y)) + b_{\text{out}} + W_U F_1(x, y)$$
$$\approx W_{\text{out}} \text{ReLU}(F_2(x, y))$$

(again ignoring the residual stream)

Then

$$\text{logits}(x, y, z)$$
$$= \sum_i \text{ReLU}((F_2(x, y))_i)(W_{\text{out}})_{zi}$$
$$\approx \sum_i \text{ReLU}(d_i \cos(k_i(x-y)/2)$$
$$\cos(k_i(x+y)/2 + \phi_i))e_i \cos(k_i z + \psi_i))$$
$$= \sum_k |\cos(k(x-y)/2|$$
$$\sum_i r_i \text{ReLU}(\cos(k(x+y)/2 + \phi_i))\cos(kz + \psi_i)$$
$$\approx \sum_k |\cos(k(x-y)/2)|$$
$$\{\sum_i r_i \text{ReLU}[\cos(k(x+y)/2 + \phi_i)]\cos(\psi_i)\}\cos(kz)$$
$$+ \{\sum_i r_i \text{ReLU}[\cos(k(x+y)/2 + \phi_i)]\sin(\psi_i)\}\sin(kz)$$

where we sum over the 'key frequencies' k (in our example $k = 12, 18, 21, 22$), $r_i = d_i e_i$, and we use again the cosine addition formula.

B. Analysis of the 'identity' component of ReLU

Recall that we broke down ReLU into two parts,

$$\text{ReLU}(x) = \frac{x}{2} + \frac{|x|}{2}$$

The integrals then split into

$$\int_{-\pi}^{\pi} \cos(-2\phi)\tfrac{1}{2}\cos(\tfrac{k}{2} + \phi)\, d\phi = \tfrac{2}{3}\cos(k)$$
$$\int_{-\pi}^{\pi} \sin(-2\phi)\tfrac{1}{2}\cos(\tfrac{k}{2} + \phi)\, d\phi = \tfrac{2}{3}\sin(k)$$
$$\int_{-\pi}^{\pi} \cos(-2\phi)\tfrac{1}{2}|\cos(\tfrac{k}{2} + \phi)|\, d\phi = 0$$
$$\int_{-\pi}^{\pi} \sin(-2\phi)\tfrac{1}{2}|\cos(\tfrac{k}{2} + \phi)|\, d\phi = 0$$

We see that the 'identity' part of the ReLU yields a zero integral. So does this part of the model contribute to the logits? It turns out that the answer is yes. To resolve this issue, we look at the discrepancy between the results suggested by previous work: Zhong et al. (2023) claim that logits are of the form

$$\text{logit}(x, y, z) \propto |\cos(k(x-y)/2)|\cos(k(x+y-z))$$

while Nanda et al. (2023) claim that logits are of the form

$$\text{logit}(x, y, z) \propto \cos(k(x+y-z))$$

To check which is correct, we regress the logits against the factors $|\cos(k(x-y)/2)|\cos(k(x+y-z))$, which

gives an R^2 of 0.86, while if we regress them against just $\cos(k(x + y - z))$, we obtain an R^2 of 0.98. So overall, Nanda et al. (2023) give a more accurate expression, but this seems to go against the analysis we did above, which led to the expression in Zhong et al. (2023). (A similar value is obtained if we just use the MLP output and drop the residual streams.) However, if we only consider the contribution to the logits from the absolute value component of ReLU, the R^2 values become 0.99 and 0.85 respectively. Therefore, although the contribution from the identity component of ReLU is small, it does make a difference towards reducing the logit dependence on $x - y$, in particular $|\cos(k(x - y)/2)|$. This is a good thing because when $\cos(k(x - y)/2)$ is small, the logit difference between the correct logit $(x + y)$ and other logits will also be small, which will lead to a higher loss. The identity component slightly counters this effect. Then

$$W_{\text{out}}\text{OV}(x)/2 + W_{\text{out}}\text{OV}(y)/2 + W_{\text{out}}\text{embed}(y)/2$$

Thus, we can store the matrices $\text{logit\_id1}[:, x] = W_{\text{out}}\text{OV}(x)/2$ and $\text{logit\_id2}[:, x] = W_{\text{out}}\text{embed}(x)/2$, then we have

$$F_2(x, y)_z = \text{residual stream} + \text{absolute value terms}$$
$$+ \text{logit\_id1}[z, x] + \text{logit\_id1}[z, y] + \text{logit\_id2}[z, y]$$

We carry out a 2D Fourier transform to find out the decomposition of the logit_id1 and logit_id2 matrices (because W_{out} and $\text{OV}(x)$ are sparse in the (1D) Fourier basis, so their product will naturally be sparse in the 2D Fourier basis). We get $\text{logit\_id1}[z, x] \approx 2\Re(\sum_k a_k e^{i(kz - 2kx)})$, where the frequencies k here are the same as section 3. Hence, the output from the identity component of ReLU is (ignoring logit_id2 for now, which comes from the residual stream and is smaller): $\sum_k D_k(\cos(kz - 2kx) + \cos(kz - 2ky)) + E_k(\sin(kz - 2kx) + \sin(kz - 2ky)) = \sum_k \cos(k(y - x))(D_k\cos(k(z - x - y)) + E_k\sin(k(z - x - y)))$.

The imaginary component of the FT is very small, $c_k \approx 0$; so the contribution is $\sum_k b_k \cos(k(y - x)) \cos(k(x + y - z))$.

Why does this happen, and why does it help explain the R^2 values we got above? We first list the approximate coefficients a_k:

Frequency	12	18	21	22
abs coefs (C_k)	13.9	15.1	12.1	11.2
id coefs (D_k)	-3.7	-3.9	-3.2	-3.3

Thus, the overall expression for the logits is

$$F_2(x, y)_z \approx \sum_k (C_k |\cos(k(y - x)/2)|$$
$$+ D_k \cos(k(y - x))) \cos(k(x + y - z))$$
$$= \sum_k (2D_k^2 |\cos(k(y - x)/2)|^2$$

$$+ C_k |\cos(k(y - x)/2)|) \cos(k(x + y - z))$$
$$- D_k \cos(k(x + y - z))$$

using double angle formula. Since $D_k < 0$, the $\sum_k -D_k \cos(k(x + y - z))$ term gives some cushion for the base performance of the model (since as we discussed, the $\cos(k(x + y - z))$ term is why the model gives the highest logit when $z = x + y$). Moreover, the $2D_k^2|\cos(k(y - x)/2)|^2$ term also further improves the model since it is always non-negative. Hence, the contribution of the identity term evens out parts of the model and improves the logit difference when $|\cos(k(y - x)/2)|$ is small (where the absolute value part doesn't do well). Note that the model would work on its own if we only use the absolute value part, but since ReLU is composed of both the absolute value and identity part and the coefficients combine both parts in a way that improve model performance.

C. Further work

There are obvious problems with generalising this sort of approach to neural network interpretation. Not only does it depend on the specifics of this problem (how we can have a specific desired formula for the logits), but also it is highly labour intensive. Thus, in order for the approach to have any practical use, we need to develop automated tools to make these approximations and interpretations. For example, we may want to use the first few terms of the Fourier expansion (or other low-rank approximations) to approximate the action of various layers in a neural network, and then combine those to get algebraic expressions for certain neuron outputs of interest. Such algebraic expressions will natural admit phenomena like the numerical integration we described above. This sort of method may be particularly fruitful on problems which Fourier transforms play a large role, such as signal processing and solutions to partial differential equations.

D. Future technical work

To complete the technical work laid out in the introduction, we must accomplish two tasks which we discuss in this appendix section: constructing a parameterisation of the MLP which is checkable in less than $\mathcal{O}(p \cdot d_{mlp})$ time, and more generally constructing a parameterisation of the entire 'pizza' model that is checkable in time that is linear in the number of parameters; and establishing a bound on the error in the model's logits that does not neglect any terms.

D.1. Linear parameterisation

Constructing a parameterisation of the model which is checkable in less than $\mathcal{O}(p \cdot d_{mlp})$ time is a relatively straightforward task, given the interpretation in the body of the paper. We expect that the parameters are:

- A choice of n_{freq} frequencies k_i.

- A splitting of the neurons into groups by frequency, and an ordering of the neurons within each group.

- An assignment of widths r_i to each neuron, and an assignment of angles ϕ_i to each neuron.

- An assignment of orthogonal planes into which each frequency is embedded by the embedding matrix, and by the unembedding matrix.

- Rotations and scaling of the low-rank subset of the hidden model dimension for each of the O and V matrices.

D.2. Bounding the error of the MLP

To bound the error of our interpreation of the MLP precisely, we'd need to include a bound on the primary frequency contribution of the identity component (which integrates to 0 symbolically), and include bounds on the residual components – OVE on x and y, the MLP bias, and the embed of y, as inputs to ReLU; and UOVE on x and y and UE on y as output logits.

We could decompose every matrix in our model as a sum of the corresponding matrix from our parameterized model and a noise term. Expanding out the resulting expression for the logits (and expanding $|x + \varepsilon|$ as $|x| + (|x + \varepsilon| - |x|)$), we will have an expression which is at top-level a sum of our parameterized model result and a noise term which is expressed recursively as the difference between the actual model and the parameterized model. We can then ask two questions:

1. What worst-case bounds can we prove on the error terms at various complexities?

2. What are the empirical worst-case bounds on the relevant error terms?