
Crafting Global Optimizers to Reasoning Tasks via Algebraic Objects in Neural Nets

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Abstract

1 We prove rich algebraic structures of the solution space for 2-layer neural net-
2 works with quadratic activation and L_2 loss, trained on reasoning tasks in Abelian
3 group (e.g., modular addition). Such a rich structure enables us to *analytically*
4 construct the global optimal solutions to the task from partial solutions that only
5 satisfy part of the loss, despite its high nonlinearity. Specifically, we show that
6 the union-ed solution space of different number of hidden nodes of the 2-layer
7 network is endowed with a semi-ring algebraic structure, and the loss function to
8 be optimized consists of *monomial potentials* which are ring homomorphism, al-
9 lowing composition of partial solutions by ring addition and multiplication. While
10 the constructed global optimizers only require small number of hidden nodes, we
11 show that overparameterization asymptotically decouples the training dynamics
12 and thus is beneficial. We further show that training dynamics move towards sim-
13 pler solutions under regularization, by proving that global optimizers algebraically
14 connected by ring multiplication are also topologically connected. Experiments
15 verify our theoretical findings.

16 1 Introduction

17 Large Language Models (LLMs) have shown impressive results in various disciplines [18, 1, 22, 4, 5,
18 11], while they also make surprising mistakes in basic reasoning tasks [17, 2]. Therefore, it remains
19 an open problem whether it can truly do reasoning tasks. On one hand, existing works demonstrate
20 that the models can learn efficient algorithm (e.g., dynamic programming [27] for language structure
21 modeling, gradient descent [24] for linear regressions, etc) and good representations [12]. Some
22 reports emergent behaviors [25] when scaling up with data and model size. On the other hand, many
23 works also show that LLMs cannot self-correct [9], and cannot generalize very well beyond the
24 training set for simple tasks [6, 28, 19], let alone complicated planning [13, 26].

25 To understand how the model performs reasoning and further improve its reasoning power, people
26 have been studying simple arithmetic reasoning problems in depth. Modular addition [16, 29], i.e.,
27 predicting $a + b \pmod d$ given a and b , is a popular one due to its simple and intuitive structure
28 yet surprising behaviors in learning dynamics (e.g., grokking [20]) and learned representations (e.g.,
29 Fourier bases [30]). Most works focus on various metrics to measure the behaviors and extracting
30 interpretable circuits from trained models [16, 23, 10]. Analytic solutions can be constructed and/or
31 reverse-engineered [8, 29, 16] but it is not clear how to generalize the results.

32 In this work, we systematically analyze 2-layer neural networks with quadratic activation and L_2 loss
33 on predicting group multiplication in Abelian group G , which is an extension of modular addition.
34 We find that global optimizers can be constructed *algebraically* from small partial solutions that are
35 optimal only for parts of the loss. We achieve this by showing that (1) for the 2-layer network, there
36 exists a *semi-ring* structure over the set of solutions *across different order* (i.e., number of hidden
37 nodes or network width), with specifically defined addition and multiplication (Def. 3), and (2) the

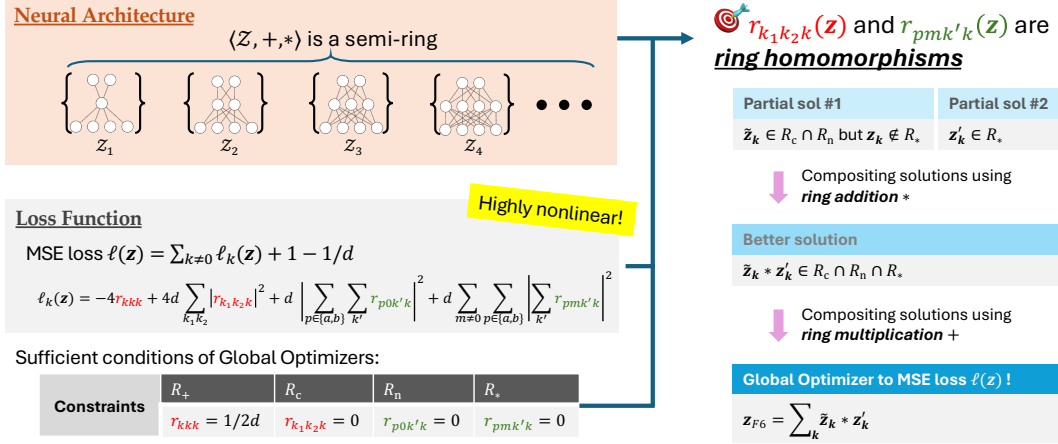


Figure 1: Overview of proposed theoretical framework CaGO. (1) The family of 1-hidden layer neural networks, \mathcal{Z} , form a *semi-ring* algebraic structure ring addition and multiplication (Theorem 2). $\mathcal{Z} = \bigcup_{q \geq 0} \mathcal{Z}_q$ where \mathcal{Z}_q is a collection of all weights (solutions) with order- q (i.e., q hidden nodes). (2) For Abelian reasoning task, the MSE loss $\ell(\mathbf{z})$ is a function of *monomial potentials* (MPs) $r_{k_1 k_2 k}(\mathbf{z})$ and $r_{pmk'k}(\mathbf{z})$ (Theorem 1), which are ring homomorphism (Theorem 3). (3) Thanks to the property of ring homomorphism, global optimizers to MSE loss $\ell(\mathbf{z})$ with quadratic activation can be constructed *algebraically* from partial solutions that only satisfy a subset of constraints (Sec. A.1) using ring addition and multiplication, instead of running gradient descent. Examples include Fourier solution \mathbf{z}_{F6} (Corollary 2) and perfect memorization solution \mathbf{z}_M (Corollary 4). In Sec. B, we analyze the role played of MPs in gradient dynamics, showing that the dynamics favors low-order global optimizers (Theorem 5) under weight decay regularization, and the dynamics of MPs become decoupled with infinite width (Theorem 6).

38 L_2 loss is a function of *monomial potentials* (MPs), which are ring homomorphisms (Theorem 1)
 39 that allow compositions of partial solutions into global ones using ring addition and multiplication.

40 As a result, our theoretical framework, named CaGO (i.e., *Crafting Global Optimizers*), successfully
 41 constructs two distinct types of Fourier-based solutions of per-frequency order 4 ($= 2 \times 2$) and
 42 order 6 ($= 2 \times 3$) that is global optimal, which are verified in the experiments, and global optimal
 43 solutions of order d^2 that correspond to perfect memorization. To our best knowledge, we are the
 44 first to discover such algebraic structures inside network training, and apply it to analyze solutions
 45 to reasoning tasks such as modular additions in details.

46 In addition, we also analyze the training dynamics of MPs. We show that the dynamics favors
 47 low-order solutions and perfect memorization is unfavorable in the dynamics, and the MP dynamics
 48 becomes decoupled when the network width goes to infinite, demystifying why overparameteriza-
 49 tion improves the performance.

50 **Most Related work.** Existing theoretical work [15] also shows group-theoretical results on alge-
 51 braic tasks related to finite groups, also for networks with one-hidden layers and quadratic activa-
 52 tions. However, they use the max-margin framework with a special regularization ($L_{2,3}$ norm) rather
 53 than MSE loss, do not characterize and leverage algebraic structures to construct solutions, and do
 54 not analyze the training dynamics.

55 2 Decoupling L_2 Loss in reasoning tasks of Abelian group

56 **Problem Setup.** We consider the following 2-layer networks with one layer of hidden nodes, trained
 57 with (projected) ℓ_2 loss on prediction of group multiplication in Abelian group G with $|G| = d$:

$$\ell = \sum_i \|P_1^\perp(\mathbf{o}[i] - l[i])\|^2, \quad \mathbf{o}[i] = V\sigma(W^\top \mathbf{f}[i]) = \sum_j \mathbf{v}_j \sigma(\mathbf{w}_j^\top \mathbf{f}[i]) \quad (1)$$

58 where $\sigma(x) = x^2$ is the quadratic activation function, $P_1^\perp = I - \frac{1}{d}\mathbf{1}\mathbf{1}^\top$ is the zero-mean projection
 59 matrix, $W = [\mathbf{w}_1, \dots, \mathbf{w}_q] \in \mathbb{R}^{d \times q}$, $V = [\mathbf{v}_1, \dots, \mathbf{v}_q]^\top \in \mathbb{R}^{d \times q}$ are learnable parameters. $\mathbf{f}[i] \in$
 60 \mathbb{R}^d are input embeddings. i is the sample index.

61 **Input and Output.** The input contains the two group elements $g_1[i]$ and $g_2[i]$, encoded as $\mathbf{f}[i] =$
62 $U_{G_1} \mathbf{e}_{g_1[i]} + U_{G_2} \mathbf{e}_{g_2[i]}$, where U_{G_1} and U_{G_2} are column orthogonal embedding matrices. The output
63 is the result $g_1[i]g_2[i] \in G$, encoded as the label $l[i] = g_1[i]g_2[i]$ to be predicted.

64 Let $\phi_k = [\phi_k(g)]_{g \in G} \in \mathbb{C}^d$ be the scaled Fourier bases (or more formally, *character function* of the
65 finite Abelian group G , see Appendix D). Then weight vector \mathbf{w}_j and \mathbf{v}_j can be written as:

$$\mathbf{w}_j = U_{G_1} \sum_{k \neq 0} z_{akj} \phi_k + U_{G_2} \sum_{k \neq 0} z_{bkj} \phi_k, \quad \mathbf{v}_j = \sum_{k \neq 0} z_{ckj} \bar{\phi}_k \quad (2)$$

66 where $\mathbf{z} := \{z_{pkj}\}$ are the complex coefficients ($p \in \{a, b, c\}$, $0 \leq k < d$ and j runs through
67 hidden nodes). Leveraging the property of quadratic activation functions, we can write down the
68 loss function analytically (see Appendix D):

69 **Theorem 1** (Analytic form of L_2 loss with quadratic activation). *The objective of 2-layer MLP*
70 *network with quadratic activation can be written as $\ell = \sum_{k \neq 0} \ell_k + (d-1)/d$, where*

$$\ell_k = -4r_{kkk} + 4d \sum_{k_1 k_2} |r_{k_1 k_2 k}|^2 + d \left| \sum_{p \in \{a, b\}} \sum_{k'} r_{p0k'k} \right|^2 + d \sum_{m \neq 0} \sum_{p \in \{a, b\}} \left| \sum_{k'} r_{pmk'k} \right|^2 \quad (3)$$

71 Here $r_{k_1 k_2 k} := \sum_j z_{ak_1 j} z_{bk_2 j} z_{ckj}$ and $r_{pmk'k} := \sum_j z_{pk'j} z_{p, m-k', j} z_{ckj}$.

72 Note that for cyclic group G , the frequency k is a mod- d integer. For general Abelian group which
73 can be decomposed into direct sum of cyclic groups according to Fundamental Theorem of Finite
74 Abelian Groups, k is a multidimensional frequency index. For convenience, we define $\phi_{-k} := \bar{\phi}_k$
75 as the conjugate representation of ϕ_k . The reason why $\phi_0 \equiv 1$ is excluded is that the constant bias
76 term has been filtered out by the top-down gradient from the loss function. Since weights are all
77 real, the Hermitian constraints holds, i.e., $\bar{z}_{ckj} = \overline{\phi_k^* \mathbf{v}_j} = \phi_{-k}^* \mathbf{v}_j = z_{c, -k, j}$ (and similar for z_{akj}
78 and z_{bkj}). Therefore, $z_{p, -k, j} = \bar{z}_{pkj}$, $r_{-k, -k, -k} = \bar{r}_{kkk}$ and ℓ is real and can be minimized.

79 **Lemma 1** (A Sufficient Conditions of Global optimizers of Eqn. 3). *If a solution \mathbf{z} to Eqn. 3 satisfies*
80 *the following, then it is a global optimizer with zero loss $\ell(\mathbf{z}) = 0$.*

$$r_{kkk}(\mathbf{z}) = \mathbb{1}(k \neq 0)/2d, \quad r_{k_1 k_2 k}(\mathbf{z}) = 0, \quad r_{pmk'k}(\mathbf{z}) = 0 \quad (4)$$

81 Lemma 1 provides a *sufficient* condition since there may exist other solutions that achieve global
82 optimum (e.g., $\sum_{k'} r_{pmk'k} = 0$). It turns out Eqn. 4 already leads to very rich algebraic structures
83 and we will not discuss more broader cases in this work.

84 3 Beyond Fixed Parameter Space: The Semi-ring structure

85 We define the *solution space* $\mathcal{Z}_q = \{\mathbf{z}\}$ to include all the weight matrices with q hidden nodes (\mathcal{Z}_0
86 means an empty network). Let $\mathcal{Z} = \bigcup_{q \geq 0} \mathcal{Z}_q$ be the solution space of all different number of hidden
87 nodes. For clarity, we use bold symbol \mathbf{z} to represent the collection of all its components $\{z_{pkj}\}$,
88 and $\mathbf{z}_1 := \{z_{pkj}^{(1)}\}$ and $\mathbf{z}_2 := \{z_{pkj}^{(2)}\}$ represent two solutions.

89 Directly finding the global optimizers to Eqn. 4 can be a bit complicated and highly non-intuitive.
90 Interestingly, the \mathcal{Z} naturally has an algebraic (semi-ring) structure, and global optimizers can be
91 composited from non-optimal ones that only satisfies a subset of terms of the loss! Both the Fourier
92 bases solution and the perfect memorization solution can be represented this way.

93 **Definition 1** (Order of \mathbf{z}). *The order $\text{ord}(\mathbf{z})$ of $\mathbf{z} \in \mathcal{Z}$ is its number of hidden nodes.*

94 **Definition 2** (Identification of \mathcal{Z}). *In \mathcal{Z} , two solutions of the same order that differ only by a per-
95 mutation along hidden dimension j are considered identical.*

96 Note that for any two solutions $\mathbf{z}_1, \mathbf{z}_2 \in \mathcal{Z}$, we can define their operations:

97 **Definition 3** (Addition and Multiplication in \mathcal{Z}). *Define $\mathbf{z} = \mathbf{z}_1 + \mathbf{z}_2$ in which $z_{pk} :=$
98 $\text{concat}(z_{pk}^{(1)}, z_{pk}^{(2)})$ and $\mathbf{z} = \mathbf{z}_1 * \mathbf{z}_2$, in which $z_{pk} := z_{pk}^{(1)} \otimes z_{pk}^{(2)}$. The addition and multipli-
99 cation respect Hermitian and the identity element $\mathbf{1}$ is the 1-order solutions with $\{z_{pk0} = 1\}$.*

100 Note that the multiplication definition is one special case of Khatri–Rao product [14]. Although
101 the Kronecker product and concatenation are not commutative, thanks to the identification (Def. 2),
102 $\mathbf{z}_1 + \mathbf{z}_2 = \mathbf{z}_2 + \mathbf{z}_1$ and $\mathbf{z}_1 * \mathbf{z}_2 = \mathbf{z}_2 * \mathbf{z}_1$ and thus both operations are commutative. Then:

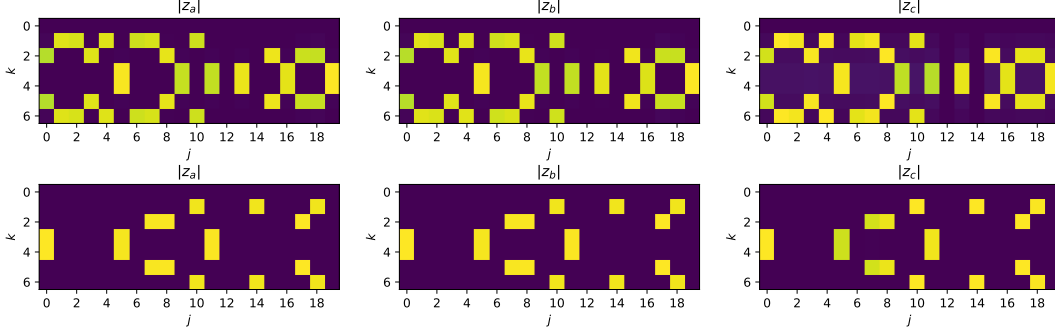


Figure 2: Solutions obtained by the Adam optimizers on ℓ_2 loss for modular addition task with $|G| = d = 7$ and $q = 20$ hidden nodes. **Top:** For each frequency $\pm k$, there are exactly 6 hidden nodes representing such a frequency, consistent with Corollary 2. **Bottom:** Optimizing Eqn. 3 without the last term $\sum_{m \neq 0} \sum_{p \in \{a, b\}} \left| \sum_{k'} r_{pmk'k} \right|^2$ (equivalently removing the constraint R_{\otimes}). Now each frequency has exactly 3 hidden nodes, which is also consistent with our analysis (Lemma 2).

103 **Theorem 2** (Algebraic Structure of \mathcal{Z}). $\langle \mathcal{Z}, +, * \rangle$ is a commutative semi-ring.

104 In the following sections, the semi-ring structure of \mathcal{Z} paves the way to construct explicitly the
 105 global optimal solutions for our ℓ_2 objectives.

106 Now let us study the structure of the loss function Eqn. 3 and how they are related to the semi-ring
 107 structure of \mathcal{Z} . For this, we first define the concept of *monomial potentials*:

108 **Definition 4** (Monomial potential (MP)). Define the monomial potential (MP) $r(\mathbf{z}) :=$
 109 $\sum_j \prod_{(p,k) \in \text{idx}(r)} z_{pkj}$ where $\text{idx}(r)$ specifies the indices involved in the monomial terms.

110 Following this definition, terms in the loss function (Theorem 1) are examples of MPs.

111 **Observation 1** (Specific MPs). $r_{k_1 k_2 k}(\mathbf{z})$ and $r_{pmk'k}(\mathbf{z})$ defined in Theorem 1 are MPs.

112 So what is the relationship between MPs, which are parts of the loss function, and the semi-ring
 113 structure of \mathcal{Z} ? The following theorem tells that, MPs are ring homomorphism.

114 **Theorem 3.** For any monomial potential $r : \mathcal{Z} \mapsto \mathbb{C}$, $r(\mathbf{1}) = 1$, $r(\mathbf{z}_1 + \mathbf{z}_2) = r(\mathbf{z}_1) + r(\mathbf{z}_2)$ and
 115 $r(\mathbf{z}_1 * \mathbf{z}_2) = r(\mathbf{z}_1)r(\mathbf{z}_2)$ and thus r is a ring homomorphism.

116 **Observation 2.** The order function $\text{ord} : \mathcal{Z} \mapsto \mathbb{N}$ is also a ring homomorphism.

117 Due to the property of ring homomorphism, we immediately know that there exists infinitely many
 118 global minimizers, via ring multiplication (Def. 3):

119 **Definition 5** (Unit). \mathbf{z} is called a unit if $r_{kkk}(\mathbf{z}) = 1$ for all $k \neq 0$.

120 **Corollary 1.** If \mathbf{z} is a global optimizer and \mathbf{y} is a unit, then $\mathbf{z} * \mathbf{y}$ is also a global optimizer.

121 More importantly, a global optimizer can be constructed from partial solutions that satisfy only some
 122 of the constraints. For example, if there exists \mathbf{z}_1 that satisfies constraint $r_1(\mathbf{z}_1) = 0$ and \mathbf{z}_2 that
 123 satisfies constraint $r_2(\mathbf{z}_2) = 0$, then their product $\mathbf{z}_1 * \mathbf{z}_2$ satisfy both constraints. In particular, we
 124 want such seed solutions to be small in order, so that the order of the final solutions is not too large.

125 4 Summary of the Appendix

126 In Appendix A, we show concrete solutions that are constructed following the semi-ring structure,
 127 including a per-frequency order-6 solution \mathbf{z}_{F6} (Corollary 2), a order-4 solution \mathbf{z}_{F4} (Corollary 3)
 128 and the perfect memorization solution \mathbf{z}_M (Corollary 4). If we remove the last term in ℓ_2 loss, then
 129 there will be order-3 solution (Lemma 2), as shown in Fig. 2.

130 We also provide gradient dynamics analysis in Appendix B that shows that the inductive bias in
 131 gradient descent prefers simpler global optimizers (Theorem 5) and overparameterization decouples
 132 gradient dynamics for each MP, and thus makes the training easier (Theorem 6). We also provide
 133 experiments to verify the claim.

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483 David Madras, Sasha Goldshtein, Willi Gierke, Tong Zhou, Yaxin Liu, Yannie Liang, Anais
484 White, Yunjie Li, Shreya Singh, Sanaz Bahargam, Mark Epstein, Sujoy Basu, Li Lao, Ad-
485 nan Ozturel, Carl Crous, Alex Zhai, Han Lu, Zora Tung, Neeraj Gaur, Alanna Walton, Lucas
486 Dixon, Ming Zhang, Amir Globerson, Grant Uy, Andrew Bolt, Olivia Wiles, Milad Nasr,
487 Iliia Shumailov, Marco Selvi, Francesco Piccinno, Ricardo Aguilar, Sara McCarthy, Misha
488 Khalman, Mrinal Shukla, Vlado Galic, John Carpenter, Kevin Vellela, Haibin Zhang, Harry
489 Richardson, James Martens, Matko Bosnjak, Shreyas Rammohan Belle, Jeff Seibert, Mah-
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491 Lenin Simicich, Laura Knight, Pulkrit Mehta, Nishesh Gupta, Chongyang Shi, Saaber Fatehi,
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493 Zhang, Damion Yates, Bhavishya Mittal, Nilesh Tripuraneni, Yannis Assael, Thomas Brov-
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496 Ruddock, Matthias Bauer, Nick Felt, Anirudh GP, Anurag Arnab, Dustin Zelle, Jonas Roth-
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499 Caswell, Carey Radebaugh, Andre Elisseeff, Pedro Valenzuela, Kay McKinney, Kim Paterson,
500 Albert Cui, Eri Latorre-Chimoto, Solomon Kim, William Zeng, Ken Durden, Priya Ponna-
501 palli, Tiberiu Sosea, Christopher A. Choquette-Choo, James Manyika, Brona Robenek, Har-
502 sha Vashisht, Sebastien Pereira, Hoi Lam, Marko Velic, Denese Owusu-Afriyie, Katherine
503 Lee, Tolga Bolukbasi, Alicia Parrish, Shawn Lu, Jane Park, Balaji Venkatraman, Alice Tal-
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505 Jessica Austin, Lu Li, Khalid Salama, Wooyeol Kim, Nandita Dukkupati, Anthony Barysh-
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507 Harry Askham, Kathryn Tunyasuvunakool, Felix Gimeno, Siim Poder, Chester Kwak, Matt
508 Miecnikowski, Vahab Mirrokni, Alek Dimitriev, Aaron Parisi, Dangyi Liu, Tomy Tsai, Toby
509 Shevlane, Christina Kouridi, Drew Garmon, Adrian Goedeckemeyer, Adam R. Brown, Anitha
510 Vijayakumar, Ali Elqursh, Sadegh Jazayeri, Jin Huang, Sara Mc Carthy, Jay Hoover, Lucy
511 Kim, Sandeep Kumar, Wei Chen, Courtney Biles, Garrett Bingham, Evan Rosen, Lisa Wang,
512 Qijun Tan, David Engel, Francesco Pongetti, Dario de Cesare, Dongseong Hwang, Lily Yu,
513 Jennifer Pullman, Srini Narayanan, Kyle Levin, Siddharth Gopal, Megan Li, Asaf Aharoni,
514 Trieu Trinh, Jessica Lo, Norman Casagrande, Roopali Vij, Loic Matthey, Bramandia Ramad-
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516 Ashraf, Kingshuk Dasgupta, Rasmus Larsen, Yicheng Wang, Manish Reddy Vuyyuru, Chong
517 Jiang, Joana Ijazi, Kazuki Osawa, Celine Smith, Ramya Sree Boppana, Taylan Bilal, Yuma
518 Koizumi, Ying Xu, Yasemin Altun, Nir Shabat, Ben Bariach, Alex Korchemniy, Kiam Choo,
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520 Cai, Shariq Iqbal, Martin Sundermeyer, Zhe Chen, Elie Bursztein, Chaitanya Malaviya, Fadi
521 Biadsy, Prakash Shroff, Inderjit Dhillon, Tejasi Latkar, Chris Dyer, Hannah Forbes, Massimo
522 Nicosia, Vitaly Nikolaev, Somer Greene, Marin Georgiev, Pidong Wang, Nina Martin, Hanie
523 Sedghi, John Zhang, Praseem Banzal, Doug Fritz, Vikram Rao, Xuezhi Wang, Jiageng Zhang,
524 Viorica Patrascu, Dayou Du, Igor Mordatch, Ivan Jurin, Lewis Liu, Ayush Dubey, Abhi
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527 Ji Liu, Madhavi Sewak, Bryce Petrini, DongHyun Choi, Ivan Philips, Ziyue Wang, Ioana
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558 A Constructing global optimizers

559 As mentioned in the main text, we find a mechanism to construct global optimizers from partial
 560 solutions that only make a subset of terms vanish in the loss function. This motivates us to find the
 561 “seed” solutions that satisfy individual constraints (MPs) in the loss, and then combine them. For
 562 this, we group MPs from the loss (Eqn. 3) into three types of constraints. Next, we discuss the partial
 563 solutions that satisfy a subset of them, which can be combined to obtain global optimizers.

564 **Definition 6** (Sets of Constraints). *Four sets of constraints exist in MSE loss (Eqn. 3):*

- 565 • *The main term constraints $R_+ := \{\mathbf{z} | r_{kkk}(\mathbf{z}) = 1/2d\}$;*
- 566 • *The cross term constraints $R_c := \{\mathbf{z} | r_{k_1 k_2 k}(\mathbf{z}) = 0 \text{ except for } k_1 = k_2 = k\}$;*
- 567 • *The norm constrains $R_n := \{\mathbf{z} | r_{p0k'k}(\mathbf{z}) = \sum_j |z_{pk'j}|^2 z_{ckj} = 0\}$;*
- 568 • *The circular convolution constraints $R_{\otimes} = \{\mathbf{z} | r_{pmk'k}(\mathbf{z}) = 0 \text{ for } m \neq 0\}$.*

569 A.1 Global Optimizers leveraging Fourier Bases

570 We first consider the case that the solution is only nonzero at frequency k_0 but not others, i.e.,
 571 $z_{pkj} = 0$ for $k \neq \pm k_0$. Such solution corresponds to Fourier bases in the original domain.

572 **Lemma 2** (Solutions satisfying R_c). *All order-1 or order-2 solutions satisfying R_c must have $r_{kkk} =$
 573 0 for all k . With small L_2 regularization, all order-3 solutions can be decomposed into $\mathbf{z} = \tilde{\mathbf{z}}_{k_0} * \mathbf{y}$
 574 for certain frequency k_0 , where $\tilde{\mathbf{z}}_{k_0} = \{\tilde{z}_{pkj}\}$ has order 3 and corresponds to Fourier bases in the
 575 original domain:*

$$\tilde{z}_{pk_0} = [1, \omega_3, \omega_3^2] / \sqrt[3]{6d} \quad (5)$$

576 where $\omega_3 := e^{-2\pi i/3}$ and \mathbf{y} is a order-1 unit.

577 Note that by simple calculation, $\tilde{\mathbf{z}}_{k_0} \in R_n$ but $\tilde{\mathbf{z}}_{k_0} \notin R_{\otimes}$. Fortunately, leveraging the property of
 578 ring homomorphism, we can construct another solution $\mathbf{z}'_{k_0} \in R_{\otimes}$ of order-2, and they combined to
 579 form global optimizers.

580 **Corollary 2** (Order-6 global optimizers of Eqn. 3). *The following “ 3×2 ” Fourier solutions satisfies
 581 the global optimality condition (Eqn. 4):*

$$\mathbf{z}_{F6} = \sum_{k=1}^{(d-1)/2} \tilde{\mathbf{z}}_k * \mathbf{z}'_k * \mathbf{y}_k \quad (6)$$

582 where \mathbf{z}'_k is order-2 (see Proof). As a result, $\text{ord}(\mathbf{z}_{F6}) = 3 \cdot 2 \cdot 1 \cdot (d-1)/2 = 3(d-1)$ and each
 583 frequency is affiliated with 6 hidden nodes (order-6).

584 Fig. 2 shows a case with $d = 7$. In this case, each frequency, out of $(d-1)/2 = 3$ total number of
 585 frequencies, is associated with 6 hidden nodes. If we remove the last term in the loss that corresponds
 586 to constraints R_{\otimes} , then an order-3 solution suffices.

587 Interestingly, there also exists a lower-order solution, 2×2 , which involves $\omega_8 := e^{-\pi i/4}$, that meets
 588 R_c and R_{\otimes} but not R_n :

589 **Corollary 3** (Order-4 “almost” global optimizers). *The following order-2 solution satisfies R_c ex-
 590 cept for $r_{k_0, k_0, -k_0} = 0$, R_{\otimes} and $r_{k_0 k_0 k_0} = 1/\sqrt{2d}$:*

$$z_{ak_0} = [1, \bar{\omega}_8^2] / \sqrt{2}, \quad z_{bk_0} = [\bar{\omega}_8, \omega_8] / \sqrt{2}, \quad z_{ck_0} = [\omega_8, \omega_8] / \sqrt{2d} \quad (7)$$

591 and the following order-2 solution satisfies $r_{k_0, k_0, -k_0} = 0$ and $r_{k_0 k_0 k_0} = 1/\sqrt{2d}$:

$$z_{ak_0} = [1, \omega_8] / \sqrt{2}, \quad z_{bk_0} = [\omega_8, \bar{\omega}_8^2] / \sqrt{2}, \quad z_{ck_0} = [\bar{\omega}_8, \omega_8] / \sqrt{2d} \quad (8)$$

592 Therefore, their product \mathbf{z}_{F4} , an “ 2×2 ” order-4 solution satisfies both R_c and R_{\otimes} .

593 Note that this solution is perceived in the experiments, in particular for larger scale problems, show-
 594 ing a strong preference of gradient descent towards lower order solutions.

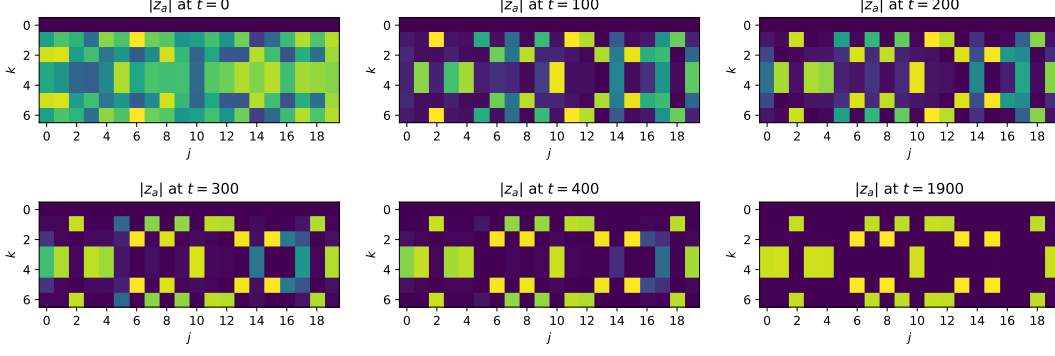


Figure 3: The convergence path of z_a , when training modular addition using Adam optimizer (learning rate 0.05, weight decay 0.005). The final solution contains 2 order-6 (z_{F6}) and 1 order-4 (z_{F4}) solutions. For each hidden node j , once a dominant frequency emerges, others fade away.

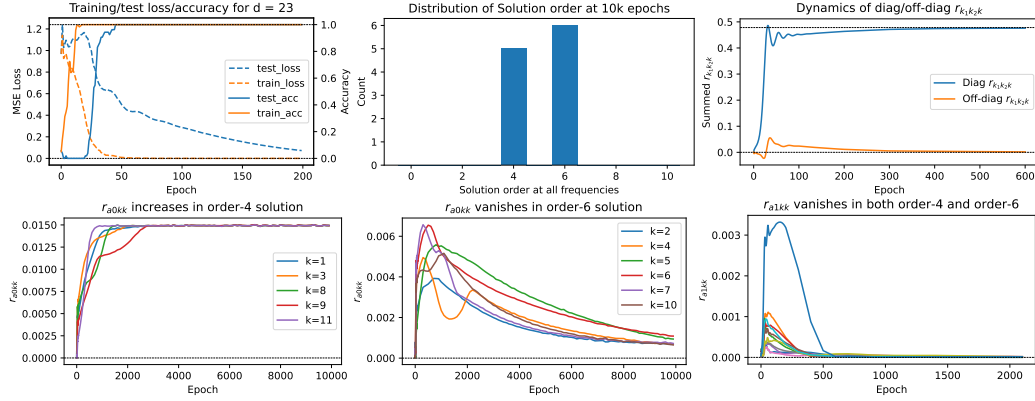


Figure 4: Dynamics of monomial potentials (MPs) over the training process for modular addition with $d = 23$ and $q = 1024$ hidden nodes. **Top Row.** *Left:* Training/test accuracy reaches 100% and loss close to 0. Test accuracy jumps after training reaches 100% (grokking). *Mid:* After 5k epochs, the distribution of solution orders are concentrated at 4 and 6 (Corollary 2,3). *Right:* Dynamics of $r_{k_1 k_2 k}$. Summation of diagonal r_{kkk} converges towards $(d-1)/2d$ (dotted line) with ripple effects, while off-diagonal $r_{k_1 k_2 k}$ converges towards 0. **Bottom Row.** Dynamics of different MPs. Note that order-4 and order-6 solutions have very different behaviors on r_{a0kk} (similar for r_{b0kk}).

595 A.2 Global Optimizers using Pure Memorization

596 We can also construct perfect memorization solutions as follows.

597 **Corollary 4** (Perfect Memorization). *Construct the following two d -order weights z_a and z_b .*
 598 *Specifically, for $0 \leq j < d$ and $k \neq 0$:*

$$z_{akj}^{(a)} = \omega_d^{kj} / \sqrt{d}, \quad z_{bkj}^{(a)} = 1 / \sqrt{d}, \quad z_{ckj}^{(a)} = \omega_d^{-kj} / \sqrt{2d} \quad (9)$$

$$z_{bkj}^{(b)} = 1 / \sqrt{d}, \quad z_{akj}^{(b)} = \omega_d^{kj} / \sqrt{d}, \quad z_{ckj}^{(b)} = \omega_d^{-kj} / \sqrt{2d} \quad (10)$$

599 where $\omega_d := e^{-2\pi i/d}$ is the d -th root of unity. Here $z_a \in R_c(k_1 \neq k) \cap R_n \cap R_{\otimes}(p = b \text{ or } m \neq k)$,
 600 $z_b \in R_c(k_2 \neq k) \cap R_n \cap R_{\otimes}(p = a \text{ or } m \neq k)$. Then $z_M = z_a * z_b$ satisfies the global optimality
 601 condition (Eqn. 4) and is the perfect memorization solution with $\text{ord}(z_M) = d^2$:

$$z_{akj_1 j_2}^{(M)} = \omega_d^{kj_1} / d, \quad z_{bkj_1 j_2}^{(M)} = \omega_d^{kj_2} / d, \quad z_{ckj_1 j_2}^{(M)} = \omega_d^{-k(j_1 + j_2)} / 2d \quad (11)$$

602 where each hidden node is indexed by $j = (j_1, j_2)$, $0 \leq j_1, j_2 < d$, $k \neq 0$.

603 To see why this corresponds to perfect memorization, simply apply an inverse Fourier transform for
 604 each hidden node (j_1, j_2) , and the original weights are (zero-mean) delta function located at j_1 , j_2
 605 and $j_1 + j_2$ accordingly.

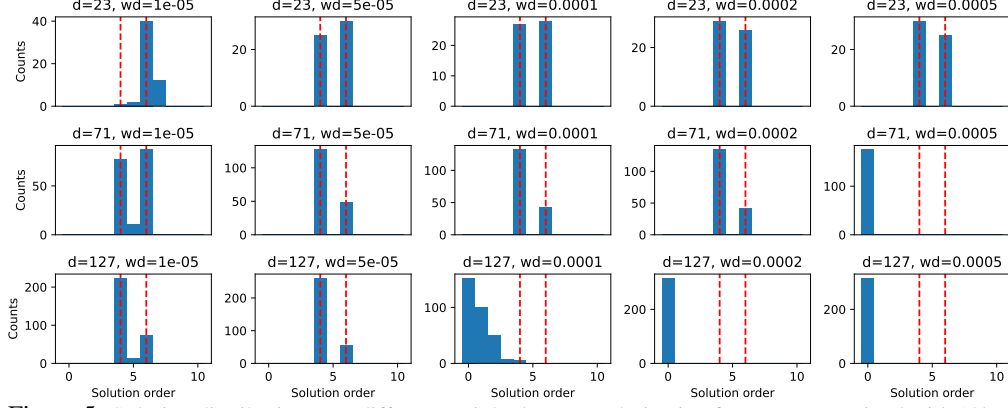


Figure 5: Solution distribution over different weight decay regularization for $q = 512$, trained with 10k epochs with Adams with learning rate 0.01 on modular addition (i.e., predicting $a+b \pmod d$) with $d \in \{23, 71, 127\}$. The two red dashed lines correspond to order-4/6 solutions. The histogram is accumulated over 5 random seeds. While heavily over-parameterized (in particular for small d), final solution order remains constant, consistent with Corollary 1. Heavy weight decay shifts the distribution to the left (i.e., low-order solutions) until model collapsing, consistent with Theorem 5.

606 B Gradient dynamics

607 Now we have characterized the structures of global optimizers. One natural question arises: why
 608 the optimization procedure does not converge to the perfect memorization solution \mathbf{z}_M , but to the
 609 Fourier solutions \mathbf{z}_{F6} and \mathbf{z}_{F4} ? The answer is given by gradient dynamics.

610 Let $\mathbf{r} = [r_{k_1 k_2 k}, r_{p m k' k}] \in \mathbb{C}^{4d^3}$ be a vector of all MPs, and $J := \frac{\partial \mathbf{r}}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathcal{W}}$ be the Jacobian matrix
 611 of the mapping $\mathbf{r} = \mathbf{r}(\mathbf{z}(\mathcal{W}))$ in which \mathcal{W} is the collection of original weights. Note that when we
 612 take derivatives with respect to \mathbf{r} and apply chain rules, we treat \mathbf{r} and its complex conjugate (e.g.,
 613 $r_{k k k}$ and $r_{-k, -k, -k} = \bar{r}_{k k k}$) as independent variables.

614 Since we run the gradient descent on \mathcal{W} , will such (indirect) optimization leads to a descent of \mathbf{r}
 615 towards the desired targets (Eqn. 4)? This is confirmed by the following theorem:

616 **Theorem 4** (Dynamics of MPs). *The dynamics of MPs satisfies $\dot{\mathbf{r}} = -J J^* \overline{\nabla_{\mathbf{r}}} \ell$, which has positive
 617 inner product with the negative gradient direction $-\overline{\nabla_{\mathbf{r}}} \ell$.*

618 Corollary 1 shows that by ring multiplication, we could create infinitely many global optima from a
 619 base one. The following theorem answers which solution gradient dynamics picks.

620 **Theorem 5** (The Occam’s Razer: Preference of low-order solutions). *If $\mathbf{z} = \mathbf{y} * \mathbf{z}'$ and both \mathbf{z} (of
 621 order q) and \mathbf{z}' are global optimal solutions, then there exists a path of zero loss connecting \mathbf{z} and \mathbf{z}'
 622 in the space of \mathcal{Z}_q . As a result, lower-order solutions are preferred if trained with L_2 regularization.*

623 This shows that gradient dynamics with weight decay will pick a lower-order (i.e., simpler) solution.
 624 Fig. 5 verifies it with experiments.

625 The following theorem shows that the dynamics also enjoys *asymptotic freedom*:

626 **Theorem 6** (Infinite Width Limits at Initialization). *Considering the modified loss of Eqn. 3 with
 627 only the first two terms: $\tilde{\ell}_k := r_{k k k} + d \sum_{k_1 k_2} |r_{k_1 k_2 k}|^2$, if the weights are i.i.d Gaussian and
 628 network width $q \rightarrow +\infty$, then $J J^*$ converge to diagonal and the dynamics of MPs is decoupled.*

629 Intuitively, this means that a large enough network width ($q \rightarrow +\infty$) makes the dynamics much
 630 easier to analyze, while the final solution may not require that large M . As analyzed in Corollary 2,
 631 for each frequency, to achieve global optimality, only 6 hidden nodes are needed.

632 **Ripple effects.** While Theorem 6 only holds at initialization, the resulting decoupled MP dynamics,
 633 e.g., $dr_{k k k}/dt = 1 - 2dr_{k k k}$ that leads to $r_{k k k}(t) = (1 - e^{-t})/2d$, already captures the rough shape
 634 of the curve (Fig. 4 top right). To capture its fine structures (e.g., ripples before stabilization), we can
 635 also model the dynamics of the diagonal element in $J J^*$. Consider a symmetric 1D case on a fixed
 636 frequency k , where all diagonal $r_{k k k} = r_0 - r$ (where $r_0 = 1/2d$) and all off-diagonal $r_{k_1 k_2 k} = r$,

637 then

$$\dot{r} = -\dot{r}_{kkk} = \kappa(r_{kkk} - r_0) = -\kappa r, \quad \dot{\kappa} = \alpha(r_0 - r_{kkk}) - (1 - \alpha)r_{k_1 k_2 k} - c_0 = (2\alpha - 1)r - c_0 \quad (12)$$

638 where $\kappa > 0$ is the diagonal element of JJ^* and α is a coefficient that characterizes the relative
639 strength of two negative gradient $-\nabla_{r_{kkk}} \ell = r_0 - r_{kkk}$ and $-\nabla_{r_{k_1 k_2 k}} \ell = -r_{k_1 k_2 k}$, and c_0 is the
640 gradient terms caused by asymmetry and/or other frequencies. This yields a second-order ODE that
641 has complex roots in the characteristic function when $c_0 > 0$.

642 C Conclusion and future work

643 In this work, we propose CaGO (*Crafting Global Optimizers*), a theoretical framework that models
644 the algebraic structure of global optimizers when training a 2-layer network on reasoning tasks of
645 Abelian group with L_2 loss. We find that the global optimizers can be algebraically composited (i.e.,
646 “crafted”) by non-optimal partial solutions that only fit to parts of the loss, using ring operations
647 defined in the solution space of the 2-layer neural networks across different network widths. Our
648 constructed solutions (i.e., z_{F4} and z_{F6} , see Corollary 3 and Corollary 2) are verified in modular
649 addition tasks. Under CaGO, we also analyze the training dynamics, show the benefit of over-
650 parameterization, and the inductive bias towards simpler solutions due to topological connectivity
651 between algebraically linked high-order (i.e., involving more hidden nodes) and low-order global
652 optimizers.

653 **Develop novel training algorithms.** Our analysis suggests that instead of applying (stochastic)
654 gradient descent to a greatly overparameterized network, we may be able to decompose the loss,
655 construct low-order solutions and combine them to achieve the final solutions on the fly using al-
656 gebraic operations. Such an approach may be more efficient (it takes a long time to get model
657 training converged), and more scalable than a holistic end2end approach using gradient descent, due
658 to its factorizable nature. Also our framework works for any loss function that is a combination of
659 monomial potentials (L_2 loss is just one example), which opens a new dimension for loss function
660 design.

661 **Putting different widths into the same framework.** Many existing theoretical works often as-
662 sume that the network has a fixed width. However, our study demonstrates that nice mathematical
663 structures can emerge when we consider networks of different widths together, which can be an
664 interesting direction to consider in the future work.

665 **Grokking.** When learning modular addition, there exists a phase transition from *memorization*
666 to *generalization* during training, known as *grokking* [23, 20], long after the training performance
667 becomes (almost) perfect. While our work focuses more on what representation is learned on a
668 uniform training data distribution, by applying it to different data distribution, grokking can be
669 studied.

670 **Extension to other activation functions.** One key assumption of our approach is that the activation
671 function is quadratic. For other activation functions (e.g., SiLU) with $\sigma(0) = 0$, we can do a Taylor
672 expansion around the origin and the same framework can still apply (with higher rank MPs).

673 **D Decoupling L_2 Loss (Proof)**

674 We use the *character function* $\phi : G \rightarrow \mathbb{C}$, which maps a group element g into a complex number.

675 **Lemma 3.** *For finite Abelian group, the character function ϕ has the following properties [7, 21]:*

- 676 • *It is a 1-dimensional (irreducible) representation of the group G , i.e., $|\phi(g)| = 1$ for $g \in G$*
677 *and for any $g_1, g_2 \in G$, $\phi(g_1 g_2) = \phi(g_1)\phi(g_2)$.*
- 678 • *There exists d character functions $\{\phi_k\}$ that satisfy the orthonormal condition*
679 *$\frac{1}{d} \sum_{g \in G} \phi_k(g) \overline{\phi_{k'}(g)} = \mathbb{1}(k = k')$. Here $\bar{\phi}$ is the complex conjugate of ϕ and is also*
680 *a character function.*
- 681 • *The set of character functions $\{\phi_k\}$ forms a character group \hat{G} under pairwise multiplication:*
682 *$\phi_{k_1+k_2} = \phi_{k_1} \circ \phi_{k_2}$.*

683 Note that the *frequency* k goes from 0 to $d - 1$, where $\phi_0 \equiv 1$ is the trivial representation (i.e., all
684 $g \in G$ maps to 1). According to the Fundamental Theorem of Finite Abelian Groups, each finite
685 Abelian group can be decomposed into a direct sum of cyclic groups, and the character function
686 of each cyclic group is exactly (scaled) Fourier bases. Therefore, in Abelian group, k is a multi-
687 dimensional frequency index. [3] shows that $\hat{G} \cong G$ (Theorem 3.13) so each character function
688 $\phi \in \hat{G}$ can also be indexed by g itself. Right now we keep the index k .

689 For convenience, we define $\phi_{-k} := \bar{\phi}_k$ as the conjugate representation of ϕ_k .

690 Let $\phi_k = [\phi_k(g)]_{g \in G} \in \mathbb{C}^d$ be the vector that contains the value of the character function ϕ_k .
691 Then $\{\phi_k\}$ form an orthogonal base in \mathbb{C}^d and we can represent the weight vector \mathbf{w}_j and \mathbf{v}_j as the
692 following:

$$\mathbf{w}_j = U_{G_1} \sum_{k \neq 0} z_{akj} \phi_k + U_{G_2} \sum_{k \neq 0} z_{bkj} \phi_k, \quad \mathbf{v}_j = \sum_{k \neq 0} z_{ckj} \bar{\phi}_k \quad (13)$$

693 where $\mathbf{z} := \{z_{pkj}\}$ are the complex coefficients ($p \in \{a, b, c\}$, $0 \leq k < d$ and j runs through hidden
694 nodes). Then it is clear that $\mathbf{w}_j^\top \mathbf{f}[i] = \sum_{k \neq 0} h_{akj} \phi_k(\iota_0(g[i])) + \sum_{k \neq 0} h_{bkj} \phi_k(x[i])$.

695 **Theorem 1** (Analytic form of L_2 loss with quadratic activation). *The objective of 2-layer MLP*
696 *network with quadratic activation can be written as $\ell = \sum_{k \neq 0} \ell_k + (d - 1)/d$, where*

$$\ell_k = -4r_{kkk} + 4d \sum_{k_1 k_2} |r_{k_1 k_2 k}|^2 + d \left| \sum_{p \in \{a, b\}} \sum_{k'} r_{p0k'k} \right|^2 + d \sum_{m \neq 0} \sum_{p \in \{a, b\}} \left| \sum_{k'} r_{pmk'k} \right|^2 \quad (3)$$

697 Here $r_{k_1 k_2 k} := \sum_j z_{ak_1 j} z_{bk_2 j} z_{ckj}$ and $r_{pmk'k} := \sum_j z_{pk'j} z_{p, m-k', j} z_{ckj}$.

698 *Proof.* Note that the objective ℓ can be written down as

$$\ell = \mathbb{E}_{g, x} [\|P_1^\perp(\mathbf{o}(g, x) - \mathbf{e}_{gx})\|^2] \quad (14)$$

$$= \mathbb{E}_{g, x} [\mathbf{o}^\top P_1^\perp \mathbf{o} - 2\mathbf{o}^\top P_1^\perp \mathbf{e}_{gx} + \mathbf{e}_{gx}^\top P_1^\perp \mathbf{e}_{gx}] \quad (15)$$

699 For $\mathbb{E}[\mathbf{o}^\top P_1^\perp \mathbf{e}_{gx}]$, since

$$\mathbf{e}_{gx}^\top P_1^\perp \mathbf{o} = \sum_j \mathbf{e}_{gx}^\top P_1^\perp \mathbf{v}_j \sigma(\mathbf{w}_j^\top \mathbf{f}(g, x)) \quad (16)$$

$$= \sum_j \left(\sum_{k' \neq 0} c_{k'j} \bar{\phi}_{k'}(gx) \right) \left(\sum_k a_{kj} \phi_k(\iota_0(g)) + b_{kj} \phi_k(x) + \mathbf{e}_g^\top \mathbf{w}_j^\perp \right)^2 \quad (17)$$

700 Note that by our previous analysis, there exists $y_1 := \iota_0(g)$ so that $gy = x_1 y$. Let $x_2 := x$. For
701 notation brevity, let $z_{akj} := a_{kj}$, $z_{bkj} := b_{kj}$ and $z_{ckj} := c_{kj}$, then we have:

$$\mathbf{e}_{gx}^\top P_1^\perp \mathbf{o} = \sum_j \left(\sum_{k' \neq 0} c_{k'j} \bar{\phi}_{k'}(x_1 x_2) \right) \left(\sum_k \sum_p z_{pkj} \phi_k(x_p) + \mathbf{e}_{x_1}^\top \mathbf{w}_j^\perp \right)^2 \quad (18)$$

702 Therefore, we have:

$$\mathbb{E}_{g,x} [\mathbf{e}_{g,x}^\top P_1^\perp \mathbf{o}] = \sum_{k_1, k_2, k' \neq 0, p_1, p_2, j} c_{k'j} z_{p_1 k_1 j} z_{p_2 k_2 j} \mathbb{E} [\bar{\phi}_{k'}(x_1) \bar{\phi}_{k'}(x_2) \phi_{k_1}(x_{p_1}) \phi_{k_2}(x_{p_2})] \quad (19)$$

703 Note that due to the fact that $\mathbb{E}_{g \in \iota_0^{-1}(x_1)} [\mathbf{e}_g^\top \mathbf{w}_j^\perp] = 0$ and $\mathbb{E}_{g \in \iota_0^{-1}(x_1)} [\mathbf{e}_g \mathbf{e}_g^\top]$ is only a function of
 704 x_1 and becomes 0 if multiplied with $\sum_{k' \neq 0} c_{k'j} \bar{\phi}_{k'}(x_1 x_2)$ and taking expectation w.r.t x_2 , in the
 705 final expression, all terms involving \mathbf{w}_j^\perp vanish.

706 Since $\mathbb{E}_x [\phi_k(x) \bar{\phi}_{k'}(x)] = \mathbb{1}(k = k')$, there are only a few cases that the summand is nonzero:

- 707 • $p_1 = 1, p_2 = 2, k' = k_1 = k_2 \neq 0$.
- 708 • $p_1 = 2, p_2 = 1, k' = k_1 = k_2 \neq 0$.

709 In both cases, the summation reduces to $\sum_{k \neq 0, j} c_{kj} z_{1kj} z_{2kj} = \sum_{k \neq 0, j} c_{kj} a_{kj} b_{kj}$. Let $r_{k_1 k_2 k'} :=$
 710 $\sum_j a_{k_1 j} b_{k_2 j} c_{k' j}$, then we have

$$\mathbb{E} [\mathbf{o}^\top P_1^\perp \mathbf{e}_{gy}] = 2 \sum_{k \neq 0, j} a_{kj} b_{kj} c_{kj} = 2 \sum_{k \neq 0} x_{kkk} \quad (20)$$

711 For $\mathbb{E} [\mathbf{o}^\top P_1^\perp \mathbf{o}]$, if $\mathbf{w}_j^\perp = 0$, then we have:

$$\mathbf{o}^\top P_1^\perp \mathbf{o} = \sum_{j, j'} \mathbf{v}_j^\top P_1^\perp \mathbf{v}_{j'} \sigma(\mathbf{w}_j^\top \mathbf{f}(g, y)) \sigma(\mathbf{w}_{j'}^\top \mathbf{f}(g, y)) \quad (21)$$

712 here

$$\mathbf{v}_j^\top P_1^\perp \mathbf{v}_{j'} = \left(\sum_{k' \neq 0} c_{k'j} \bar{\phi}_{k'} \right)^\top \left(\sum_{k'' \neq 0} \bar{c}_{k''j'} \phi_{k''} \right) = d \sum_{k' \neq 0} c_{k'j} \bar{c}_{k'j'} \quad (22)$$

713 due to the fact that $\bar{\phi}_k^\top \phi_{k'} = \sum_y \bar{\phi}_k(y) \phi_{k'}(y) = d \mathbb{1}(k = k')$.

714 Then the key part is to compute the following terms:

$$\mathbb{E}_{y_1, y_2} [z_{p_1 k_1 j_1} z_{p_2 k_2 j_1} z_{p_3 k_3 j_2} z_{p_4 k_4 j_2} c_{k' j_1} \bar{c}_{k' j_2} \phi_{k_1}(y_{p_1}) \phi_{k_2}(y_{p_2}) \phi_{k_3}(y_{p_3}) \phi_{k_4}(y_{p_4})] \quad (23)$$

715 summing over $\{p_1, p_2, p_3, p_4, k_1, k_2, k_3, k_4, k' \neq 0, j_1, j_2\}$. Note that since each $p \in \{a, b\}$, there
 716 are $2^4 = 16$ choices of (p_1, p_2, p_3, p_4) . For notation brevity, we use $(1, 3)$ to represent the subset of
 717 p that takes the value of a (e.g., $(1, 3)$ means that $p_1 = p_3 = a$ and $p_2 = p_4 = b$). It is clear that for
 718 odd assignments such as $(1, 2, 3)$, since $z_{p_0 j} = 0$, the summation is zero. Then, we only discuss the
 719 even cases as follows:

720 **Case 1:** $(1, 3), (2, 4), (1, 4), (2, 3)$. The 4 cases are identical so we only need to analyze one. We
 721 take $(1, 3)$ as an example. For $(1, 3)$, $p_1 = p_3 = a, p_2 = p_4 = b$ and the only nonzero terms is when
 722 $k_1 + k_3 = 0 \pmod d, k_2 + k_4 = 0 \pmod d$, since $\mathbb{E}_{y_1} [\phi_{k_1}(y_1) \phi_{k_3}(y_1)] = \mathbb{1}(k_1 + k_3 = 0 \pmod d)$
 723 (and similar in other cases). Then Eqn. 23 becomes:

$$\sum_{k_1, k_2, k' \neq 0} \sum_{j_1, j_2} z_{a k_1 j_1} z_{b k_2 j_1} z_{a, -k_1, j_2} z_{b, -k_2, j_2} c_{k' j_1} \bar{c}_{k' j_2} \quad (24)$$

$$= \sum_{k_1, k_2, k' \neq 0} \sum_{j_1} z_{a k_1 j_1} z_{b k_2 j_1} c_{k' j_1} \overline{\sum_{j_2} z_{a k_1 j_2} z_{b k_2 j_2} c_{k' j_2}} \quad (25)$$

$$= \sum_{k_1, k_2, k' \neq 0} \sum_{j_1} a_{k_1 j_1} b_{k_2 j_1} c_{k' j_1} \overline{\sum_{j_2} a_{k_1 j_2} b_{k_2 j_2} c_{k' j_2}} \quad (26)$$

$$= \sum_{k_1, k_2, k' \neq 0} r_{k_1 k_2 k'} \overline{r_{k_1 k_2 k'}} = \sum_{k_1, k_2, k' \neq 0} |r_{k_1 k_2 k'}|^2 \quad (27)$$

724 Since there are 4 such cases, we have:

$$\epsilon_1 = 4 \sum_{k' \neq 0} \sum_{k_1, k_2} |r_{k_1 k_2 k'}|^2 \quad (28)$$

725 **Case 2:** (1, 2) and (3, 4). The two cases are identical. Take (1, 2) as an example. In this case,
 726 $p_1 = p_2 = a$ and $p_3 = p_4 = b$. The only non-zero terms are when $k_1 + k_2 = 0$, $k_3 + k_4 = 0$. Then
 727 Eqn. 23 becomes:

$$\sum_{k_1, k_3, k' \neq 0} \sum_{j_1 j_2} z_{ak_1 j_1} \bar{z}_{ak_1 j_1} z_{bk_3 j_2} \bar{z}_{bk_3 j_2} c_{k' j_1} \bar{c}_{k' j_2} \quad (29)$$

$$= \sum_{k_1, k_3, k' \neq 0} \sum_{j_1} |a_{k_1 j_1}|^2 c_{k' j_1} \sum_{j_2} |b_{k_3 j_2}|^2 \bar{c}_{k' j_2} \quad (30)$$

$$= \sum_{k' \neq 0} \left[\sum_{j_1} \left(\sum_{k_1} |a_{k_1 j_1}|^2 \right) c_{k' j_1} \right] \left[\sum_{j_2} \left(\sum_{k_3} |b_{k_3 j_2}|^2 \right) \bar{c}_{k' j_2} \right] \quad (31)$$

728 Let $r_{amk'}^\circledast := \sum_j \left(\sum_{k_1+k_2=m} a_{k_1 j} a_{k_2 j} \right) c_{k' j}$ (similar for $r_{bmk'}^\circledast$), then the above becomes
 729 $\sum_{k' \neq 0} r_{a0k'}^\circledast \bar{r}_{b0k'}^\circledast$.

730 Similarly, for (3, 4), the above equation becomes $\sum_{k' \neq 0} \bar{r}_{a0k'}^\circledast r_{b0k'}^\circledast$. Therefore, we have:

$$\epsilon_2 = \sum_{k' \neq 0} r_{a0k'}^\circledast \bar{r}_{b0k'}^\circledast + \bar{r}_{a0k'}^\circledast r_{b0k'}^\circledast \quad (32)$$

731 Note that this term can be negative. However, we will see that when it is combined with the following
 732 terms, all terms will be non-negative.

733 **Case 3:** (1, 2, 3, 4) and (). In this case we have:

$$\sum_{k' \neq 0} \sum_{j_1 j_2} \sum_{p \in \{1, 2\}} \sum_{k_1+k_2+k_3+k_4=0} z_{pk_1 j_1} z_{pk_2 j_1} z_{pk_3 j_2} z_{pk_4 j_2} c_{k' j_1} \bar{c}_{k' j_2} \quad (33)$$

$$= \sum_{k' \neq 0} \sum_{j_1 j_2} \sum_{p \in \{1, 2\}} \sum_{k_1+k_2=k_3+k_4} z_{pk_1 j_1} z_{pk_2 j_1} \bar{z}_{pk_3 j_2} \bar{z}_{pk_4 j_2} c_{k' j_1} \bar{c}_{k' j_2} \quad (34)$$

$$= \sum_{k' \neq 0} \sum_m \sum_{p \in \{1, 2\}} \sum_{j_1 j_2} \sum_{p \in \{1, 2\}} \sum_{k_1+k_2=m} \sum_{k_3+k_4=m} z_{pk_1 j_1} z_{pk_2 j_1} \bar{z}_{pk_3 j_2} \bar{z}_{pk_4 j_2} c_{k' j_1} \bar{c}_{k' j_2} \quad (35)$$

$$= \sum_{k' \neq 0} \sum_m \sum_{p \in \{1, 2\}} \left[\sum_{j_1} \left(\sum_{k_1+k_2=m} z_{pk_1 j_1} z_{pk_2 j_1} \right) c_{k' j_1} \right] \left[\sum_{j_2} \left(\sum_{k_3+k_4=m} \overline{z_{pk_3 j_2} z_{pk_4 j_2}} \right) \bar{c}_{k' j_2} \right] \quad (36)$$

$$= \sum_{k' \neq 0} \sum_m |r_{amk'}^\circledast|^2 + |r_{bmk'}^\circledast|^2$$

734 In particular, when $m = 0$, we have $\sum_{k' \neq 0} |r_{a0k'}^\circledast|^2 + |r_{b0k'}^\circledast|^2$. Therefore, we have

$$\epsilon_2 + \epsilon_{3, m=0} = \sum_{k' \neq 0} |r_{a0k'}^\circledast|^2 + |r_{b0k'}^\circledast|^2 \quad (37)$$

735 Finally, putting them together, we have:

$$\mathbb{E} [\mathbf{o}^\top P_1^\perp \mathbf{o}] = d(\epsilon_1 + \epsilon_2 + \epsilon_3) = d(\epsilon_1 + (\epsilon_2 + \epsilon_{3, m=0}) + \epsilon_{3, m \neq 0}) \quad (38)$$

$$= d \sum_{k' \neq 0} \left(4 \sum_{k_1 k_2} |r_{k_1 k_2 k'}|^2 + |r_{a0k'}^\circledast|^2 + |r_{b0k'}^\circledast|^2 + \sum_{m \neq 0} |r_{amk'}^\circledast|^2 + |r_{bmk'}^\circledast|^2 \right) \quad (39)$$

$$\geq 0$$

736 \square

737 **Lemma 1** (A Sufficient Conditions of Global optimizers of Eqn. 3). *If a solution \mathbf{z} to Eqn. 3 satisfies*
 738 *the following, then it is a global optimizer with zero loss $\ell(\mathbf{z}) = 0$.*

$$r_{kkk}(\mathbf{z}) = \mathbb{1}(k \neq 0)/2d, \quad r_{k_1 k_2 k}(\mathbf{z}) = 0, \quad r_{pmk'k}(\mathbf{z}) = 0 \quad (4)$$

739 *Proof.* Note that $d^{-1} \sum_k r_{kkk} - \sum_k |r_{kkk}|^2$ has a minimizer $r_{kkk} = 1/2d$. Therefore, the best loss
 740 value any assignment of weights is able to achieve is the following:

$$r_{k_1 k_2 k'} = \sum_j a_{k_1 j} b_{k_2 j} c_{k' j} = \frac{1}{2d} \mathbb{1}(k_1 = k_2 = k') \quad k' \neq 0 \quad (40)$$

$$r_{a_0 k'}^{\otimes} + r_{b_0 k'}^{\otimes} := \sum_j \left(\sum_k |a_{k j}|^2 + |b_{k j}|^2 \right) c_{k' j} = 0 \quad k' \neq 0 \quad (41)$$

$$r_{a m k'}^{\otimes} := \sum_j \left(\sum_{k_1 + k_2 = m} a_{k_1 j} a_{k_2 j} \right) c_{k' j} = 0 \quad k' \neq 0, m \neq 0 \quad (42)$$

$$r_{b m k'}^{\otimes} := \sum_j \left(\sum_{k_1 + k_2 = m} b_{k_1 j} b_{k_2 j} \right) c_{k' j} = 0 \quad k' \neq 0, m \neq 0 \quad (43)$$

741 Therefore the sufficient conditions (Eqn. 4) will make all above come true. \square

742 E Semi-ring structure of \mathcal{Z} (Proof)

743 **Theorem 2** (Algebraic Structure of \mathcal{Z}). $\langle \mathcal{Z}, +, * \rangle$ is a commutative semi-ring.

744 *Proof.* Straightforward from the definition of addition and multiplication (Def. 3) and identification
 745 of hidden nodes under permutation (Def. 2). Note that ring addition (i.e., concatenation) does not
 746 have inverse and thus it is a semi-ring. \square

747 **Theorem 3.** For any monomial potential $r : \mathcal{Z} \mapsto \mathbb{C}$, $r(\mathbf{1}) = 1$, $r(\mathbf{z}_1 + \mathbf{z}_2) = r(\mathbf{z}_1) + r(\mathbf{z}_2)$ and
 748 $r(\mathbf{z}_1 * \mathbf{z}_2) = r(\mathbf{z}_1)r(\mathbf{z}_2)$ and thus r is a ring homomorphism.

749 *Proof.* Let $r(\mathbf{z}) = \sum_j \prod_{(p,k) \in \text{idx}(r)} z_{pkj}$. Since the ring identity $\mathbf{1}$ is order-1 and all $z_{pkj} = 1$, it is
 750 obvious that $r(\mathbf{1}) = 1$.

751 Let $\text{supp}(\mathbf{z}_1)$ be the subset of the hidden nodes that corresponds to \mathbf{z}_1 in the concatenated solution
 752 $\mathbf{z}_1 + \mathbf{z}_2$, similar for $\text{supp}(\mathbf{z}_2)$. Note that

$$r(\mathbf{z}_1 + \mathbf{z}_2) = \sum_{j \in \text{supp}(\mathbf{z}_1)} \prod_{(p,k) \in \text{idx}(r)} z_{pkj}^{(1)} + \sum_{j \in \text{supp}(\mathbf{z}_2)} \prod_{(p,k) \in \text{idx}(r)} z_{pkj}^{(2)} = r(\mathbf{z}_1) + r(\mathbf{z}_2) \quad (44)$$

753 On the other hand, we have

$$r(\mathbf{z}_1 * \mathbf{z}_2) = \sum_{j_1 j_2} \prod_{(p,k) \in \text{idx}(r)} \left(z_{pkj_1}^{(1)} z_{pkj_2}^{(2)} \right) \quad (45)$$

$$= \sum_{j_1 j_2} \left(\prod_{(p,k) \in \text{idx}(r)} z_{pkj_1}^{(1)} \right) \left(\prod_{(p,k) \in \text{idx}(r)} z_{pkj_2}^{(2)} \right) \quad (46)$$

$$= \left(\sum_{j_1} \prod_{(p,k) \in \text{idx}(r)} z_{pkj_1}^{(1)} \right) \left(\sum_{j_2} \prod_{(p,k) \in \text{idx}(r)} z_{pkj_2}^{(2)} \right) \quad (47)$$

$$= r(\mathbf{z}_1)r(\mathbf{z}_2) \quad (48)$$

754 \square

755 **Corollary 1.** If \mathbf{z} is a global optimizer and \mathbf{y} is a unit, then $\mathbf{z} * \mathbf{y}$ is also a global optimizer.

756 *Proof.* Straightforward by leveraging the property of ring homomorphism. E.g.,

$$r_{kkk}(\mathbf{z} * \mathbf{y}) = r_{kkk}(\mathbf{z})r_{kkk}(\mathbf{y}) = r_{kkk}(\mathbf{z}) \quad (49)$$

757 and the proof is complete. \square

758 **F Solution Construction (Proof)**

759 **Lemma 2** (Solutions satisfying R_c). *All order-1 or order-2 solutions satisfying R_c must have $r_{kkk} =$*
 760 *0 for all k . With small L_2 regularization, all order-3 solutions can be decomposed into $\mathbf{z} = \tilde{\mathbf{z}}_{k_0} * \mathbf{y}$*
 761 *for certain frequency k_0 , where $\tilde{\mathbf{z}}_{k_0} = \{\tilde{z}_{pkj}\}$ has order 3 and corresponds to Fourier bases in the*
 762 *original domain:*

$$\tilde{z}_{pk_0} = [1, \omega_3, \omega_3^2] / \sqrt[3]{6d} \quad (5)$$

763 where $\omega_3 := e^{-2\pi i/3}$ and \mathbf{y} is a order-1 unit.

764 *Proof.* We first prove that $\tilde{\mathbf{z}}_{k_0}$ satisfies R_c . To see this, we have

$$r_{k_1 k_2 k} = \sum_j \mathbb{1}(k_1 = k_2 = k = k_0) \omega_3^{3j} + \sum_j \mathbb{1}(-k_1 = k_2 = k = k_0) \omega_3^j \quad (50)$$

$$+ \dots + \sum_j \mathbb{1}(-k_1 = -k_2 = -k = k_0) \bar{\omega}_3^{3j} \quad (51)$$

$$= 3\mathbb{1}(k_1 = k_2 = k = k_0) + 3\mathbb{1}(k_1 = k_2 = k = -k_0) \quad (52)$$

765 Note that all cross terms are gone since $\sum_j \omega_3^j = 0$. It is clear that $r_{k_1 k_2 k} \neq 0$ unless $k_1 = k_2 = k$
 766 so \mathbf{z}_0 satisfies R_c .

767 To show the reverse direction, first notice that for any order-1 solution, for any k , in order to make
 768 $r_{k, -k, k} = z_{ak0} z_{b, -k, 0} z_{ck0} = z_{ak0} \bar{z}_{bk0} z_{ck0} = 0$, either z_{ak0} , z_{bk0} or z_{ck0} has to be zero, which
 769 means that $r_{kkk} = 0$.

770 For order-2, first of all if any $z_{pk0} = 0$ for any $p \in \{a, b, c\}$, then a constraint like $r_{k, k, -k} =$
 771 $z_{ak0} z_{bk0} \bar{z}_{ck0} + z_{ak1} z_{bk1} \bar{z}_{ck1} = 0$ yields $z_{ak1} z_{bk1} z_{ck1} = 0$ and thus $r_{kkk} = 0$. If not, then for any two
 772 complex numbers z_{pk0} and z_{pk1} , there always exist four real numbers $\theta_p \in (-\pi, \pi]$, $\theta'_p \in (-\pi, \pi]$,
 773 $m_{p0} > 0$ and $m_{p1} > 0$ so that

$$z_{pk0} = m_{p0} e^{i\theta'_p} e^{i\theta_p}, \quad z_{pk1} = m_{p1} e^{i\theta'_p} e^{-i\theta_p} \quad (53)$$

774 Then a constraint like $r_{k, k, -k} = z_{ak0} z_{bk0} \bar{z}_{ck0} + z_{ak1} z_{bk1} \bar{z}_{ck1} = 0$ can be written as $z_{ak0} z_{bk0} \bar{z}_{ck0} =$
 775 $-z_{ak1} z_{bk1} \bar{z}_{ck1}$, or equivalently:

$$m_{a0} m_{b0} m_{c0} e^{i(\theta'_a + \theta'_b + \theta'_c)} e^{i(\theta_a + \theta_b - \theta_c)} = -m_{a1} m_{b1} m_{c1} e^{i(\theta'_a + \theta'_b + \theta'_c)} e^{-i(\theta_a + \theta_b - \theta_c)} \quad (54)$$

$$m_{a0} m_{b0} m_{c0} e^{i\theta_a} e^{i\theta_b} e^{-i\theta_c} = -m_{a1} m_{b1} m_{c1} e^{-i\theta_a} e^{-i\theta_b} e^{i\theta_c} \quad (55)$$

776 Comparing their magnitude and phase, we have $m_{a0} m_{b0} m_{c0} = m_{a1} m_{b1} m_{c1}$ and

$$\theta_a + \theta_b - \theta_c = \pm\pi/2 \pmod{2\pi} \quad (56)$$

777 Similarly, we have:

$$\theta_a + \theta_c - \theta_b = \pm\pi/2 \pmod{2\pi}, \quad \theta_b + \theta_c - \theta_a = \pm\pi/2 \pmod{2\pi} \quad (57)$$

778 Solving the three equations and we have 6 solutions:

$$(\theta_a, \theta_b, \theta_c) = (0, 0, \pm\pi/2) \pmod{2\pi} \quad (58)$$

$$(\theta_a, \theta_b, \theta_c) = (0, \pm\pi/2, 0) \pmod{2\pi} \quad (59)$$

$$(\theta_a, \theta_b, \theta_c) = (\pm\pi/2, 0, 0) \pmod{2\pi} \quad (60)$$

779 For all such solutions, we have $r_{kkk} = 0$.

780 For order-3 solutions, for each k , let $a_j := z_{akj}$, $b_j := z_{bkj}$ and $c_j := z_{ckj}$. Let $\mathbf{a} = [a_j] \in \mathbb{C}^3$,
 781 $\mathbf{b} = [b_j] \in \mathbb{C}^3$ and $\mathbf{c} = [c_j] \in \mathbb{C}^3$. Then the conditions yield that

$$(\mathbf{a} \circ \bar{\mathbf{b}})^\top \mathbf{c} = 0, \quad (\mathbf{a} \circ \bar{\mathbf{b}})^\top \bar{\mathbf{c}} = 0, \quad (\bar{\mathbf{a}} \circ \mathbf{b})^\top \mathbf{c} = 0, \quad (\bar{\mathbf{a}} \circ \mathbf{b})^\top \bar{\mathbf{c}} = 0 \quad (61)$$

782 which means that in \mathbb{R}^3 space, the following condition holds:

$$\text{span}(\Re(\mathbf{a} \circ \bar{\mathbf{b}}), \Im(\mathbf{a} \circ \bar{\mathbf{b}})) \perp \text{span}(\Re(\mathbf{c}), \Im(\mathbf{c})) \quad (62)$$

783 where $\Re(\cdot)$ and $\Im(\cdot)$ are real and imaginary parts of a complex vector. Since Eqn. 62 holds in \mathbb{R}^3 ,
 784 it must be the case that either $\Re(\mathbf{a} \circ \bar{\mathbf{b}})$ is co-linear with $\Im(\mathbf{a} \circ \bar{\mathbf{b}})$, or $\Re(\mathbf{c})$ is co-linear with $\Im(\mathbf{c})$.

785 If the former is true (i.e., there exists β so that $\Re(\mathbf{c}) = \beta\Im(\mathbf{c})$), then there exists a scalar θ so that
 786 $\mathbf{c}e^{-i\theta} = \mathbf{c}_R \in \mathbb{R}^3$, since all angles in the components of \mathbf{c} are the same. Then we have:

$$r_{kkk} = (\mathbf{a} \circ \mathbf{b})^\top \mathbf{c} = (\mathbf{a} \circ \mathbf{b})^\top \bar{\mathbf{c}}e^{2i\theta} = 0 \quad (63)$$

787 If the latter is true, then there exists $\theta_{a\bar{b}}$ so that

$$(\mathbf{a} \circ \bar{\mathbf{b}})e^{-i\theta_{a\bar{b}}} \in \mathbb{R}_+^3 \quad (64)$$

788 Applying the same reasoning symmetrically, in order to find cases such that $r_{kkk} \neq 0$, a necessary
 789 condition is that

$$(\mathbf{a} \circ \bar{\mathbf{b}})e^{-i\theta_{a\bar{b}}} \in \mathbb{R}_+^3, \quad (\mathbf{b} \circ \bar{\mathbf{c}})e^{-i\theta_{b\bar{c}}} \in \mathbb{R}_+^3, \quad (\mathbf{c} \circ \bar{\mathbf{a}})e^{-i\theta_{c\bar{a}}} \in \mathbb{R}_+^3 \quad (65)$$

790 with the condition that $\theta_{a\bar{b}} + \theta_{b\bar{c}} + \theta_{c\bar{a}} = 0 \pmod{2\pi}$. To determine these angles, we look at a_0, b_0
 791 and c_0 and their angles $\theta_{a_0}, \theta_{b_0}$, and θ_{c_0} , it is clear that

$$\theta_{a\bar{b}} = \theta_{a_0} - \theta_{b_0} \pmod{2\pi} \quad (66)$$

$$\theta_{b\bar{c}} = \theta_{b_0} - \theta_{c_0} \pmod{2\pi} \quad (67)$$

$$\theta_{c\bar{a}} = \theta_{c_0} - \theta_{a_0} \pmod{2\pi} \quad (68)$$

792 Therefore, if we multiple \mathbf{a}, \mathbf{b} and \mathbf{c} with $e^{-i\theta_{a_0}}, e^{-i\theta_{b_0}}$ and $e^{-i\theta_{c_0}}$, and still note the resulting vectors
 793 to be \mathbf{a}, \mathbf{b} and \mathbf{c} , then we have:

$$\mathbf{a} \circ \bar{\mathbf{b}} \in \mathbb{R}_+^3, \quad \mathbf{b} \circ \bar{\mathbf{c}} \in \mathbb{R}_+^3, \quad \mathbf{c} \circ \bar{\mathbf{a}} \in \mathbb{R}_+^3 \quad (69)$$

794 Note that is equivalent to a decomposition of \mathbf{z} into a multiplication of 1-order term and another
 795 3-order term. Then we have $\theta_{a_0} = \theta_{b_0} = \theta_{c_0} = \theta_0 = 0, \theta_{a_1} = \theta_{b_1} = \theta_{c_1} = \theta_1, \theta_{a_2} = \theta_{b_2} = \theta_{c_2} =$
 796 θ_2 .

797 Letting $m_j := |a_j||b_j||c_j|$, then the corresponding r_{kkk} can be written as:

$$r_{kkk} = \sum_{j=0}^2 m_j e^{3i\theta_j} \quad (70)$$

798 with the constraints that $\sum_{j=0}^2 m_j e^{i\theta_j} = 0$ imposed by R_A . One interesting question is that what
 799 is the minimal norm representation that achieves the highest objective? For this we can solve the
 800 following optimization problem:

$$\max_{\{m_j, \theta_j\}} \sum_j m_j (e^{3i\theta_j} + e^{-3i\theta_j}) - \epsilon \sum_j m_j^2 \quad \text{s.t.} \quad \sum_j m_j e^{i\theta_j} = 0 \quad (71)$$

801 which achieves the maximal when $m_j = 1/\epsilon, \theta_1 = 2\pi j/3$ and $\theta_2 = 4\pi j/3$ (or vice versa). Note
 802 that θ_j is fixed no matter how small the regularization ϵ is.

803 To see that, let $u_j := e^{i\theta_j}$. Then we have:

$$\sum_j m_j (u_j + \bar{u}_j)^3 = \sum_j m_j [u_j^3 + 3u_j\bar{u}_j(u_j + \bar{u}_j) + \bar{u}_j^3] = \sum_j m_j (u_j^3 + \bar{u}_j^3) \quad (72)$$

804 Therefore, we can instead solve the following optimization in \mathbb{R} :

$$\max_{\{m_j, -2 \leq x_j \leq 2, x_0=2\}} \sum_j m_j x_j^3 - \epsilon \sum_j m_j^2 \quad \text{s.t.} \quad \sum_j m_j x_j = 0 \quad (73)$$

805 whose solutions give a sufficient condition. Using Lagrangian multiplier, we have:

$$\frac{\partial L}{\partial x_j} = m_j(3x_j^2 - \lambda) = 0, \quad \frac{\partial L}{\partial m_j} = x_j^3 - 2\epsilon m_j - \lambda x_j = 0 \quad (74)$$

806 which leads to $\lambda = 3, m_j = 1/\epsilon$ and $x_1 = x_2 = -1$. Therefore, $u_1 = \omega_3$ and $u_2 = \omega_3^2$ for 3-th root
 807 of unity $\omega_3 = e^{2\pi i/3}$ (or vice versa).

808 **Constructing $\mathbf{z}' \in R_{\otimes}$.** It is clear that $r_{pmk_0k_0}(\tilde{\mathbf{z}}_{k_0}) \neq 0$ for $m = \pm 2k_0$ so $\tilde{\mathbf{z}}_{k_0} \notin R_{\otimes}$. We
 809 construct \mathbf{z}' of order-2 so that $r_{pmk_0k_0}(\mathbf{z}'_{k_0}) = 0$:

$$\mathbf{z}'_{pk1} = \mathbb{I}(k = k_0)\xi_p + \mathbb{I}(k = -k_0)\bar{\xi}_p, \quad \mathbf{z}'_{pk2} = \mathbb{I}(k = k_0)\bar{\xi}_p + \mathbb{I}(k = -k_0)\xi_p \quad (75)$$

810 with the constraint that $\Re(\xi_p^2 \xi_c) = 0$ (i.e., pure imaginary) for $p \in \{a, b\}$ so that $r_{pmk_0k_0}(\mathbf{z}') =$
 811 $\xi_p^2 \xi_c + \bar{\xi}_p^2 \bar{\xi}_c = 0$, but $\Re(\xi_a \xi_b \xi_c) > 0$ so that $r_{k_0k_0k_0} = \xi_a \xi_b \xi_c + \bar{\xi}_a \bar{\xi}_b \bar{\xi}_c > 0$. This is possible, e.g.,
 812 by setting $\xi_b = \bar{\xi}_a = e^{\pm \pi i/4}$ (i.e., ω_8 or $\bar{\omega}_8$), $\xi_c = 1$. \square

813 **Corollary 4** (Perfect Memorization). *Construct the following two d -order weights \mathbf{z}_a and \mathbf{z}_b .*
 814 *Specifically, for $0 \leq j < d$ and $k \neq 0$:*

$$z_{akj}^{(a)} = \omega_d^{kj} / \sqrt{d}, \quad z_{bkj}^{(a)} = 1 / \sqrt{d}, \quad z_{ckj}^{(a)} = \omega_d^{-kj} / \sqrt{2d} \quad (9)$$

$$z_{bkj}^{(b)} = 1 / \sqrt{d}, \quad z_{akj}^{(b)} = \omega_d^{kj} / \sqrt{d}, \quad z_{ckj}^{(b)} = \omega_d^{-kj} / \sqrt{2d} \quad (10)$$

815 *where $\omega_d := e^{-2\pi i/d}$ is the d -th root of unity. Here $\mathbf{z}_a \in R_c(k_1 \neq k) \cap R_n \cap R_{\otimes}(p = b \text{ or } m \neq k)$,*
 816 *$\mathbf{z}_b \in R_c(k_2 \neq k) \cap R_n \cap R_{\otimes}(p = a \text{ or } m \neq k)$. Then $\mathbf{z}_M = \mathbf{z}_a * \mathbf{z}_b$ satisfies the global optimality*
 817 *condition (Eqn. 4) and is the perfect memorization solution with $\text{ord}(\mathbf{z}_M) = d^2$:*

$$z_{akj_1j_2}^{(M)} = \omega^{kj_1} / d, \quad z_{bkj_1j_2}^{(M)} = \omega^{kj_2} / d, \quad z_{ckj_1j_2}^{(M)} = \omega^{-k(j_1+j_2)} / 2d \quad (11)$$

818 *where each hidden node is indexed by $j = (j_1, j_2)$, $0 \leq j_1, j_2 < d$, $k \neq 0$.*

819 *Proof.* Simply plugging in the solution and check whether the equations specified the equations. For
 820 \mathbf{z}_a , for $k = 0$ everything is zero; for $k \neq 0$, we have:

$$r_{k_1k_2k}(\mathbf{z}_a) = \sum_j a_{k_1j} b_{k_2j} c_{kj} = \frac{1}{d\sqrt{2d}} \sum_j \omega^{j(k_1-k)} = \frac{1}{\sqrt{2d}} \mathbb{1}(k_1 = k \neq 0) \quad (76)$$

$$r_{amk'k}(\mathbf{z}_a) = \sum_j a_{k'j} a_{m-k',j} c_{kj} = \frac{1}{d\sqrt{2d}} \sum_j \omega^{j(m-k)} = \frac{1}{\sqrt{2d}} \mathbb{1}(m = k \neq 0) \quad (77)$$

$$r_{bmk'k}(\mathbf{z}_a) = \sum_j b_{k'j} b_{m-k',j} c_{kj} = \frac{1}{d\sqrt{2d}} \sum_j \omega^{-jk} = \frac{1}{\sqrt{2d}} \mathbb{1}(k = 0) = 0 \quad (78)$$

(79)

821 Therefore, $\mathbf{z}_a \in R_c(k_1 \neq k) \cap R_n \cap R_{\otimes}(p = b \text{ or } m \neq k)$. Similar for \mathbf{z}_b . For $\mathbf{z}_M := \mathbf{z}_a * \mathbf{z}_b$,
 822 it satisfies all constraints (i.e., for any r , either \mathbf{z}_a satisfies with $r(\mathbf{z}_a) = 0$, or \mathbf{z}_b satisfies with
 823 $r(\mathbf{z}_b) = 0$) and we have:

$$r_{kkk}(\mathbf{z}_a * \mathbf{z}_b) = r_{kkk}(\mathbf{z}_a) r_{kkk}(\mathbf{z}_b) = 1/2d \quad (80)$$

824 So \mathbf{z}_M satisfies the sufficient conditions (Eqn. 4). \square

825 G Gradient Dynamics (Proof)

826 **Theorem 4** (Dynamics of MPs). *The dynamics of MPs satisfies $\dot{\mathbf{r}} = -JJ^* \overline{\nabla_{\mathbf{r}} \ell}$, which has positive*
 827 *inner product with the negative gradient direction $-\overline{\nabla_{\mathbf{r}} \ell}$.*

828 *Proof.* By gradient descent of \mathcal{W} , we have $\dot{\mathcal{W}} = -\overline{\nabla_{\mathcal{W}} \ell}$. By chain rule, we have:

$$\dot{\mathcal{W}} = -\overline{\nabla_{\mathcal{W}} \ell} = -\overline{J^{\top} \nabla_{\mathbf{r}} \ell} = -J^* \overline{\nabla_{\mathbf{r}} \ell} \quad (81)$$

829 Then the dynamics of $\mathbf{r} = \mathbf{r}(\mathcal{W})$, as driven by the dynamics of \mathcal{W} , is given by

$$\dot{\mathbf{r}} = J \dot{\mathcal{W}} = -JJ^* \overline{\nabla_{\mathbf{r}} \ell} \quad (82)$$

830 To show positive inner product, we have:

$$-\overline{\nabla_{\mathbf{r}} \ell}^* \dot{\mathbf{r}} = \overline{\nabla_{\mathbf{r}} \ell}^* JJ^* \overline{\nabla_{\mathbf{r}} \ell} = \|J^* \overline{\nabla_{\mathbf{r}} \ell}\|_2^2 \geq 0 \quad (83)$$

831 \square

832 **Theorem 5** (The Occam's Razer: Preference of low-order solutions). *If $\mathbf{z} = \mathbf{y} * \mathbf{z}'$ and both \mathbf{z} (of*
 833 *order q) and \mathbf{z}' are global optimal solutions, then there exists a path of zero loss connecting \mathbf{z} and \mathbf{z}'*
 834 *in the space of \mathcal{Z}_q . As a result, lower-order solutions are preferred if trained with L_2 regularization.*

835 *Proof.* Let $\text{ord}(\mathbf{z}) = q$ and $\text{ord}(\mathbf{z}') = q'$. Then $q' | q$. Since both \mathbf{z} and \mathbf{z}' are global optimal. Since
 836 r_{kkk} is ring homomorphism, we know that $r_{kkk}(\mathbf{z}) = r_{kkk}(\mathbf{z}') r_{kkk}(\mathbf{y}) = 1/2d = r_{kkk}(\mathbf{z}')$ and
 837 thus $r_{kkk}(\mathbf{y}) = 1$ for all $k \neq 0$.

838 Let the augmented identity $e \in \mathcal{Z}_q$ be $e_{pmj} = \mathbb{1}(j = 0)$. Then $r_{kkk}(e) = 1$ for all $k \neq 0$.

839 We want to construct a path in \mathcal{Z}_q , the space of order- q solutions as follows:

$$\tilde{z}(t) = \tilde{y}(t) * z', \quad 0 \leq t \leq 1 \quad (84)$$

840 in which $\tilde{y}(0) = e$, $\tilde{y}(1) = y$, and $r_{kkk}(\tilde{y}(t)) = 1$ for any t . To see why this is possible, pick a
841 continuous family of trajectories $\hat{y}(t; \lambda)$ with $\lambda \in [0, 1]$ so that they satisfies

$$\hat{y}(0; \lambda) = e, \quad \hat{y}(1; \lambda) = y, \quad r_{kkk}(\hat{y}(t; 0)) \leq 1, \quad r_{kkk}(\hat{y}(t; 1)) \leq 1 \quad (85)$$

842 which can always be achieved by scaling some trajectory with a factor that depends on λ . Then
843 by intermediate theorem, there exists $\lambda(t)$ so that $r_{kkk}(\hat{y}(t; \lambda(t))) = 1$ for some k . Note that for
844 different frequency k and k' , r_{kkk} and $r_{k'k'k'}$ involves disjoint components of z so we could find
845 such a path for all $k \neq 0$.

846 Therefore, for any monomial potential r included in MSE loss (Eqn. 3), we have

$$r(\tilde{z}(t)) = r(\tilde{y}(t))r(z') = \begin{cases} \text{finite} \cdot 0 = 0 & r \neq r_{kkk} \\ 1 \cdot 1/2d = 1/2d & r = r_{kkk} \end{cases} \quad (86)$$

847 and thus the entire trajectory $\tilde{z}(t) = \tilde{y}(t) * z' \in \mathcal{Z}_q$ connecting z and $e * z'$, which is z' in the space
848 of \mathcal{Z}_q , is also globally optimal.

849 To see why weight decay regularization leads to lower-order solution, we could simply compare the
850 ℓ_2 norm of $z = y * z'$ and $e * z'$. At each frequency k , this reduces to the following optimization
851 problem:

$$\min \sum_j |a_j|^2 + |b_j|^2 + |c_j|^2, \quad \text{s.t.} \sum_j a_j b_j c_j = 1 \quad (87)$$

852 where $a_j := y_{akj}$, $b_j := y_{bkj}$ and $c_j := y_{ckj}$. Since we know that arithmetic mean is no less than
853 geometric mean:

$$\frac{|a_j|^2 + |b_j|^2 + |c_j|^2}{3} \geq \sqrt[3]{|a_j b_j c_j|^2} \quad (88)$$

854 We have:

$$\sum_j |a_j|^2 + |b_j|^2 + |c_j|^2 \geq 3 \sum_j |a_j b_j c_j|^{2/3} \geq 3 \quad (89)$$

855 The last inequality holds because (1) if any $|a_j b_j c_j| \geq 1$, then it holds, (2) if all $|a_j b_j c_j| < 1$, then
856 since a^x is a decreasing function for $a < 1$, $\sum_j |a_j b_j c_j|^{2/3} \geq \sum_j |a_j b_j c_j| \geq |\sum_j a_j b_j c_j| = 1$.

857 The minimizer is reached when $|a_j| = |b_j| = |c_j|$. Note that if $a_j b_j c_j$ has any complex phase or
858 negative, then in order to satisfy $\sum_j a_j b_j c_j = 1$, objective function needs to be larger. So without
859 loss of generality, we could study $a_j = b_j = c_j = x_j \geq 0$ and the optimization problem becomes

$$\min \sum_j x_j^2, \quad \text{s.t.} \sum_j x_j^3 = 1, \quad x_j \geq 0 \quad (90)$$

860 which has a minimizer at the corners $(1, 0, \dots)$. This corresponds to $a_j = b_j = c_j = \mathbb{1}(j = 0)$,
861 which is the augmented identity $e \in \mathcal{Z}_q$. \square

862 **Theorem 6** (Infinite Width Limits at Initialization). *Considering the modified loss of Eqn. 3 with
863 only the first two terms: $\tilde{\ell}_k := r_{kkk} + d \sum_{k_1 k_2} |r_{k_1 k_2 k}|^2$, if the weights are i.i.d Gaussian and
864 network width $q \rightarrow +\infty$, then JJ^* converge to diagonal and the dynamics of MPs is decoupled.*

865 *Proof.* For each component of $H = JJ^*$, after computation, they can be written as the following:

$$h_{k_1 k_2 k_3, k'_1 k'_2 k'_3} = \sum_{pmj} \frac{\partial r_{k_1 k_2 k_3}}{\partial z_{pmj}} \frac{\partial r_{k'_1 k'_2 k'_3}}{\partial z_{pmj}} \quad (91)$$

$$= \mathbb{1}(k_1 = k'_1) \sum_j b_{k_2 j} \bar{b}_{k'_2 j} c_{k_3 j} \bar{c}_{k'_3 j} \quad (92)$$

$$+ \mathbb{1}(k_2 = k'_2) \sum_j a_{k_1 j} \bar{a}_{k'_1 j} c_{k_3 j} \bar{c}_{k'_3 j} \quad (93)$$

$$+ \mathbb{1}(k_3 = k'_3) \sum_j a_{k_1 j} \bar{a}_{k'_1 j} b_{k_2 j} \bar{b}_{k'_2 j} \quad (94)$$

866 where $a_{kj} := z_{akj}$, $b_{kj} := z_{bkj}$ and $c_{kj} := z_{ckj}$. Then for component $(k_1 k_2 k_3, k'_1, k'_2, k'_3)$, if any
 867 $k_p \neq k'_p$ for some $p \in \{a, b, c\}$, then the corresponding $z_{pk_p j} \bar{z}_{pk'_p j}$ has random phase for hidden
 868 node j , and $h_{k_1 k_2 k_3, k'_1 k'_2 k'_3} \rightarrow 0$ when $q \rightarrow +\infty$. \square