## On Computational Limits of Modern Hopfield Models: A Fine-Grained Complexity Analysis

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#### Abstract

We investigate the computational limits of the memory retrieval dynamics of modern Hopfield models from the fine-grained complexity analysis. Our key contribution is the characterization of a phase transition behavior in the efficiency of all possible modern Hopfield models based on the norm of patterns. Specifically, we establish an upper bound criterion for the norm of input query patterns and memory patterns. Only below this criterion, sub-quadratic (efficient) variants of the modern Hopfield model exist, assuming the Strong Exponential Time Hypothesis (SETH). To showcase our theory, we provide a formal example of efficient constructions of modern Hopfield models using low-rank approximation when the efficient criterion holds. This includes a derivation of a lower bound on the computational time, scaling linearly with  $\max\{\# \text{ of stored memory} \}$ patterns, length of input query sequence}. In addition, we prove its memory retrieval error bound and exponential memory capacity.

#### 1. Introduction

We investigate the computational limits of modern Hopfield models (Wu et al., 2024a;b; Hu et al., 2024a;b; 2023; Ramsauer et al., 2021) from a fine-grained complexity analysis, and characterize a norm-based phase transition for all possible efficient modern Hopfield model. This analysis holds practical significance. Modern Hopfield models are a type of associative memory model compatible with deep learning. More precisely, their deep learning derivatives offer robust alternatives to attention mechanisms in various transformer- and Hopfield-based methods (Hofmann et al., 2024; Xu et al., 2024; Wu et al., 2024a;b; Hu et al., 2024a; Schimunek et al., 2023; Fürst et al., 2022; Paischer et al., 2022; Seidl et al., 2022; Widrich et al., 2020). However, these models currently lack efficient implementations for large-scale applications (Hu et al., 2023, Section C.2). This issue becomes more relevant with the rise of Large Foundation Models (Bommasani et al., 2021), where expansive attention-based architectures, pre-trained on vast datasets, are pivotal across multiple scientific fields, including natural language processing (Brown et al., 2020; Floridi and Chiriatti, 2020), financial analytics (Wu et al., 2023), genomic research (Zhou et al., 2024; 2023; Ji et al., 2021), medical science (Thirunavukarasu et al., 2023; Singhal et al., 2023; Moor et al., 2023) and more. This work makes a timely theoretical analysis of their computational limits, aimed at advancing (Hopfield-based) large foundation models.

Let  $\mathbf{x} \in \mathbb{R}^d$  be the input query pattern. The memory patterns are stored in a matrix  $\mathbf{\Xi} = [\boldsymbol{\xi}_1, \cdots, \boldsymbol{\xi}_M] \in \mathbb{R}^{d \times M}$ . Hopfield models are energy-based associative memory models. These models store memory patterns  $\mathbf{\Xi}$  on the local minima of their energy landscapes, i.e. energy functions E. For any input query  $\mathbf{x}$ , they retrieve its closest memory pattern through some energy minimization algorithms, i.e. retrieval dynamics  $\mathcal{T}$ , initialized at  $\mathbf{x}$ .

Ramsauer et al. (2021) propose the Modern Hopfield Model with a specific set of energy function E and memory retrieval dynamics  $\mathcal{T}$ , and integrate it into deep learning architectures via its connection with the transformer attention (Vaswani et al., 2017), offering enhanced performance, and theoretically guaranteed exponential memory capacity. Specifically, they introduce the energy function:

$$E(\mathbf{x}) = -\operatorname{lse}(\beta, \mathbf{\Xi}^{\mathsf{T}} \mathbf{x}) + \frac{1}{2} \langle \mathbf{x}, \mathbf{x} \rangle, \qquad (1.1)$$

where the retrieval dynamics is given by

$$\mathbf{x}^{\text{new}} = \mathcal{T}_{\text{Dense}}(\mathbf{x}) = \mathbf{\Xi} \cdot \text{Softmax}(\beta \mathbf{\Xi}^{\mathsf{T}} \mathbf{x}).$$
 (1.2)

The function lse  $(\beta, \mathbf{z}) \coloneqq \log \left( \sum_{\mu=1}^{M} \exp\{\beta z_{\mu}\} \right) / \beta$  is the log-sum-exponential for any given vector  $\mathbf{z} \in \mathbb{R}^{M}$  and  $\beta >$ 

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0. Let  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_L] \in \mathbb{R}^{d \times L}$  be a sequence of input queries, such that (1.2) becomes  $\mathbf{Z} \coloneqq [\mathbf{x}_1^{\text{new}}, \dots, \mathbf{x}_L^{\text{new}}] = \mathcal{T}_{\text{Dense}}(\mathbf{X})$ , and hence

$$\mathcal{T}_{\text{Dense}}(\mathbf{X}) = \underbrace{\widehat{\Xi}}_{\in \mathbb{R}^{d \times M}} \cdot \text{Softmax}(\beta \underbrace{\underbrace{\Xi}_{\in \mathbb{R}^{M \times d}}^{\mathbf{T}} \underbrace{\mathbf{X}}_{\in \mathbb{R}^{d \times L}}) \in \mathbb{R}^{d \times L},$$

where the Softmax(·) applies column-wise normalization<sup>1</sup>. Here we assume  $d = L^{o(1)}$ , i.e., the growth rate of this function is sub-polynomial concerning L.

To motivate the study of possible efficient implementations, we make the following observation on (1.1):

The bottleneck of Hopfield-based methods is the time to perform matrix multiplication in memory retrieval:  $\mathcal{O}(dML)$ . Namely, (1.1) is inefficient with  $M = \Omega(e^d)$  (large memory set) and  $L = \Omega(e^d)$  (long query sequences).

Explicitly, if the associative space is *d*-dimensional, this necessitates *d* multiplication operations for the inner products of  $\{\mathbf{x}\}$  and  $\{\boldsymbol{\xi}\}$ . Consequently, the complexity of computing a dot product is  $\mathcal{O}(d)$ . Each pattern in  $\mathbf{Z}$  must associate with every pattern in  $\Xi$ . Therefore, the time complexity for sequences of length *L* and *M* with a pattern dimension of *d* is  $\mathcal{O}(dML)$ . In this regard, this work aims to characterize the fundamental limits on improving  $\mathcal{O}(dML)$ . Specifically, we ask the following questions:

**Question 1.** Is it possible to improve the time complexity O(dML) with a controllable approximation error?

**Question 2.** More aggressively, is it possible to perform memory retrieval computations in almost linear time  $L^{1+o(1)}$  or  $M^{1+o(1)}$  or  $(L+M)^{1+o(1)}$ ?

To address these questions, we explore approximate retrieval computations with precision guarantees. We aim to find a surrogate  $\mathcal{T}_{approx.}$  (also denoted as  $\tilde{\mathcal{T}}_{Dense}$ ) for  $\mathcal{T}_{Dense}$  such that

$$\|\mathcal{T}_{approx.} - \mathcal{T}_{Dense}\|_{max} \leq \delta_{approx.},$$

for some  $\delta_{\text{approx.}} > 0$ , where  $\|\mathbf{A}\|_{\max} \coloneqq \max_{i,j} |a_{ij}|$ .

To be concrete, we study the following approximation problem with the realistic setting  $\delta_{approx.} = 1/\text{poly}(L)$ .

**Problem 1** (Approximate Modern Hopfield Memory Retrieval Dynamics  $AHop(d, M, L, \beta, B, \delta_H)$ ). Let  $\delta_H > 0$ . Given  $\Xi \in \mathbb{R}^{d \times M}$  and  $\mathbf{X} \in \mathbb{R}^{d \times L}$  such that  $\|\Xi\|_{max} \leq B$  and  $\|\mathbf{X}\|_{max} \leq B$ . We aim to study an approximation problem  $AHop(d, M, L, \beta, B, \delta_H)$ , that approximates  $\mathbf{Z}$  with a

matrix 
$$\widetilde{\mathbf{Z}} \coloneqq \widetilde{\mathcal{T}}_{Dense}(\mathbf{X})$$
 such that

$$\left\| \widetilde{\mathbf{Z}} - \mathbf{\Xi} \mathbf{D}^{-1} \mathbf{A} \right\|_{\max} \leq \delta_H,$$

where  $\mathbf{\Xi}\mathbf{D}^{-1}\mathbf{A} = \mathbf{Z}$  with

$$\mathbf{A} = \exp\{\beta \mathbf{\Xi}^{\mathsf{T}} \mathbf{X}\}, \quad \mathbf{D} = \operatorname{diag}(\mathbf{A} \mathbf{1}_M).$$

In this work, we aim to investigate the computational limits and potential efficient algorithms of AHop.

Contributions. Our contributions are threefold:

- Computational Limits. We answer Question 1 by identifying a phase transition behavior on the norm of query and memory patterns assuming the Strong Exponential Time Hypothesis (SETH). Explicitly, let  $\tau = \max \{M, L\}$  be the upper bound of the patterns' lengths. We prove an upper bound criterion  $B^* = \Theta(\sqrt{\log \tau})$  for  $\|\mathbf{\Xi}\|_{\max}$  and  $\|\mathbf{X}\|_{\max}$  such that, only below which, solving AHop in  $\tau^{2-\Omega(1)}$  (sub-quadratic) time is possible.
- Efficient Model. We answer Question 2 by providing an efficient algorithm for AHop based on low-rank approximation: an almost linear time modern Hopfield model. Explicitly, we prove that the algorithm, under realistic settings, performs the computation in almost linear time  $\tau^{1+o(1)}$ .
- Exponential Memory Capacity. Focusing on the almostlinear-time modern Hopfield model, we derive its retrieval error bound and show that this model achieves almostlinear-time efficiency while maintaining the exponential memory capacity characteristic of modern Hopfield models.

#### **Background and Related Works**

Modern Hopfield Models for Deep Learning. Classical Hopfield models (Hopfield, 1984; 1982; Krotov and Hopfield, 2016) emulate human brain associative memory by focusing on storing and retrieving memory patterns. In machine learning community, a noticeable interest in these models arises from (i) improved memory storage capacities (from linear to polynomial (Krotov and Hopfield, 2016), to exponential (Demircigil et al., 2017) and to kernelized (Wu et al., 2024a)), (ii) novel architectures (Hoover et al., 2023; Seidl et al., 2022; Fürst et al., 2022), and (iii) their biological plausibility (Kozachkov et al., 2022; Krotov and Hopfield, 2021). Notably, the modern Hopfield models (Hu et al., 2024a;b; 2023; Wu et al., 2024a;b; Burns and Fukai, 2023; Brandstetter, 2021; Ramsauer et al., 2021) offer fast convergence and expanded memory capacity. Importantly, they serve as advanced extensions of attention mechanisms to Transformer architecture. They have extensive applications in diverse fields like tabular learning (Xu et al., 2024), drug

<sup>&</sup>lt;sup>1</sup>Many existing works denote  $\mathbf{Z}$  by  $\mathbf{X}^{new}$ .

discovery (Schimunek et al., 2023), immunology (Widrich et al., 2020), time series forecasting (Wu et al., 2024b; Auer et al., 2024), reinforcement learning (Paischer et al., 2022), and large foundation models (Hu et al., 2024a; Fürst et al., 2022).

Theory of Modern Hopfield Models. Besides empirical successes, Modern Hopfield Models provide a model-based theoretical framework for analyzing transformer attention and Transformer architectures. (Hu et al., 2023) and Wu et al. (2024b) propose a unified framework to analyze and derive modern Hopfield models via entropic regularizers. Significantly, their work presents sparse variants (sparse and generalized sparse models) and incorporates the standard modern Hopfield model (Ramsauer et al., 2021) as a particular example in their framework. Yet, they also note that the modern Hopfield paradigm is incomplete and lacks efficient implementations or variants (Hu et al., 2023, Section E). Extending this foundation, Hu et al. (2024b) introduces a principled construction of efficient variants from the nonparametric perspective, including linear, top-K, and random feature modern Hopfield models. This study aims to refine this research direction towards efficient models. We believe that this study is critical in guiding future research toward a Hopfield-driven design paradigm, especially for large-scale models.

**Fine-Grained Complexity.** Much of fine-grained complexity theory relies on hypotheses concerning the time complexity of three problems: Conjunctive Normal Form Satisfiability (CNFSAT), All-Pairs Shortest Paths (APSP), and 3-SUM (Williams, 2018). Impagliazzo and Paturi (2001) introduce the Strong Exponential Time Hypothesis (SETH) to address the complexity of CNF-SAT. SETH is a stronger form of the  $P \neq NP$  conjecture, suggesting that our current best SAT algorithms are optimal. It states as follows:

**Hypothesis 1** (SETH). For every  $\epsilon > 0$ , there is a positive integer  $k \ge 3$  such that k-SAT on formulas with n variables cannot be solved in  $\mathcal{O}(2^{(1-\epsilon)n})$  time, even by a randomized algorithm.

SETH is a popular conjecture for proving fine-grained lower bounds for a wide variety of algorithmic problems, such as k-Hitting Set and k-NAE-SAT (Cygan et al., 2016). See Williams (2018) for a comprehensive review. Along this line, we utilize the fine-grained reduction under SETH to analyze the computational limits. In previous fine-grained reduction works, Backurs et al. (2017) analyze the computational complexity for multiple Empirical Risk Minimization problems, such as kernel SVMs and kernel ridge. Alman et al. (2020) study the applicability of efficient spectral graph theory on geometric graphs under SETH. Aggarwal and Alman (2022) focus on the computational limits of Batch Gaussian Kernel Density Estimation problems. Alman et al. (2023) utilize the weight-data correlation in a tree data structure for fast neural network training. Alman and Song (2023; 2024b) extend the previous work to transformer attention and introduce a tensor generalization. Compared to existing works, this work is, to the best of our knowledge, the first analysis of computational limits for modern Hopfield (associative memory) models (Hu et al., 2024a;b; Wu et al., 2024a;b; Hu et al., 2023; Ramsauer et al., 2021). In addition, it offers a more general characterization, encompassing computational analyses of self-attention (Alman and Song, 2024b; 2023) and cross-attention as special cases.

**Notations.** We denote (column) vectors by lower case bold letters, and matrices by upper case bold letters. We write  $\langle \mathbf{a}, \mathbf{b} \rangle \coloneqq \mathbf{a}^{\mathsf{T}} \mathbf{b}$  as the inner product for vectors  $\mathbf{a}, \mathbf{b}$ . Let  $\mathbf{a}[i]$  denotes the *i*-th component of vector  $\mathbf{a}$ . The index set  $\{1, \dots, I\}$  is denoted by [I], where  $I \in \mathbb{N}_+$ . Let  $\|\mathbf{A}\|_{\max} \coloneqq \max_{i,j} |\mathbf{A}_{ij}|$  for any matrix  $\mathbf{A}$ . We denote the memory patterns by  $\boldsymbol{\xi} \in \mathbb{R}^d$  and the query pattern by  $\mathbf{x} \in \mathbb{R}^d$ , and  $\boldsymbol{\Xi} \coloneqq [\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_M] \in \mathbb{R}^{d \times M}$  as shorthand for stored memory patterns  $\{\boldsymbol{\xi}_\mu\}_{\mu \in [M]}$ . We denote  $\{\underline{\tau}_1, \dots, \underline{\tau}_d\} \subset \mathbb{R}^{1 \times n}$  for each row in the matrix  $\mathbf{Z} \in \mathbb{R}^{d \times n}$ .

### 2. Computational Limits

In this section, we characterize the computational limits of all possible efficient variants of modern Hopfield models, i.e. AHop, via fine-grained reduction. Our primary technique involves casting the AHop problem (Problem 1) as a subroutine in the Approximate Nearest Neighbor Search Problem and deducing the hardness through reduction.

#### 2.1. Background: Approximate Nearest Neighbor Search Problem

Approximate Nearest Neighbor Search (ANNS) problem (Indyk and Motwani, 1998; Arya et al., 1998; Muja and Lowe, 2014; Li et al., 2019) shares the same objective with the Altop problem of identifying a pattern closely resembling a query pattern as a memory retrieval process. Furthermore, the ANNS problem, which is particularly useful in highdimensional spaces, seeks an approximate nearest neighbor within acceptable bounds to avoid the prohibitive computational costs of finding the exact nearest neighbor (Indyk and Motwani, 1998; Muja and Lowe, 2014). In this work, we observe that ANNS aligns with the goal of memory retrieval to efficiently find and recall the most relevant memory pattern in response to a specific input query. In our context, this translates to approximating the largest entry of Softmax( $\Xi^{\mathsf{T}}\mathbf{x}$ ) in (1.2) for each query  $\mathbf{x}$ , while maintaining a bounded error.

In ANNS, one is given as input n vectors of dimension d, and an error parameter  $\delta > 0$ , and the goal is to find a

pair of vectors whose distance is at most  $(1 + \delta)$  times the *minimum* distance between any pair of the vectors. The straightforward algorithm for ANNS runs in quadratic time, and it is known that it is impossible to solve ANNS in truly sub-quadratic time assuming SETH (Rubinstein, 2018).

To be concrete, we state the ANNS problem considered in this work as follows.

**Definition 2.1** (Approximate Nearest Neighbor Search ANNS). Given  $\delta > 0$ ,  $(1 + \delta)$ -ANNS for sets  $A, B \subset \{0, 1\}^d$ , with |A| = |B| = n requires finding  $\mathbf{a}^* \in A$ ,  $\mathbf{b}^* \in B$  such that:

$$\|\mathbf{a}^* - \mathbf{b}^*\|_2^2 \le (1+\delta) \min_{\mathbf{a} \in A, \mathbf{b} \in B} \|\mathbf{a} - \mathbf{b}\|_2^2.$$
 (2.1)

Next, we present the hardness results from Rubinstein (2018) as an auxiliary lemma for later use. Specifically, Rubinstein (2018) show that no sub-quadratic-time algorithms exist for the ANNS.

**Lemma 2.1** (Hardness for ANNS, Theorem 4.1 of (Rubinstein, 2018)). Assuming Hypothesis 1, for every q > 0, there exist  $\delta \in (0, 0.1)$  and C > 0 such that  $(1 + \delta)$ -ANNS with dimension  $d = C \log n$  requires  $\Omega(n^{2-q})$  time.

#### 2.2. Fine-Grained Reduction for AHop

To study the computational limits, our proof strategy involves connecting AHop to the hardness of ANNS (see Lemma 2.1) through a fine-grained reduction. We do this by introducing a decision problem Gap-ANNS as a  $(1 + \delta)$ -gap reduction (Demaine, 2014) of the ANNS optimization problem (2.1), making the analysis more tractable while maintaining the same level of hardness. To be more precise, if we prove AHop is a reduction of Gap-ANNS, we also prove AHop is a  $(1 + \delta)$ -gap reduction of ANNS. We start with Gap-ANNS in below.

**Definition 2.2** (Gap Approximate Nearest Neighbor Search Gap-ANNS $(d, n, t, \delta)$ ). Given two sets of n input vectors  $A = \{\mathbf{a}_1, \ldots, \mathbf{a}_n\} \subset \{0, 1\}^d$  and  $B = \{\mathbf{b}_1, \ldots, \mathbf{b}_n\} \subset \{0, 1\}^d$ , the Gap-ANNS $(d, n, t, \delta)$  problem requires, for each  $i \in [n]$ , distinguish between the following two cases:

- **Case 1:** There exists at least one pair  $(\mathbf{a}_i, \mathbf{b}_j) \in A \times B$ such that  $\|\mathbf{a}_i - \mathbf{b}_j\|_2^2 < t$ .
- Case 2: For all  $\mathbf{b}_j \in B$ , it holds that  $\|\mathbf{a}_i \mathbf{b}_j\|_2^2 \ge (1+\delta) \cdot t$ .

An algorithm for Gap-ANNS $(d, n, t, \delta)$  with  $\log(nd)$  time can binary search the answer of ANNS (Williams, 2018).

Then, we show that AHop serves as a subroutine within Gap-ANNS, thereby establishing a connection between the computational complexities of both problems.

**Theorem 2.1** (Reduction from ANNS to AHop). Consider Gap-ANNS with two sets of n input vectors, for every q > 0, for any chosen constants  $C, C_0 > 0$ , there exist  $\delta \in (0, 0.1)$  and constants  $C_{\alpha}, C_{\beta} > 0$  such that: Gap-ANNS $(d = C \log n, n, t = C_0 \log n, \delta)$  requires  $\mathcal{O}(T + n^{2-q})$  time if AHop $(2d, M = 2n, L = 2n, \beta = 1/2d, B = C_{\beta}\sqrt{\log n}, \delta_H = n^{-C_{\alpha}})$  requires time T.

*Proof Sketch.* To solve Gap-ANNS, we employ different approaches for two scenarios, either through

- Scenario 1: a brute-force approach, or
- Scenario 2: reducing Gap-ANNS to an AHop problem, and translating AHop's solution to Gap-ANNS's solution (i.e. distinguish the 2 cases in Definition 2.2).

The proof of **Scenario 1** employs a brute-force algorithm for Gap-ANNS. This algorithm iterates over vectors within a Hamming distance of t from each input vector and checks for a match in the target set. It results in a manageable time complexity  $O(n^{2-q})$ .

The proof for **Scenario 2** adopts a complex strategy. Initially, an AHop instance is formulated to encompass the Gap-ANNS problem. This formulation involves selecting specific parameters to ensure that resolving the AHop problem concurrently addresses the Gap-ANNS challenge. Next, we introduce  $\tilde{t}$ , a threshold exceeding the AHop algorithm's error bound, to effectively bridge the conditions of the Gap-ANNS problem with the compound inequality derived from AHop. Finally, by considering an illustrative set of input vectors under the premise of a uniform distribution, the method for resolving the Gap-ANNS is elucidated with the established value of  $\tilde{t}$ . This approach simplifies the decision-making process in solving Gap-ANNS.

**Main Proof.** Here is the main proof of Theorem 2.1.

*Proof.* Let  $\{\mathbf{a}_1, \dots, \mathbf{a}_n, \mathbf{b}_1, \dots, \mathbf{b}_n\} \subseteq \{0, 1\}^d$  denote the input vectors of Gap-ANNS $(d = C \log n, n, t, \delta)$ . For any given c satisfying

$$\begin{cases} c\left(\log C+1\right) \le 1-q\\ 0 < c \le \frac{1}{2}C, \end{cases}$$
(2.2)

we categorize two scenarios based on whether  $t < c \log n$ .

**Scenario 1:**  $t < c \log n$ .

The brute-force algorithm is described below:

- 1. For each  $i \in [n]$ , iterate over all vectors  $\mathbf{b}' \in \{0, 1\}^d$  which have Hamming distance at most t from  $\mathbf{a}_i$ .
- 2. Check whether  $\mathbf{b}' \in {\mathbf{b}_1, \cdots, \mathbf{b}_n}$ .

Since  $t < \frac{1}{2}C \log n < d$ , there are  $\binom{d}{t}$  choices for the vector **b**', so the algorithm takes  $\mathcal{O}(n \cdot \binom{d}{t})$  time. We know:

$$n \cdot \binom{d}{t} \le n \cdot \binom{C \log n}{c \log n} \le \left(e \frac{C}{c}\right)^{c \log n} \le n^{1+c \log(Ce)}.$$

Therefore, if we choose constant c satisfying (2.2), the algorithm requires  $\mathcal{O}(n^{2-q})$  time.

#### **Scenario 2:** $t \ge c \log n$ .

Scenario 2 - Part 1. This part shows the associated AHop problem. Our objective is to construct an instance of the AHop problem in such a way that solving it also addresses the Gap-ANNS problem. To this end, we configure the  $AHop(\tilde{d}, \tilde{n}, \tilde{n}, \beta, B, \delta_H)$  problem by selecting a specific set of parameters:

$$\widetilde{d} \coloneqq 2d, \quad \widetilde{n} \coloneqq 2n, \quad \beta \coloneqq 1/\widetilde{d}$$

$$C_{\beta} > 2\sqrt{C/(C_0\delta)}, \quad C_{\alpha} > \frac{C_{\beta}^2}{4}(3+C_0/C)+1, \quad (2.3)$$

$$B \coloneqq C_{\beta} \sqrt{\log n}, \quad \delta_H \coloneqq n^{-C_{\alpha}}, \tag{2.4}$$

Note that  $\delta_H$  is dependent on but not equal to  $\delta$ .

We parametrize AHop's input,  $\Xi$  and X, with Gap-ANNS input  $\{a_1, \dots, a_n, b_1, \dots, b_n\}$ :

$$\begin{split} \mathbf{\Xi} &\coloneqq B \cdot \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \cdots & \mathbf{a}_n & \mathbf{0}_d & \mathbf{0}_d & \cdots & \mathbf{0}_d \\ \mathbf{1}_d & \mathbf{1}_d & \cdots & \mathbf{1}_d & \mathbf{1}_d & \mathbf{1}_d & \mathbf{1}_d & \cdots & \mathbf{1}_d \end{bmatrix} \in \mathbb{R}^{\widetilde{d} \times \widetilde{n}}, \\ \mathbf{X} &\coloneqq B \cdot \begin{bmatrix} \mathbf{b}_1 & \mathbf{b}_2 & \cdots & \mathbf{b}_n & \mathbf{0}_d & \mathbf{0}_d & \cdots & \mathbf{0}_d \\ \mathbf{0}_d & \mathbf{0}_d & \cdots & \mathbf{0}_d & \mathbf{1}_d & \mathbf{1}_d & \cdots & \mathbf{1}_d \end{bmatrix} \in \mathbb{R}^{\widetilde{d} \times \widetilde{n}} \end{split}$$

By construction, we have  $\|\mathbf{\Xi}\|_{\max} \leq B$  and  $\|\mathbf{X}\|_{\max} \leq B$ . This follows that:

$$\left\|\beta \mathbf{\Xi}^{\mathsf{T}} \mathbf{X}\right\|_{\max} \leq \beta B^2 \widetilde{d} = B^2.$$

Consider the matrix  $\mathbf{A} \coloneqq \exp\{\beta \mathbf{\Xi}^{\mathsf{T}} \mathbf{X}\} \in \mathbb{R}^{\widetilde{n} \times \widetilde{n}}$ :

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_1 & \mathbf{A}_2 \\ \mathbf{A}_3 & \mathbf{A}_4 \end{bmatrix}, \tag{2.5}$$

where  $\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3, \mathbf{A}_4 \in \mathbb{R}^{n \times n}$ :

$$\begin{split} \mathbf{A}_{1} &\coloneqq \left[ \exp \left\{ \beta B^{2} \left\langle \mathbf{a}_{i}, \mathbf{b}_{j} \right\rangle \right\} \right]_{i \in [1,n], j \in [1,n]}, \\ \mathbf{A}_{2} &\coloneqq \left[ \exp \left\{ B^{2} \right\} \right]_{i \in [1,n], j \in [n+1,2n]}, \\ \mathbf{A}_{3} &\coloneqq \left[ 0 \right]_{i \in [n+1,2n], j \in [1,n]}, \\ \mathbf{A}_{4} &\coloneqq \left[ \exp \left\{ B^{2} \right\} \right]_{i \in [n+1,2n], j \in [n+1,2n]}. \end{split}$$

We provide the explicit form of (2.5) in (B.1).

For each  $(i, j) \in [n] \times [n]$ , it holds

$$\begin{aligned} \mathbf{A}_{i,j} &= \exp\{\beta B^2 \langle \mathbf{a}_i, \mathbf{b}_j \rangle\} \\ &\leq \exp\{\beta B^2 \widetilde{d} \|\mathbf{a}_i\|_{\max} \|\mathbf{b}_j\|_{\max}\} \leq \exp\{B^2\}. \end{aligned}$$

Thus,

$$0 \le \mathbf{A}_{i,j} \le \exp\left\{B^2\right\}$$

Since  $\mathbf{D} = \operatorname{diag}(\mathbf{A1}_{\widetilde{n}})$ , for each  $i \in [\widetilde{n}]$ , we get

$$n\exp\{B^2\} \le \mathbf{D}_{i,i} \le 2n\exp\{B^2\}.$$
 (2.6)

Scenario 2 - Part 2. This part shows the Gap-ANNS is a part of the associated AHop problem. Given input matrices  $\mathbf{D} \in \mathbb{R}^{\tilde{n} \times \tilde{n}}$ ,  $\mathbf{A} \in \mathbb{R}^{\tilde{n} \times \tilde{n}}$ , if we have an algorithm  $AHop(\tilde{d}, \tilde{n}, \tilde{n}, \beta, B, \delta_H)$  such that its output  $\tilde{\mathbf{Z}}$  satisfies

$$\left\| \widetilde{\mathbf{Z}} - \mathbf{\Xi} \mathbf{D}^{-1} \mathbf{A} \right\|_{\max} \le \delta_H.$$
 (2.7)

To connect (2.7) to Gap-ANNS, we define  $\tilde{t}$  as

$$\tilde{t} \coloneqq \frac{1}{3} \frac{\exp\{\frac{1}{4}B^2(1-t/d)\}}{2n\exp\{B^2\}}.$$

It follows that

Since  $\tilde{t} \geq \delta_H$ , the last row vector of  $\widetilde{\mathbf{Z}}$ , i.e  $\underline{\widetilde{\mathbf{z}}}_{\tilde{d}} \in \mathbb{R}^{1 \times \tilde{n}}$  for all  $j \in [\tilde{n}]$ , satisfying

$$\left| \underline{\widetilde{\mathbf{z}}}_{\widetilde{d}}[j] - \left( \underline{\boldsymbol{\xi}}_{\widetilde{d}} \mathbf{D}^{-1} \mathbf{A} \right) [j] \right| \le \widetilde{t}, \tag{2.8}$$

where  $\boldsymbol{\xi}_{\tilde{d}} = \mathbf{1}_{\tilde{n}}^{\mathsf{T}}$  is the last row of  $\boldsymbol{\Xi}$ .

Scenario 2 - Part 3. This part shows how to distinguish the 2 cases in the Gap-ANNS with  $\underline{\widetilde{z}}_{\tilde{d}}$  constructed in the previous AHop $(\tilde{d}, \tilde{n}, \tilde{n}, \beta, B, \delta_H)$  problem.

For the sake of convenience, we assume each input vector has an equal probability of being either 0 or 1, that is,

$$\begin{cases} \|\mathbf{a}_i\|_2^2 = d/2, & \forall i \in [n], \\ \|\mathbf{b}_j\|_2^2 = d/2, & \forall j \in [n]. \end{cases}$$

Hence, for each  $(i, j) \in [n] \times [n]$ ,

$$\beta B^{2} \langle \mathbf{a}_{i}, \mathbf{b}_{j} \rangle = \frac{B^{2}}{4d} (\|\mathbf{a}_{i}\|_{2}^{2} + \|\mathbf{b}_{j}\|_{2}^{2} - \|\mathbf{a}_{i} - \mathbf{b}_{j}\|_{2}^{2})$$
$$= \frac{B^{2}}{4d} \left( d - \|\mathbf{a}_{i} - \mathbf{b}_{j}\|_{2}^{2} \right).$$
(2.9)

Our goal of solving Gap-ANNS $(d, n, t, \delta)$  is to determine, for each  $i \in [n]$ , whether there is a  $j \in [n]$  such that  $\|\mathbf{a}_i - \mathbf{b}_j\|_2^2 \le t$ , or whether  $\|\mathbf{a}_i - \mathbf{b}_j\|_2^2 > (1 + \delta)t$  for all  $j \in [n]$ .

**Case 1:** If there exists an  $(i, j) \in [n] \times [n]$  such that  $\|\mathbf{a}_i - \mathbf{b}_j\|_2^2 \leq t$ , then

$$\beta B^2 \langle \mathbf{a}_i, \mathbf{b}_j \rangle \ge \frac{1}{4} B^2 (1 - t/d). \qquad (By (2.9))$$

In this case,

$$\widetilde{\underline{\mathbf{z}}}_{\widetilde{d}}[j] \geq \sum_{\iota}^{n} \mathbf{D}_{\iota,\iota}^{-1} \mathbf{A}_{\iota,j} - \widetilde{t} \qquad (By (2.8))$$
$$\geq \mathbf{D}_{i,i}^{-1} \exp\{\beta B^{2} \langle \mathbf{a}_{i}, \mathbf{b}_{j} \rangle\} - \widetilde{t}$$
$$\geq \frac{\exp\{\frac{1}{4}B^{2}(1 - t/d)\}}{2n \exp\{B^{2}\}} - \widetilde{t} \qquad (By (2.6))$$
$$= 2\widetilde{t}.$$

**Case 2:** If  $\|\mathbf{a}_i - \mathbf{b}_j\|_2^2 > (1 + \delta)t$  for all  $(i, j) \in [n] \times [n]$ , then

$$\beta B^2 \langle \mathbf{a}_i, \mathbf{b}_j \rangle < \frac{1}{4} B^2 (1 - (1 + \delta)t/d). \qquad (\text{By (2.9)})$$

In this case,

$$\begin{split} \widetilde{\mathbf{z}}_{\widetilde{d}}[j] &\leq \sum_{\iota}^{n} \mathbf{D}_{\iota,\iota}^{-1} \mathbf{A}_{\iota,j} + \widetilde{t} & (\text{By (2.8)}) \\ &= \sum_{\iota}^{n} \mathbf{D}_{\iota,\iota}^{-1} \exp\{\beta B^{2} \langle \mathbf{a}_{\iota}, \mathbf{b}_{j} \rangle\} + \widetilde{t} \\ &< \frac{n \exp\{\frac{1}{4}B^{2}(1 - (1 + \delta)t/d)\}}{n \exp\{B^{2}\}} + \widetilde{t} & (\text{By (2.6)}) \\ &= \frac{\exp\{\frac{1}{4}B^{2}(1 - t/d)\}}{2n \exp\{B^{2}\}} \frac{2n}{\exp\{\frac{\delta}{4}B^{2}t/d\}} + \widetilde{t} \\ &= 3\widetilde{t} \cdot \frac{2n}{\exp\{\frac{\delta}{4}C_{\beta}^{2}\log nC_{0}/C\}} + \widetilde{t} & (\text{By (2.3)}) \\ &< 2\widetilde{t}. \end{split}$$

Therefore, by determining whether  $\widetilde{\mathbf{z}}_{\widetilde{d}}[j] \geq 2\widetilde{t}$ , we distinguish the two cases, or solve the Gap-Ann $(n, d, t, \delta)$ . Furthermore, the entire algorithm take T time, the same as the time required for  $\operatorname{AHop}(\widetilde{d}, \widetilde{n}, \beta, B, \delta_H)$ .

**Corollary 2.1.1.** Assuming Hypothesis 1, for every q > 0, for any chosen  $C, C_0 > 0$ , there exist  $\delta \in (0, 0.1)$  and  $C_{\alpha}, C_{\beta} > 0$  satisfying (2.3) such that  $\operatorname{AHop}(2d, M = 2n, L = 2n, \beta = 1/2d, B = C_{\beta}\sqrt{\log n}, \delta_H = n^{-C_{\alpha}})$  requires  $\Omega(n^{2-q})$  time.

*Proof.* By Lemma 2.1, suppose  $\delta \in (0, 0.1), (1 + \delta)$ -ANNS with dimension  $d = C \log n$  requires  $\Omega(n^{2-q})$  time. By Theorem 2.1, Gap-ANNS requires  $\mathcal{O}(T + n^{2-q})$  time with T being the computation time of AHop $(d, M, L, \beta, B, \delta_H)$ . For Gap-ANNS to have the same precision  $\delta$  as  $(1 + \delta)$ -ANNS, we need  $\mathcal{O}(T + n^{2-q}) = \Omega(n^{2-q})$ . Consequently, AHop $(d, M, L, \beta, B, \delta_H)$  requires  $T = \Omega(n^{2-q})$  time. This completes the proof. □

Interestingly, Corollary 2.1.1 characterizes a phase transition behavior in AHop problems assuming Hypothesis 1. To extend the applicability of this corollary beyond the specific case where M = L = n, we introduce  $\tau := \max\{M, L\}$  to capture the larger dimension. That is, regardless of whether M or L is larger,  $\tau$  ensures that the hardness result considers the worst-case scenario (i.e. extending the shorter one). To sum up, we establish a criterion  $B^* = \Theta(\sqrt{\log \tau})$  for  $\|\mathbf{\Xi}\|_{\max}$  and  $\|\mathbf{X}\|_{\max}$  such that, only below which, solving AHop in  $\tau^{2-\Omega(1)}$  (sub-quadratic) time is possible.

#### 3. An Almost Linear Modern Hopfield Model

To showcase our theory, this section presents an example of an almost linear-time modern Hopfield model using lowdegree polynomial approximation. We show its almost linear lower bound on computational time in Section 3.2 and its upper bound on memory retrieval error in the same section. Additionally, we show that this model possesses a marginally smaller, yet still exponential-in-d memory capacity in Section 3.3, compared to standard modern Hopfield associative memory models (Wu et al., 2024b; Hu et al., 2023; Ramsauer et al., 2021).

#### 3.1. Background: Polynomial Method for Low-Rank Approximation

Consider a matrix  $\mathbf{A} \in \mathbb{R}^{p \times q}$ , and a function  $f : \mathbb{R} \to \mathbb{R}$ . We define  $f(\mathbf{A}) : \mathbb{R}^{p \times q} \to \mathbb{R}^{p \times q}$  as the matrix obtained by applying f entry-wise to  $\mathbf{A}$ . The polynomial method aims to find a low-rank approximation for  $f(\mathbf{A})$ . Under this method, if  $\mathbf{A}$  possesses a low rank, and if function fcan be well-approximated by a low-degree polynomial, then the matrix  $f(\mathbf{A})$  can be approximated by a low-rank matrix. Furthermore, this low-rank approximation can be efficiently computed in terms of its low-rank decomposition.

Aggarwal and Alman (2022) provide the bounds on the degrees of the polynomial required for low-rank approx-

imation of  $f(\mathbf{A})$ , particularly when f is the exponential function. Leveraging these results, we construct a low-rank approximation for  $\operatorname{Softmax}(\beta \Xi^{\mathsf{T}} \mathbf{X})$  in (1.1), satisfying the following definition:

**Definition 3.1** ( $(\delta_A, r)$  Low-Rank Approximation). Let  $r \in \mathbb{N}_+ \geq 1$  and  $\delta_A \in (0, 0.1)$ . For a given  $\mathbf{A} \in \mathbb{R}^{p \times q}$ , we say  $\widetilde{\mathbf{A}} \in \mathbb{R}^{p \times q}$  is an  $(\delta_A, r)$ -approximation of  $\mathbf{A}$  if

- $\widetilde{\mathbf{A}} = \mathbf{U}\mathbf{V}^{\mathsf{T}}$  with  $\mathbf{U} \in \mathbb{R}^{p \times r}$  and  $\mathbf{V} \in \mathbb{R}^{q \times r}$ , and
- $\left|\widetilde{\mathbf{A}}_{ij} \mathbf{A}_{ij}\right| \leq \delta_A \cdot \mathbf{A}_{ij} \text{ for each } i \in [p] \text{ and } j \in [q].$

#### 3.2. Low-Rank Matrix Approximation for AHop

This section includes our linear time result for AHop via lowrank approximation. Let  $\|\mathbf{X}\|_{\max} \leq B$  and  $\|\mathbf{\Xi}\|_{\max} \leq B$ . Let  $T_{\max}(a, b, c)$  denote the time required for multiplication between an  $\mathbb{R}^{a \times b}$  matrix and an  $\mathbb{R}^{b \times c}$  matrix. In fact,  $T_{\max}(a, b, c) \leq \mathcal{O}(abc)$ .

We compute  $\widetilde{\mathbf{A}}$  as a  $(\delta_A, r)$ -approximation of  $\mathbf{A}$ :

**Lemma 3.1.** Suppose B > 1 and matrices  $\Xi \in \mathbb{R}^{d \times M}$ ,  $\mathbf{X} \in \mathbb{R}^{d \times L}$  have  $\|\mathbf{X}\|_{\max} \leq B$  and  $\|\mathbf{\Xi}\|_{\max} \leq B$ . Given  $\mathbf{A} = \exp\{\beta \mathbf{\Xi}^{\mathsf{T}} \mathbf{X}\} \in \mathbb{R}^{M \times L}$ , for  $\delta_A \in (0, 0.1)$ , there is a positive integer g upper bounded by

$$g = \mathcal{O}\left(\max\left\{B^2\beta d, \frac{\log(1/\delta_A)}{\log\left[1/(B^2\beta d) \cdot \log(1/\delta_A)\right]}\right\}\right),$$

and a  $r \in \mathbb{N}_+$  upper bounded by  $r \leq \binom{2(g+d)}{2g}$  such that: There is a matrix  $\widetilde{\mathbf{A}} \in \mathbb{R}^{M \times L}$  that is an  $(\delta_A, r)$ -approximation of  $\mathbf{A} \in \mathbb{R}^{M \times L}$ . Furthermore, the matrices  $\mathbf{U}_1$  and  $\mathbf{U}_2$  defining  $\widetilde{\mathbf{A}}$  can be computed in  $\mathcal{O}(\max{\{M, L\}} \cdot rg)$  time.

*Proof.* For each  $(i, j) \in [M] \times [L]$ , we have

$$\left| (\mathbf{\Xi}^{\mathsf{T}} \mathbf{X})_{i,j} \right| = \left| \sum_{l=1}^{d} \mathbf{\Xi}_{l,i} \mathbf{X}_{l,j} \right| \le \|\mathbf{\Xi}\|_{\max} \|\mathbf{X}\|_{\max} d \le B^2 d.$$

Thus, the entries of the exp in **A** have upper bound:

$$\left\|\beta \mathbf{\Xi}^{\mathsf{T}} \mathbf{X}\right\|_{\max} \leq B^2 \beta d.$$

Applying Lemma A.2 with bound  $B^2\beta d$ , there is a polynomial function P(x) of degree g such that:

$$\sup_{\mathbf{\Xi},\mathbf{X}} \left| P((\beta \mathbf{\Xi}^{\mathsf{T}} \mathbf{X})_{ij}) - \mathbf{A}_{ij} \right| < \delta_A \cdot \mathbf{A}_{ij}.$$

Applying Lemma A.3 with  $\Xi$ , X, there exists an algorithm constructing  $\mathbf{U}_1, \mathbf{U}_2$  in  $\mathcal{O}(\max \{M, L\} \cdot rg)$  time such that  $P(\beta \Xi^{\mathsf{T}} \mathbf{X}) = \mathbf{U}_1 \mathbf{U}_2^{\mathsf{T}}$ .

Therefore, by Definition 3.1,  $\widetilde{\mathbf{A}} := P(\beta \mathbf{\Xi}^{\mathsf{T}} \mathbf{X})$  is an  $(\delta_A, r)$ -approximation of  $\mathbf{A}$ .

Prior to solving AHop, we compute the approximation error bound for  $\widetilde{\mathbf{Z}}$  by utilizing a low-rank approximation (Lemma 3.1) applied to Problem 1.

**Lemma 3.2** (Approximation Error). Let  $\delta_A \in (0, 0.1)$ ,  $\beta > 0, B > 0, \|\mathbf{X}\|_{\max} \leq B$ , and  $\|\mathbf{\Xi}\|_{\max} \leq B$ . Let  $\mathbf{A} = \exp\{\beta \mathbf{\Xi}^{\mathsf{T}} \mathbf{X}\} \in \mathbb{R}^{M \times L}$ , and let  $\widetilde{\mathbf{A}} \in \mathbb{R}^{M \times L}$  such that, for each  $(l, j) \in [M] \times [L]$ ,

$$\widetilde{\mathbf{A}}_{l,j} - \mathbf{A}_{l,j} \bigg| \le \delta_A \cdot \mathbf{A}_{l,j}.$$
(3.1)

Let  $\mathbf{D} = \operatorname{diag}(\mathbf{A}\mathbf{1}_M) \in \mathbb{R}^{M \times M}$  and  $\widetilde{\mathbf{D}} = \operatorname{diag}(\widetilde{\mathbf{A}}\mathbf{1}_M) \in \mathbb{R}^{M \times M}$ , for each  $l \in [M]$ , we have

$$\left| \widetilde{\mathbf{D}}_{l,l} - \mathbf{D}_{l,l} \right| \le \delta_A \cdot \mathbf{D}_{l,l}.$$
(3.2)

Hence, we have

$$\left\|\widetilde{\mathbf{Z}} - \mathbf{Z}\right\|_{\max} = \left\|\Xi\widetilde{\mathbf{D}}^{-1}\widetilde{\mathbf{A}} - \Xi\mathbf{D}^{-1}\mathbf{A}\right\|_{\max} \le 2MB\delta_A.$$
(3.3)

*Proof.* To see (3.2), we observe

$$\left| \widetilde{\mathbf{D}}_{l,l} - \mathbf{D}_{l,l} \right| = \left| \sum_{j=1}^{n} \widetilde{\mathbf{A}}_{l,j} - \sum_{j=1}^{n} \mathbf{A}_{l,j} \right|$$
$$\leq \sum_{j=1}^{n} \left| \widetilde{\mathbf{A}}_{l,j} - \mathbf{A}_{l,j} \right|$$
$$\leq \sum_{j=1}^{n} \delta_{A} \cdot \mathbf{A}_{l,j} = \delta_{A} \cdot \mathbf{D}_{l,l}. \quad (By (3.1))$$

By triangle inequality, we have

$$\leq \underbrace{\left\| \Xi \widetilde{\mathbf{D}}^{-1} \widetilde{\mathbf{A}} - \Xi \mathbf{D}^{-1} \mathbf{A} \right\|_{max}}_{(I)} + \underbrace{\left\| \Xi \widetilde{\mathbf{D}}^{-1} \widetilde{\mathbf{A}} - \Xi \mathbf{D}^{-1} \widetilde{\mathbf{A}} \right\|_{max}}_{(II)}$$

Consider the (I) term; for each  $(i, j) \in [d] \times [L]$ , we have

$$\begin{aligned} \left| \left( \Xi \widetilde{\mathbf{D}}^{-1} \widetilde{\mathbf{A}} - \Xi \mathbf{D}^{-1} \widetilde{\mathbf{A}} \right)_{i,j} \right| \\ &= \left| \sum_{l=1}^{M} \Xi_{i,l} \left( \widetilde{\mathbf{D}}_{l,l}^{-1} - \mathbf{D}_{l,l}^{-1} \right) \widetilde{\mathbf{A}}_{l,j} \right| \\ &\leq \sum_{l=1}^{M} \left| \left( \widetilde{\mathbf{D}}_{l,l}^{-1} - \mathbf{D}_{l,l}^{-1} \right) \widetilde{\mathbf{A}}_{l,j} \right| \cdot \|\Xi\|_{\max} \\ &= \sum_{l=1}^{M} \left| \frac{\mathbf{D}_{l,l} - \widetilde{\mathbf{D}}_{l,l}}{\mathbf{D}_{l,l} \widetilde{\mathbf{D}}_{l,l}} \widetilde{\mathbf{A}}_{l,j} \right| \cdot \|\Xi\|_{\max} \\ &\leq \delta_A B \sum_{l=1}^{M} \widetilde{\mathbf{D}}_{l,l}^{-1} \widetilde{\mathbf{A}}_{l,j} \qquad (\text{By } \|\Xi\|_{\max} \le B \text{ and } (3.2)) \\ &\leq \delta_A B \cdot M. \end{aligned}$$

### Algorithm 1 The algorithm to solve AHop

Input: matrices  $\Xi \in \mathbb{R}^{d \times M}$ ,  $\mathbf{X} \in \mathbb{R}^{d \times L}$ , with  $\beta, d, M, L, B$ , and error margin  $\delta_A$ . Let  $\tau := \max\{M, L\}$ . 1:  $g \leftarrow \mathcal{O}\left(\max\left\{B^2\beta d, \frac{\log(1/\delta_A)}{\log[1/(B^2\beta d) \cdot \log(1/\delta_A)]}\right\}\right)$  by Lemma 3.1 2:  $r \leftarrow \binom{2(g+d)}{2g}$  by Lemma 3.1 3: Compute  $\mathbf{U}_1 \in \mathbb{R}^{M \times r}$ ,  $\mathbf{U}_2 \in \mathbb{R}^{L \times r}$  by Lemma A.3 4: Compute  $\widetilde{\mathbf{D}}^{-1} = \operatorname{diag}\left(\mathbf{U}_1(\mathbf{U}_2^T \mathbf{1}_L)\right) \in \mathbb{R}^{M \times M}$ 5:  $\widetilde{\mathbf{Z}} \leftarrow \Xi \widetilde{\mathbf{D}}^{-1} \mathbf{U}_1 \mathbf{U}_2^T \in \mathbb{R}^{d \times M}$  // Time:  $\mathcal{O}(\tau rd)$ return  $\widetilde{\mathbf{Z}}$ 

Consider the (II) term; for each  $(i, j) \in [d] \times [L]$ , we have

$$\begin{aligned} \left| \left( \Xi \widetilde{\mathbf{D}}^{-1} \widetilde{\mathbf{A}} - \Xi \mathbf{D}^{-1} \mathbf{A} \right)_{i,j} \right| \\ &= \left| \sum_{l=1}^{M} \Xi_{i,l} \mathbf{D}_{l,l}^{-1} \left( \widetilde{\mathbf{A}}_{l,j} - \mathbf{A}_{l,j} \right) \right| \\ &\leq \sum_{l=1}^{M} \left| \mathbf{D}_{l,l}^{-1} \right| \cdot \left| \left( \widetilde{\mathbf{A}}_{l,j} - \mathbf{A}_{l,j} \right) \right| \cdot \left\| \Xi \right\|_{\max} \\ &\leq \delta_A B \sum_{l=1}^{M} \mathbf{D}_{l,l}^{-1} \mathbf{A}_{l,j} \qquad (\text{By } \| \Xi \|_{\max} \le B \text{ and } (3.1)) \\ &\leq \delta_A B \cdot M. \end{aligned}$$

Combining (I) and (II), we obtain

$$\left\|\mathbf{\Xi}\widetilde{\mathbf{D}}^{-1}\widetilde{\mathbf{A}}-\mathbf{\Xi}\mathbf{D}^{-1}\mathbf{A}\right\|_{\max}\leq 2MB\delta_A.$$

This completes the proof of (3.3).

Lemma 3.2 states that the controllable approximation error in Problem 1 takes the form of  $\delta_H = 2MB\delta_A$  by low-rank approximation. Here M is the size of stored memory set  $\Xi$ ,  $\delta_A$  is the precision of low-rank approximation and B is the upper bound of  $\|\mathbf{X}\|_{\max}$  and  $\|\Xi\|_{\max}$ .

Next, we show that AHop utilizing  $(\delta_A, r)$ -approximation requires only almost linear computational time.

**Theorem 3.1** (Almost Linear AHop, Algorithm 1). Let  $\tau := \max \{M, L\}$  and  $\delta_H := 2MB\delta_A$ . For  $\beta > 0$ ,  $d, M, L \in \mathbb{N}_+, \delta_A > 0$ ,  $\|\mathbf{X}\|_{\max} \leq B$  and  $\|\mathbf{\Xi}\|_{\max} \leq B$  with  $B \geq 1$ , there are  $g = \mathcal{O}\left(\max\left\{B^2\beta d, \frac{\log(1/\delta_A)}{\log[1/(B^2\beta d) \cdot \log(1/\delta_A)]}\right\}\right) \in \mathbb{N}_+$  and  $r = \binom{2(g+d)}{2g} \in \mathbb{N}_+$  such that: There exists an Algorithm 1 that runs in  $\mathcal{O}(\tau rg + \tau rd)$  time to solve AHop $(d, M, L, \beta, B, \delta_H)$ . Thus, under realistic settings where  $d = \mathcal{O}(\log \tau), \beta = \Theta(1/d), \delta_H = MB/poly(\tau)$ , if  $B = o(\sqrt{\log \tau})$ , Algorithm 1 requires time  $\tau^{1+o(1)}$ .

*Proof.* In Algorithm 1, step 3 requires  $\mathcal{O}(\tau rg)$  time by Lemma 3.1; step 4 requires  $T_{mat}(r, L, 1) + T_{mat}(M, r, 1) = \mathcal{O}(\tau r)$  time; step 5 requires  $dM + T_{mat}(d, M, r) + T_{mat}(d, M, r)$   $T_{mat}(d, r, L) = O(\tau r d)$  time. Thus, Algorithm 1 requires  $O(\tau r g + \tau r d)$  time.

If the parameters satisfy  $d = \mathcal{O}(\log \tau), \beta = \Theta(1/d), B = o(\sqrt{\log \tau})$ , and  $\delta_A = 1/poly(\tau) = \tau^{-\mathcal{O}(1)}$ , we have

$$g = \mathcal{O}\left(\max\left\{B^2\beta d, \frac{\log(1/\delta_A)}{\log\left[1/(B^2\beta d) \cdot \log(1/\delta_A)\right]}\right\}\right)$$
$$= \mathcal{O}\left(\max\left\{o(\log\tau), \frac{\log\tau}{\log(\log\tau)}\right\}\right) = o(\log\tau).$$

We write g as  $\log \tau / f$  with any  $f = \omega(1)$ , then

$$r = \binom{2(d+g)}{2g} \leq \left(\frac{e(d+g)}{g}\right)^{2g} = 2^{\mathcal{O}(g \log((d+g)/g))}$$
$$\leq 2^{\mathcal{O}(g \log(\log \tau/g))} = 2^{\mathcal{O}(\log \tau \log f/f)}$$
$$< 2^{o(\log \tau)} < \tau^{o(1)}.$$

We know  $(\log \tau)^{\mathcal{O}(1)} \leq \tau^c$  for all a, c > 0 and b > 1, so

$$\mathcal{O}(\tau^a(\log \tau)^b) \le \tau^a \cdot \tau^{o(1)} = \tau^{a+o(1)},$$

where  $\tau^{a+o(1)}$  means  $\tau^{a+o(1)}$  grows slightly larger than  $\tau^a$ . Since  $d, r, g = \mathcal{O}(\log \tau)$ , there exists some constant K such that  $d, r, g \leq K \log \tau$ . Thus, Algorithm 1 requires time:

$$\mathcal{O}\left(\tau rd + \tau rg\right) \le \mathcal{O}\left(\tau(\log \tau)^2\right) \le \tau^{1+o(1)}.$$

This completes the proof.

Theorem 3.1 provides a formal example of efficient computation Algorithm 1 for AHop using low-rank approximation (Lemma 3.1) within a controllable approximation error (Lemma 3.2). This corresponds to Corollary 2.1.1 when the efficient criterion holds. Specifically, to achieve efficient computation under realistic settings, we require  $B = o(\sqrt{\log \tau})$ , leading to almost linear running time  $\tau^{1+o(1)}$ .

#### 3.3. Memory Retrieval Error Bound

Considering the standard modern Hopfield retrieval dynamics with length-L query sequences from (1.1):

$$\mathbf{Z} = \mathbf{\Xi} \operatorname{Softmax} \left( \beta \mathbf{\Xi}^{\mathsf{T}} \mathbf{X} \right).$$

Let  $\widetilde{\mathbf{Z}} \in \mathbb{R}^{d \times L}$  be the output of the *efficient* memory retrieval dynamics by Algorithm 1 retrieving  $\mathbf{X}^{\text{new}}$  from stored memory set  $\mathbf{\Xi} \in \mathbb{R}^{d \times M}$  based on given query  $\mathbf{X} \in \mathbb{R}^{d \times L}$ .

To see how this approximate model stores and retrieves memory patterns, we first introduce the following definitions.

**Definition 3.2.** Given a function  $\mathcal{T} : \mathbb{R}^d \to \mathbb{R}^d$ . A generalized fixed point of  $\mathcal{T}$  is a point  $\mathbf{x} \in \mathbb{R}^d$  for which  $\mathbf{x} \in \mathcal{T}(\mathbf{x})$ .

**Definition 3.3** (Memory Storage and Retrieval). For each  $\mu \in [M]$ , let  $R := \frac{1}{2} \operatorname{Min}_{\mu,\nu \in [M]; \mu \neq \nu} \| \boldsymbol{\xi}_{\mu} - \boldsymbol{\xi}_{\nu} \|$  be the finite radius of each sphere  $S_{\mu}$  centered at memory pattern  $\boldsymbol{\xi}_{\mu}$ . We say  $\boldsymbol{\xi}_{\mu}$  is *stored* if all  $\mathbf{x} \in S_{\mu}$  are generalized fixed points of  $\mathcal{T}, \mathbf{x}_{\mu}^{\star} \in S_{\mu}$ , and  $S_{\mu} \cap S_{\nu} = \emptyset$  for  $\mu \neq \nu$ . We say  $\boldsymbol{\xi}_{\mu}$  is  $\epsilon$ -retrieved by  $\mathcal{T}$  with  $\mathbf{x}$  for an error  $\epsilon$ , if  $\|\mathcal{T}(\mathbf{x}) - \boldsymbol{\xi}_{\mu}\| \leq \epsilon$ .

**Remark 3.1.** A direct implication from Definition 3.3 is that the approximation error of AHop (see Equation (2.7)) must satisfy  $\delta_H = 2MB\delta_A < R$  for successful memory retrieval (and storage).

Additionally, we recall the following definition regarding the separation between memory patterns.

**Definition 3.4** (Separation of Patterns). The separation of a memory pattern  $\boldsymbol{\xi}_{\mu}$  from all other memory patterns  $\boldsymbol{\Xi}$  is defined as its minimal inner product difference to any other patterns:  $\Delta_{\mu} := \operatorname{Min}_{\nu,\nu\neq\mu} [\langle \boldsymbol{\xi}_{\mu}, \boldsymbol{\xi}_{\mu} \rangle - \langle \boldsymbol{\xi}_{\mu}, \boldsymbol{\xi}_{\nu} \rangle].$ 

Next, we present the retrieval error bound of  $\widetilde{\mathbf{Z}}$ .

**Theorem 3.2** (Retrieval Error). Let  $\overline{\Xi}$  be the ground truth memory sequence corresponding to X. Suppose  $\mathbf{x}_l \in S_\mu$ with some  $\mu \in [M]$  for each  $l \in [L]$ , it holds

$$\left\| \widetilde{\mathbf{Z}} - \overline{\mathbf{\Xi}} \right\|_{\max}$$

$$\leq 2B(M-1)e^{-\beta \left( \langle \boldsymbol{\xi}_{\mu}, \mathbf{x} \rangle - \operatorname{Max}_{\nu \in [M]} \langle \boldsymbol{\xi}_{\mu}, \boldsymbol{\xi}_{\nu} \rangle \right)} + 2MB\delta_{A}.$$
(3.4)

*Proof.* We first decompose the RHS of (3.4) as

$$\left\| \widetilde{\mathbf{Z}} - \overline{\Xi} \right\|_{\max} = \left\| \underbrace{\left( \widetilde{\mathbf{Z}} - \mathbf{Z} \right)}_{\text{Approximation Error}} + \underbrace{\left( \mathbf{Z} - \overline{\Xi} \right)}_{\text{Retrieval Error}} \right\|_{\max}. (3.5)$$

Then, we bound the approximation error with Lemma 3.2 and bound the retrieval error with (Hu et al., 2023, eqn. 2.7). By triangle inequality, we complete the proof.  $\Box$ 

**Remark 3.2.** By definition of  $\|\cdot\|_{max}$ , this bound also holds for retrieval based on single pattern x.

**Remark 3.3.** Similar to standard results of modern Hopfield models (Wu et al., 2024a;b; Hu et al., 2023; Ramsauer et al., 2021), (3.4) indicates that with sufficiently large  $\Delta_{\mu}$ and sufficiently small approximation error, Algorithm 1 retrieves memory patterns in a single *iteration*. This allows this efficient modern Hopfield model to serve as a network layer with a single activation, enabling its integration into deep learning, similar to (Hu et al., 2024a; Xu et al., 2024; Schimunek et al., 2023; Hoover et al., 2023; Seidl et al., 2022; Fürst et al., 2022; Paischer et al., 2022).

Surprisingly, this model achieves almost linear time efficiency while maintaining the exponential memory capacity characteristic of modern Hopfield models.

**Corollary 3.2.1** (Capacity Lower Bound, Informal). Suppose all memory patterns are sampled from a sphere of radius m. This efficient modern Hopfield (approximate (1.1) with Algorithm 1) exhibits a *exponential-in-d* lower bound M on the number of patterns it can store and retrieve.

*Proof Sketch.* We first derive the necessary condition for a pattern to be stored and retrieved in the model, i.e., the well-separation condition. Next, we combine it with the separation analysis of random patterns (Hu et al., 2023). See Appendix B.3 for a formal version and a detailed proof.  $\Box$ 

**Remark 3.4.** While the capacity M is slightly smaller than those of (Wu et al., 2024b; Hu et al., 2023; Ramsauer et al., 2021), it still scales exponentially in pattern dimension d. Namely, AHop as per Algorithm 1 achieves almost linear computation time with only a marginal sacrifice in memory capacity.

## 4. Discussion and Conclusion

We apply the fine-grained reduction under the SETH hypothesis to study the computational limits of the retrieval dynamics of modern Hopfield associative memory models (Hu et al., 2024a;b; Wu et al., 2024a;b; Hu et al., 2023; Ramsauer et al., 2021). This work holds practical significance because of the robust link between transformer attention mechanisms and modern Hopfield models. We make a key observation by framing associative memory retrieval as an Approximate Nearest Neighbor Search (ANNS) problem, enabling the application of fine-grained reduction. This allows us to identify a phase transition behavior on the efficiency of all possible variants of modern Hopfield models (Corollary 2.1.1) by tuning the norm bound of queries X and memories  $\Xi$ . In addition, we showcase our theory with an almost linear time variant of modern Hopfield models (Theorem 3.1). We show this efficient model inherits the defining characteristic of modern Hopfield models: exponential memory capacity (Corollary 3.2.1 and Theorem B.1).

**Limitation.** By the formal nature of this work, our results do not lead to practical implementations. However, we anticipate that our findings will offer valuable insights for future efficient Hopfield-centric and transformer-based foundation models and deep learning implementations.

## **Impact Statement**

This theoretical work, as outlined in the introduction and related works, aims to elucidate the foundations of large Hopfield- and transformer-based foundation models and is not expected to have negative social impacts.

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# **Supplementary Material**

## A. Supplementary Theoretical Backgrounds

#### A.1. Low-Degree Approximation of exp Function

Here we present some useful known results for later convenience.

**Lemma A.1** (Approximation Degree of  $e^x$ , Theorem 1.3 of (Aggarwal and Alman, 2022)). For any real number  $B \ge 1$  and  $\delta \in (0, 1)$ , and function  $f : [0, B] \to \mathbb{R}$ , there is a polynomial function  $P : \mathbb{R} \to \mathbb{R}$  of degree tightly bounded by

$$d_{B,\delta}(f = e^x) = \Theta\left(\max\left\{B, \frac{\log(1/\delta)}{\log\left[1/B \cdot \log(1/\delta)\right]}\right\}\right)$$

such that  $\sup_{x \in [0,B]} |P(x) - \exp\{x\}| < \delta$ .

The polynomial P(x) with degree  $d_{B,\delta}(e^x)$  can be computed in poly $(d_{B,\delta}(e^x))$  time.

**Lemma A.2** (Corollary 2.2 of (Alman and Song, 2023)). For any real number  $B \ge 1$  and  $\delta \in (0, 1)$ , and function  $f : [-B, B] \to \mathbb{R}$ , there is a polynomial function  $P : \mathbb{R} \to \mathbb{R}$  of degree tightly bounded by

$$d_{B,\delta}(f = e^x) = \Theta\left(\max\left\{B, \frac{\log(1/\delta)}{\log\left[1/B \cdot \log(1/\delta)\right]}\right\}\right),$$

such that  $\sup_{x \in [0,B]} |P(x) - \exp\{x\}| < \delta \cdot \exp\{x\}.$ 

For more related topics and techniques, please see (Gao et al., 2023a;b; Song et al., 2023; Reddy et al., 2022) for fast approximation algorithms of attention and tensor regression via tensor trick, (Gu et al., 2024d) for low-rank matrix completion, (Song et al., 2024a; Deng et al., 2023; Brand et al., 2023; Song et al., 2021) for attention kernel regression, and (Gu et al., 2024a;b;c; Alman and Song, 2024a; Song et al., 2024b) for low-rank gradient computation in machine learning and large foundation models.

#### A.2. Additional Theoretical Results: Matrix Multiplication Polynomial Approximation

Here, we introduce a helper lemma for approximating an exponential function where the exponent involves matrix multiplication in the context of cross-attention. This lemma is instrumental in proving Lemma 3.1.

**Lemma A.3** (Generalized from Lemma 3.2 of (Alman and Song, 2023)). Consider a polynomial function P(x) representing a degree-g polynomial. Given matrices  $\mathbf{X} \in \mathbb{R}^{M \times d}$  and  $\mathbf{Y} \in \mathbb{R}^{L \times d}$ , there exists an algorithm with a running complexity  $\mathcal{O}(\max \{M, L\} \cdot rg)$ , where  $r = \binom{2(g+d)}{2g}$ . This algorithm, upon receiving matrices  $\mathbf{X}$ ,  $\mathbf{Y}$  as input, constructs matrices  $\mathbf{U}_1, \mathbf{U}_2$  that satisfy the equality  $P(\mathbf{X}\mathbf{Y}^\mathsf{T}) = \mathbf{U}_1\mathbf{U}_2^\mathsf{T}$ , where  $\mathbf{U}_1 \in \mathbb{R}^{M \times r}$  and  $\mathbf{U}_2 \in \mathbb{R}^{L \times r}$ .

*Proof.* See Appendix **B.1** for a detailed proof.

## **B.** Proofs of Main Text

#### B.1. Proof of Lemma A.3

*Proof.* For vectors  $\mathbf{u}, \mathbf{v} \in \mathbb{R}^d$ , define the union of the components  $\mathcal{V} := \{u_1, \cdots, u_d, v_1, \cdots, v_d\}$ . Define  $\mathcal{F}$  as the set of functions f such that:

$$\mathcal{F} \coloneqq \left\{ f: \mathcal{V} \to \{0, 1, 2, \cdots, 2g\} \Big| \sum_{v \in \mathcal{V}} f(v) \le 2g \right\}.$$

The cardinality of  $\mathcal{F}$  is derived by solving combination-with-repetition problems, leading to the expression:

$$|\mathcal{F}| = \binom{2d+2g}{2g}.$$

P(x) can be written as:

$$P(x) = \sum_{i=0}^{g} c_i \cdot x^i.$$

Let  $\mathbf{u} \coloneqq [u_1, \cdots, u_d] \in \mathbb{R}^d$  and  $\mathbf{v} \coloneqq [v_1, \cdots, v_d] \in \mathbb{R}^d$ . Consider the polynomial  $P(\langle \mathbf{u}, \mathbf{v} \rangle)$ :

$$P(\langle \mathbf{u}, \mathbf{v} \rangle) = \sum_{i=0}^{g} c_i \cdot (\langle \mathbf{u}, \mathbf{v} \rangle)^i.$$

There exists a set of constant  $c_f$  associated with each function  $f \in \mathcal{F}$ , such that:

$$\sum_{i=0}^{g} c_i \cdot (\langle \mathbf{u}, \mathbf{v} \rangle)^i = \sum_{f \in \mathcal{F}} c_f \cdot \prod_{v \in \mathcal{V}} v^{f(v)}.$$

Define two vector-valued functions  $\phi_u, \phi_v : \mathbb{R}^d \to \mathbb{R}^{|\mathcal{F}|}$ . For each  $f \in \mathcal{F}$ , we define the elements of  $\phi_u, \phi_v$  as follows:

$$\phi_{u,f}(\mathbf{u}) = c_f \cdot \prod_{l=1}^d u_l^{f(u_l)}, \quad \phi_{v,f}(\mathbf{v}) = \prod_{l=1}^d v_l^{f(v_l)}.$$

Thus,  $P(\langle \mathbf{u}, \mathbf{v} \rangle)$  becomes:

$$P(\langle \mathbf{u}, \mathbf{v} \rangle) = \langle \boldsymbol{\phi}_u(\mathbf{u}), \boldsymbol{\phi}_v(\mathbf{v}) \rangle.$$

Since  $f \leq 2g$ , both  $\phi_{u,f}$  and  $\phi_{v,f}$  require  $\mathcal{O}(g)$  time. Furthurmore, the inner product  $\langle \phi_u(\mathbf{u}), \phi_v(\mathbf{v}) \rangle$  requires  $\mathcal{O}(rg)$  time, where  $r = |\mathcal{F}|$ .

Consider the input matrices  $\mathbf{X}$ ,  $\mathbf{Y}$ . Let  $\{\mathbf{x}_i\}_{i \in [L]}$ ,  $\{\mathbf{y}_i\}_{i \in [L]}$  be the i-th row vector of matrix  $\mathbf{X}$ ,  $\mathbf{Y}$ . The polynomial can be generalized to:

$$P(\mathbf{X}\mathbf{Y}^{\mathsf{T}}) = \begin{bmatrix} P(\langle \mathbf{x}_{1}, \mathbf{y}_{1} \rangle) & P(\langle \mathbf{x}_{1}, \mathbf{y}_{2} \rangle) & \dots & P(\langle \mathbf{x}_{1}, \mathbf{y}_{L} \rangle) \\ P(\langle \mathbf{x}_{2}, \mathbf{y}_{1} \rangle) & P(\langle \mathbf{x}_{2}, \mathbf{y}_{2} \rangle) & \dots & P(\langle \mathbf{x}_{2}, \mathbf{y}_{L} \rangle) \\ \vdots & \vdots & \ddots & \vdots \\ P(\langle \mathbf{x}_{M}, \mathbf{y}_{1} \rangle) & P(\langle \mathbf{x}_{M}, \mathbf{y}_{2} \rangle) & \dots & P(\langle \mathbf{x}_{M}, \mathbf{y}_{L} \rangle) \end{bmatrix} \\ = \begin{bmatrix} \langle \phi_{u}(\mathbf{x}_{1}), \phi_{v}(\mathbf{y}_{1}) \rangle & \langle \phi_{u}(\mathbf{x}_{1}), \phi_{v}(\mathbf{y}_{2}) \rangle & \dots & \langle \phi_{u}(\mathbf{x}_{1}), \phi_{v}(\mathbf{y}_{L}) \rangle \\ \langle \phi_{u}(\mathbf{x}_{2}), \phi_{v}(\mathbf{y}_{1}) \rangle & \langle \phi_{u}(\mathbf{x}_{2}), \phi_{v}(\mathbf{y}_{2}) \rangle & \dots & \langle \phi_{u}(\mathbf{x}_{2}), \phi_{v}(\mathbf{y}_{L}) \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \phi_{u}(\mathbf{x}_{M}), \phi_{v}(\mathbf{y}_{1}) \rangle & \langle \phi_{u}(\mathbf{x}_{M}), \phi_{v}(\mathbf{y}_{2}) \rangle & \dots & \langle \phi_{u}(\mathbf{x}_{M}), \phi_{v}(\mathbf{y}_{L}) \rangle \end{bmatrix} \end{bmatrix}$$

Therefore, we can constuct matrices  $\mathbf{U}_1 \in \mathbb{R}^{M \times |\mathcal{F}|}$  and  $\mathbf{U}_2 \in \mathbb{R}^{L \times |\mathcal{F}|}$  as follows:

$$\mathbf{U}_1 = \begin{bmatrix} \phi_u(\mathbf{X}_1) \ \phi_u(\mathbf{X}_2) \ \cdots \ \phi_u(\mathbf{X}_M) \end{bmatrix}^{\mathsf{T}}, \\ \mathbf{U}_2 = \begin{bmatrix} \phi_v(\mathbf{Y}_1) \ \phi_v(\mathbf{Y}_2) \ \cdots \ \phi_v(\mathbf{Y}_L) \end{bmatrix}^{\mathsf{T}}.$$

It's trivial to observe  $P(\mathbf{X}\mathbf{Y}^{\mathsf{T}}) = \mathbf{U}_1\mathbf{U}_2^{\mathsf{T}}$ . Moreover, constructing  $\mathbf{U}_1, \mathbf{U}_2$  require time  $\mathcal{O}(\max{\{M, L\}} \cdot rg)$ .

#### B.2. A Matrix in Proof of Theorem 2.1

$$\mathbf{A} = \begin{bmatrix} \exp\left\{\frac{B^{2}}{\tilde{d}}\langle a_{1}, b_{1}\rangle\right\} & \exp\left\{\frac{B^{2}}{\tilde{d}}\langle a_{1}, b_{2}\rangle\right\} & \cdots & \exp\left\{\frac{B^{2}}{\tilde{d}}\langle a_{1}, b_{n}\rangle\right\} & \exp\left\{B^{2}\right\} & \exp\left\{B^{2}\right\} & \cdots & \exp\left\{B^{2}\right\} \\ \exp\left\{\frac{B^{2}}{\tilde{d}}\langle a_{2}, b_{1}\rangle\right\} & \exp\left\{\frac{B^{2}}{\tilde{d}}\langle a_{2}, b_{2}\rangle\right\} & \cdots & \exp\left\{\frac{B^{2}}{\tilde{d}}\langle a_{2}, b_{n}\rangle\right\} & \exp\left\{B^{2}\right\} & \exp\left\{B^{2}\right\} & \cdots & \exp\left\{B^{2}\right\} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \exp\left\{\frac{B^{2}}{\tilde{d}}\langle a_{n}, b_{1}\rangle\right\} & \exp\left\{\frac{B^{2}}{\tilde{d}}\langle a_{n}, b_{2}\rangle\right\} & \cdots & \exp\left\{\frac{B^{2}}{\tilde{d}}\langle a_{n}, b_{n}\rangle\right\} & \exp\left\{B^{2}\right\} & \exp\left\{B^{2}\right\} & \cdots & \exp\left\{B^{2}\right\} \\ 0 & 0 & \cdots & 0 & \exp\left\{B^{2}\right\} & \exp\left\{B^{2}\right\} & \cdots & \exp\left\{B^{2}\right\} \\ 0 & 0 & \cdots & 0 & \exp\left\{B^{2}\right\} & \exp\left\{B^{2}\right\} & \cdots & \exp\left\{B^{2}\right\} \\ 0 & 0 & \cdots & 0 & \exp\left\{B^{2}\right\} & \exp\left\{B^{2}\right\} & \cdots & \exp\left\{B^{2}\right\} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & \exp\left\{B^{2}\right\} & \exp\left\{B^{2}\right\} & \cdots & \exp\left\{B^{2}\right\} \\ \end{bmatrix} . \tag{B.1}$$

#### B.3. Formal Statement and Proof of Corollary 3.2.1

Let 
$$\delta \coloneqq -2MB\delta_A \leq 0$$
.

**Theorem B.1** (Memory Capacity Lower Bound, Formal). Suppose the probability of successfully storing and retrieving memory pattern is given by 1 - p. The number of memory patterns sampled from a sphere of radius m that the textitefficient modern Hopfield model (approximate (1.1) with Algorithm 1) can store and retrieve has a lower bound:  $M \ge \sqrt{p}C^{\frac{d-1}{4}}$ , where C is the solution for  $C = b/W_0(\exp\{a+\ln b\})$  with  $W_0(\cdot)$  being the principal branch of Lambert W function,  $a \coloneqq 4/d-1\{\ln [2m(\sqrt{p}-1)/(R-2MB\delta_A)]+1\}$  and  $b \coloneqq 4m^2\beta/5(d-1)$ .

Remark B.1. For details and background of Lambert W function, we refer the readers to (Olver et al., 2010).

Before the main proof, we introduce the following helper lemma. Let  $m := \text{Max}_{\mu \in [M]} \| \boldsymbol{\xi}_{\mu} \|$ .

Lemma B.1. Then, the well-separation condition of memory patterns is:

$$\Delta_{\mu} \ge \frac{1}{\beta} \ln \left( \frac{2(M-1)m}{R - 2MB\delta_A} \right) + 2mR.$$
(B.2)

If  $2MB\delta_A = 0$ , (B.2) reduces to well-separation condition of Softmax-based Hopfield model (Ramsauer et al., 2021).

*Proof of Lemma B.1.* Let  $\mathcal{T}_{Dense}$  be the retrieval dynamics given by the dense modern Hopfield model (Ramsauer et al., 2021), and  $\|\mathcal{T}(\mathbf{x}) - \boldsymbol{\xi}_{\mu}\|$  and  $\|\mathcal{T}_{Dense}(\mathbf{x}) - \boldsymbol{\xi}_{\mu}\|$  be the approximated efficient and dense modern Hopfield model, respectively. By (Ramsauer et al., 2021, Lemma A.4), we have

$$\begin{split} &\|\mathcal{T}_{\text{Dense}}(\mathbf{x}) - \boldsymbol{\xi}_{\mu}\|\\ &\leq 2m(M-1) \exp\left\{-\beta \left(\langle \boldsymbol{\xi}_{\mu}, \mathbf{x} \rangle - \max_{\nu \in [M]} \langle \boldsymbol{\xi}_{\mu}, \boldsymbol{\xi}_{\nu} \rangle \right)\right\},\\ &\leq 2m(M-1) \exp\{-\beta \left(\Delta_{\mu} - 2mR\right)\}, \end{split}$$

where R is radius of the sphere  $S_{\mu}$ .

By Theorem 3.2, the retrieval error  $\|\mathcal{T}(\mathbf{x}) - \boldsymbol{\xi}_{\mu}\|$  has an upper bound:

$$|\mathcal{T}(\mathbf{x}) - \boldsymbol{\xi}_{\mu}|| \le 2(M-1)\exp\{-\beta\left(\Delta_{\mu} - 2mR + \delta\right)\}m - \delta$$

Therefore, for  $\mathcal{T}$  to be a mapping  $\mathcal{T}: S_{\mu} \to S_{\mu}$ , we need

$$2(M-1)\exp\{-\beta\left(\Delta_{\mu}-2mR+\delta\right)\}m-\delta\leq R$$

This deduces the well-separation condition for this almost linear time model

$$\Delta_{\mu} \ge \frac{1}{\beta} \ln \left( \frac{2(M-1)m}{R - 2MB\delta_A} \right) + 2mR.$$

This completes the proof.

Now we start the main proof of Theorem B.1.

*Proof of Theorem B.1.* We first observe that (B.1) has a slightly tighter lower bound compared to its original counterpart (Ramsauer et al., 2021), we note that under the condition identified in Remark 3.1, the new well-separation condition Lemma B.1 features a smaller denominator inside the logarithmic term. Following a similar approach to that in (Wu et al., 2024b, Lemma 3.4), we complete the proof and obtain a slightly smaller, yet still exponential-in-*d*, memory capacity lower bound. This is an expected consequence of an efficient-accuracy tradeoff.