UNMASKING TRANSFORMERS: A THEORETICAL APPROACH TO DATA RECOVERY VIA ATTENTION WEIGHTS

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Paper under double-blind review

ABSTRACT

In the realm of deep learning, transformers have emerged as a dominant architecture, particularly in both natural language processing and computer vision tasks. However, with their widespread adoption, concerns regarding the security and privacy of the data processed by these models have arisen. In this paper, we address a pivotal question: Can the data fed into transformers be recovered using their attention weights and outputs? We introduce a theoretical framework to tackle this problem. Specifically, we present an algorithm that aims to recover the input data $X \in \mathbb{R}^{d \times n}$ from given attention weights $W = QK^\top \in \mathbb{R}^{d \times d}$ and output $B \in \mathbb{R}^{n \times n}$ by minimizing the loss function $L(X)$. This loss function captures the discrepancy between the expected output and the actual output of the transformer. Our findings have significant implications for preventing privacy leakage from attacking open-sourced model weights, suggesting potential vulnerabilities in the model's design from a security and privacy perspective - you may need only a few steps of training to force LLMs to tell their secrets.

1 INTRODUCTION

In the intricate and constantly evolving domain of deep learning, the transformer architecture has emerged as a game-changing innovation Vaswani et al. (2017). This novel architecture has propelled the state-of-the-art performance in a myriad of tasks, and its potency lies in the underlying mechanism known as the "attention mechanism". The essence of this mechanism can be distilled into its unique interaction between three distinct matrices: the **Query** (Q), the **Key** (K), and the **Value** (V), where the **Query** matrix (Q) represents the questions or the aspects we're interested in, the **Key** matrix (K) denotes the elements against which these questions are compared or matched, and the **Value** matrix (V) encapsulates the information we want to retrieve based on the comparisons. These matrices are not just mere multidimensional arrays; they play vital roles in encoding, comparing, and extracting pertinent information from the data.

Given this context, the attention mechanism can be mathematically captured as follows:

Definition 1.1 (Attention matrix computation)**.** *Let $Q, K \in \mathbb{R}^{n \times d}$ be two matrices that respectively represent the query and key. Similarly, for a matrix $V \in \mathbb{R}^{n \times d}$ denoting the value, the attention matrix is defined as*

$$\mathrm{Att}(Q, K, V) := D^{-1}AV,$$

In this equation, two matrices are introduced: $A \in \mathbb{R}^{n \times n}$ and $D \in \mathbb{R}^{n \times n}$, defined as:

$$A := \exp(QK^\top) \ \text{and} \ D := \mathrm{diag}(A\mathbf{1}_n).$$

Here, the matrix A represents the relationship scores between the query and key, and D ensures normalization. The computation hence, deftly combines these relationships with the value matrix to output the final attended representation.

In practical large-scale language models ChatGPT (2022); OpenAI (2023), there might be multi-levels of the attention computation. For those multi-level architecture, the feed-forward training can be represented as

$$X_{\ell+1}^\top \leftarrow D(X_\ell)^{-1} \exp(X_\ell^\top Q_\ell K_\ell X_\ell) X_\ell^\top V_\ell$$

Algorithm 1 Sketch of inverse attack to transformer-based models

Input: Ideal model prediction $B \in \mathbb{R}^{n \times d}$
Parameters: Model function f, pretrained weights W, training steps T
Output: Leaked input $X \in \mathbb{R}^{n \times d}$ for output B
procedure INVERSEATTACK(B, f, W, T)
  Initialize each entry of $X_0 \in \mathbb{R}^{n \times d}$ from Gaussian distribution $\mathcal{N}(0, 1)$.
  $t \leftarrow 1$
  for $t < T$ **do**
    Compute loss by some specific metric $\ell(\cdot, \cdot)$, such that $L_t := \ell(f(W, X_{t-1}), B)$
    Compute gradient $g_t := \nabla_{X_{t-1}} L_t$
    Compute update for X via first-order or second order algorithm using g_t, denote ΔX
    Update $X_t \leftarrow X_{t-1} - \Delta X$
    $t \leftarrow t + 1$
  end for
  return X_T with guaranteed $L_t \leq \epsilon$ (Theorem 4.3 and Theorem 4.4)
end procedure

where X_ℓ is the input of ℓ-th layer, and $X_{\ell+1}$ is the output of ℓ-th layer, and Q_ℓ, K_ℓ, V_ℓ are the attention weights in ℓ-th layer.

This architecture has particularly played a pivotal role in driving progress across various sub-disciplines of natural language processing (NLP) Firat et al. (2016); Choi et al. (2018); Usama et al. (2020); Naseem et al. (2020); Martin et al. (2019); ChatGPT (2022); OpenAI (2023). This trajectory of influence is most prominently embodied by the creation and widespread adoption of Large Language Models (LLMs) like GPT-4 and Claude-3. These models are hallmarks due to their staggering number of parameters and complex architectural designs.

Yet, the very complexity and architectural sophistication that propel the success of transformers come with a host of consequential challenges, making their effective and responsible usage nontrivial. Prominent among these challenges is the overarching imperative of ensuring data security and privacy Pan et al. (2020); Brown et al. (2022); Kandpal et al. (2022). Within the corridors of the research community, an increasingly pertinent question is emerging regarding the inherent vulnerabilities of these architectures. Specifically,

is it possible to know the input data by analyzing the attention weights and model outputs?

To put it in mathematical terms, given a language model represented as $B = f(W; X)$, if one has access to the output B and the attention weights W, is it possible to mathematically invert the model to obtain the original input data X?

Addressing this line of inquiry extends far beyond the realm of academic speculation; it has direct and significant implications for practical, real-world applications. This is especially true when these transformer models interact with data that is either sensitive in nature, like personal health records Cascella et al. (2023), or proprietary, as in the financial sector Wu et al. (2023). With the broader deployment of Large Language Models into environments that adhere to stringent data confidentiality regulations, the mandate for achieving data security becomes essential. In this work, we aim to delve deeply into this issue, striving to offer a nuanced understanding of these potential vulnerabilities while suggesting pathways for ensuring safety in the development, training, and utilization of transformer technologies.

This paper addresses a distinct *attention-based regression model* that differs from the conventional task of finding optimal weights for a given input and output. Specifically, we assume that the weights are already known, and our objective is to invert the output to recover the original data. The key focus of our investigation lies in *identifying the conditions* under which successful inversion of the original input is feasible. This problem holds significant relevance in the context of addressing security concerns associated with attention networks.

Our contribution In this paper, we formulate the formal regression model for the inverse attack on the soft-max attention layer. Utilizing simplified notations of the loss function, we are able to calculate a close-form representation of its Hessian. By assuming bounded parameters and adding a moderate regularizer, we prove the smoothness (Lipschitz continuity) and strongly-convexity (Positive Semi-definiteness) of our regression problem, which leads to the convergence of gradient-based and Hessian-based methods that approach the approximate optimal. Therefore, we apply these algorithms to invert the attention weights to the input data. We provided numerical experiments to verify the reliability of our methods.

Roadmap. We arrange the rest of our paper as follows. In Section 2 we present some works related our topic. In Section 3, we state an overview of our techniques, summarizing the method we use to recover data via attention weights. We state our main theories in Section 4. We provide our experiment results in Section 5. We conclude our work in Section 6.

2 Related Works

This section discusses related works in the LLM community. We summarize the current research on LLM security and inversion attack in Section 2.1. We concern about attention computation theory and LLM-based regression theory in Section 2.2.

2.1 LLM Security

Security concerns about LLM. Amid LLM advancements, concerns about misuse have arisen Pan et al. (2020); Brown et al. (2022); Kandpal et al. (2022); Kirchenbauer et al. (2023); Vyas et al. (2023); Chu et al. (2023a); Xu et al. (2023); Gao et al. (2023d); Kirchenbauer et al. (2023); He et al. (2022a;b); Gao et al. (2023f); Shen et al. (2023a). Pan et al. (2020) assesses the privacy risks of capturing sensitive data with eight models and introduces defensive strategies, balancing performance and privacy. Brown et al. (2022) asserts that current methods fall short in guaranteeing comprehensive privacy for language models, recommending training on publicly intended text. Kandpal et al. (2022) reveals that the vulnerability of large language models to privacy attacks is significantly tied to data duplication in training sets, emphasizing that deduplicating this data greatly boosts their resistance to such breaches. Kirchenbauer et al. (2023) devised a way to watermark LLM output without compromising quality or accessing LLM internals. Meanwhile, Vyas et al. (2023) introduced near access-freeness (NAF), ensuring generative models, like transformers and image diffusion models, don't closely mimic copyrighted content by over k-bits.

Inverting the neural network. Originating from the explosion of deep learning, there have been a series of works focused on inverting the neural network Jensen et al. (1999); Lu et al. (1999); Mahendran & Vedaldi (2015); Dosovitskiy & Brox (2016); Zhang et al. (2020d). Jensen et al. (1999) surveys various techniques for neural network inversion, which involves finding input values that produce desired outputs, and highlights its applications in query-based learning, sonar performance analysis, power system security assessment, control, and codebook vector generation. Lu et al. (1999) presents a method for inverting trained neural networks by formulating the problem as a mathematical programming task, enabling various network inversions and enhancing generalization performance.. Mahendran & Vedaldi (2015) explores the reconstruction of image representations, including CNNs, to assess the extent to which it's possible to recreate the original image, revealing that certain layers in CNNs retain accurate visual information with varying degrees of geometric and photometric invariance. Zhang et al. (2020d) presents a novel generative model-inversion attack method that can effectively reverse deep neural networks, particularly in the context of face image reconstruction, and explores the connection between a model's predictive ability and vulnerability to such attacks while noting limitations in using differential privacy for defense.

Attacking the Neural Networks. During the development of artificial intelligence, there have been many works on attaching the neural networks Zhu et al. (2019); Wei et al. (2020); Rigaki & Garcia (2020); Huang et al. (2020); Yin et al. (2021); Huang et al. (2021b); Gao et al. (2023c). Several studies Zhu et al. (2019); Wei et al. (2020); Rigaki & Garcia (2020); Yin et al. (2021) have warned that local training data can be compromised using only exchanged gradient information. These methods start with dummy data and gradients, and through gradient descent, they empirically show that the original data can be fully reconstructed. A follow-up study Zhao et al. (2020) specifically focuses on classification tasks and finds that the real labels can also be accurately recovered. Other types of attacks include membership and property inference Shokri et al. (2017); Melis et al. (2019), the use of Generative Adversarial Networks (GANs) Hitaj et al. (2017); Goodfellow et al. (2014), and additional machine-learning techniques McPherson et al. (2016); Papernot et al. (2016). A recent paper Wang et al. (2023) uses tensor decomposition for gradient leakage attacks but is limited by its inefficiency and focus on over-parametrized networks.

2.2 Attention Computation and Regression

Attention Computation Theory. Following the rise of LLM, numerous studies have emerged on attention computation Kitaev et al. (2020); Tay et al. (2020); Chen et al. (2021); Zandieh et al. (2023); Tarzanagh et al. (2023); Sanford et al. (2023); Panigrahi et al. (2023a); Zhang et al. (2020a); Arora & Goyal (2023); Tay et al. (2021); Deng et al. (2023b); Xia et al. (2023); Kacham et al. (2023). LSH techniques approximate attention, and based on them, the KDEformer offers a notable dot-product attention approximation Zandieh et al. (2023). Recent works Alman & Song (2023); Brand et al. (2023); Deng et al. (2023c) explored diverse attention computation methods and strategies to enhance model efficiency. On the optimization front, Zhang et al. (2020b) highlighted that adaptive methods excel over SGD due to heavy-tailed noise distributions. Other insights include the emergence of the KTIW property Snell et al. (2021) and various regression problems inspired by attention computation Gao et al. (2023a); Li et al. (2023c;b), revealing deeper nuances of attention models.

Theoretical Approaches to Understanding LLMs. Recent strides have been made in understanding and optimizing regression models using various activation functions. Research on overparameterized neural networks has examined exponential and hyperbolic activation functions for their convergence properties and computational efficiency Gao et al. (2023a); Li et al. (2023c); Deng et al. (2023b); Gao et al. (2023d); Li et al. (2023a); Gao et al. (2023e); Song et al. (2023); Sinha et al. (2023); Chu et al. (2023a;b); Shen et al. (2023b). Modifications such as regularization terms and algorithmic innovations, like a convergent approximation Newton method, have been introduced to enhance their performance Li et al. (2023c); Deng et al. (2022). Studies have also leveraged tensor tricks to vectorize regression models, allowing for advanced Lipschitz and time-complexity analyses Gao et al. (2023b); Deng et al. (2023a). Simultaneously, the field is seeing innovations in optimization algorithms tailored for LLMs. Techniques like block gradient estimators have been employed for huge-scale optimization problems, significantly reducing computational complexity Cai et al. (2021). Unique approaches like Direct Preference Optimization bypass the need for reward models, fine-tuning LLMs based on human preference data Rafailov et al. (2023). Additionally, advancements in second-order optimizers have relaxed the conventional Lipschitz Hessian assumptions, providing more flexibility in convergence proofs Liu et al. (2023). Also, there is a series of work on understanding fine-tuning Malladi et al. (2023a;b); Panigrahi et al. (2023b). Collectively, these theoretical contributions are refining our understanding and optimization of LLMs, even as they introduce new techniques to address challenges such as non-guaranteed Hessian Lipschitz conditions.

Optimization and Convergence of Deep Neural Networks. Prior research Li & Liang (2018); Du et al. (2018); Allen-Zhu et al. (2019a;b); Arora et al. (2019a;b); Song & Yang (2019); Cai et al. (2019); Zhang et al. (2019); Cao & Gu (2019); Zou & Gu (2019); Oymak & Soltanolkotabi (2020); Ji & Telgarsky (2019); Lee et al. (2020); Huang et al. (2021a); Zhang et al. (2020c); Brand et al. (2020); Zhang et al. (2020a); Song et al. (2021); Alman et al. (2023); Munteanu et al. (2022); Zhang (2022); Gao et al. (2023a); Li et al. (2023c); Qin et al. (2023) on the optimization and convergence of deep neural networks has been crucial in understanding their exceptional performance across various tasks. These studies have also contributed to enhancing the safety and efficiency of AI systems. In Gao et al. (2023a) they define a neural function using an exponential activation function and apply the gradient descent algorithm to find optimal weights. In Li et al. (2023c), they focus on the exponential regression problem inspired by the attention mechanism in large language models. They address the non-convex nature of standard exponential regression by considering a regularization version that is convex. They propose an algorithm that leverages input sparsity to achieve efficient computation. The algorithm has a logarithmic number of iterations and requires nearly linear time per iteration, making use of the sparsity of the input matrix.

3 Recovering Data via Attention Weights

In this section, we propose our theoretical method to recover the training data from trained transformer weights and outputs. In Section 3.1, we provide a detailed description of our approach. In Section 3.2, we introduce our simplified notations to calculate the Hessian of the loss function. In Section 3.3, we state the decomposed expression of the Hessian.

3.1 Training Objective of Attention Inversion Attack

In this study, we propose a novel technique for inverting the attention weights of a transformer model using Hessian-based algorithms. We consider the single-layer soft-max attention function

$$f(W;X) := D(X)^{-1}\exp(X^\top W X)V$$

, where $W = KQ^\top \in \mathbb{R}^{d\times d}$ represents the attention weights and $D(X) = \mathrm{diag}(\exp(X^\top W X)) \in \mathbb{R}^{n\times n}$ is the diagonal matrix for normalization.

Our aim is to find the input $X \in \mathbb{R}^{d\times n}$ that minimizes the Frobenius norm of the difference between $f(W;X)$ and the output B. Here, dimension d denotes the length of a token, dimension n denotes the total number of the tokens in X. To achieve this, we introduce an algorithm that minimizes the loss function $L(X)$, defined as follows:

Definition 3.1 (Regression model)**.** *Given the attention weights $W = KQ^\top \in \mathbb{R}^{d\times d}$, $V \in \mathbb{R}^{d\times d}$ and output $B \in \mathbb{R}^{n\times d}$, the goal is find $X \in \mathbb{R}^{d\times n}$ such that*

$$L(X) := \|D(X)^{-1}\exp(X^\top W X)X^\top V - B\|_F^2 + L_{\mathrm{reg}}, \tag{1}$$

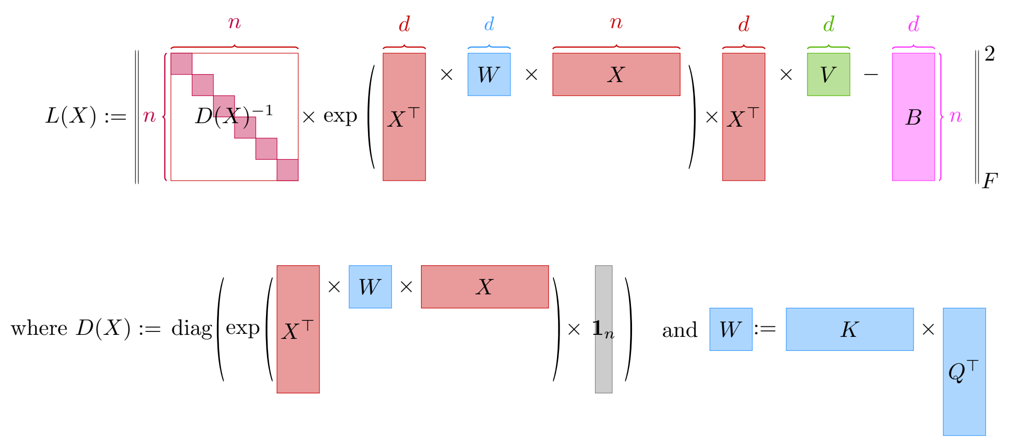


Figure 1: Visualization of our loss function.

L_{reg} captures the additional regularization terms which we introduce later. This loss function quantifies the discrepancy between the expected output and the actual output of the transformer.

In our approach, we leverage Hessian decomposition to efficiently compute the Hessian matrix and apply a second-order method to approximate the optimal input X. Utilizing the Hessian, we can gain insights into the curvature of the loss function, which improves the efficiency of finding the approximate optimal solution.

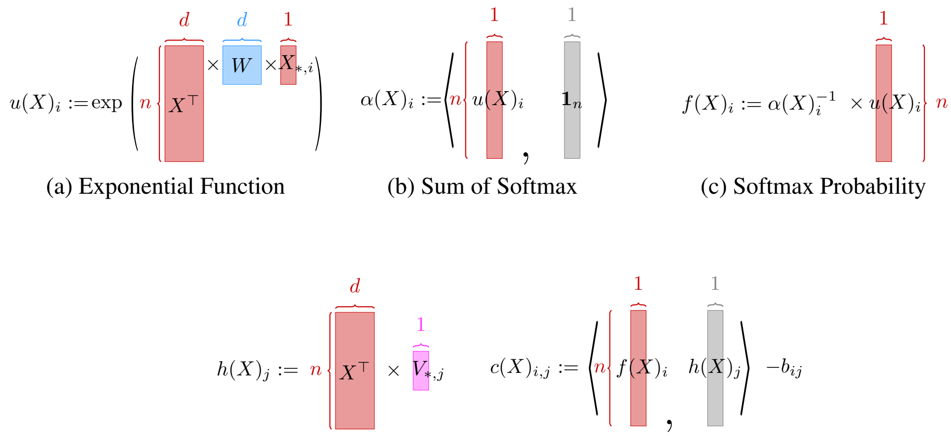
By integrating Hessian decomposition and second-order optimization techniques (Anstreicher (2000); Lee et al. (2019); Cohen et al. (2019); Jiang et al. (2021); Huang et al. (2022); Gu & Song (2022); Gu et al. (2023)), our proposed algorithm provides a promising approach for addressing the challenging task of inverting attention weights in transformer models.

3.2 Model simplification

Due to the complexity of the loss function (Eq. (1)), it is challenging to give the explicit formula of its Hessian. To simplify the computation, we introduce several notations (See Figure 2 for visualization):

$$\text{Exponential Function: } u(X)_i := \exp(X^\top W X_{*,i})$$

$$\text{Sum of Softmax: } \alpha(X)_i := \langle u(X)_i, \mathbf{1}_n \rangle$$
$$\text{Softmax Probability: } f(X)_i := \alpha(X)_i^{-1} u(X)_i$$
$$\text{Value Function: } h(X)_j := X^\top V_{*,j}$$
$$\text{One-entry Loss Function: } c(X)_{i,j} := \langle f(X)_i, h(X)_j \rangle - b_{i,j}.$$



(a) Exponential Function (b) Sum of Softmax (c) Softmax Probability

(d) Value Function (e) One-unit Loss Function

Figure 2: Visualization of Notations We Defined

Using these terms, we can express the loss function $L(X)$ as the sum over the loss in each entry as below, which allows us to break down the computation into several steps. $L(X) = \sum_{i=1}^n \sum_{j=1}^d (c(X)_{i,j})^2$.

3.3 Hessian Decomposition

This section provides our technique to decompose the Hessian. By decomposing the Hessian into several cases, we can give a close-form expression, which enables us to comprehend and analyze the Hessian. We use variables $i_k \in [n], j_k \in [d], k = 1, 2, 3$ to denote the indexes.

Now, we split $\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}}$ (the gradient of $c(X)_{i_0,j_0}$) into two cases:

- *Case 1:* The situation when $i_0 = i_1$.
- *Case 2:* The situation when $i_0 \neq i_1$.

Similar, we break down the computation of $\frac{\mathrm{d}^2 c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1} \mathrm{d}x_{i_2,j_2}}$ into five cases to handle different scenarios:

- *Case 1:* The situation when $i_0 = i_1 = i_2$.
- *Case 2:* The situation when $i_0 = i_1 \neq i_2$.
- *Case 3:* The situation when $i_0 = i_2 \neq i_1$.
- *Case 4:* The situation when $i_0 \neq i_1$, $i_0 \neq i_2$ and $i_1 = i_2$.
- *Case 5:* The situation when $i_0 \neq i_1$, $i_0 \neq i_2$ and $i_1 \neq i_2$.

It is worth mentioning that the second case and the third case are equivalent by switching indexes. By considering these cases, we can calculate the Hessian for each element in X. This allows us to gain further insights into the curvature of the loss function and optimize the parameters more effectively.

Since our decision variable X is a $n \times d$ matrix, we define the Hessian of $c(X)_{i_0,j_0}$ by considering its Hessian with respect to $x = \mathrm{vec}(X)$. This means that, $\nabla^2 c(X)_{i_0,j_0}$ is a $nd \times nd$ matrix with its $i_1 \cdot j_1, i_2 \cdot j_2$-th entry being $\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_2} x_{i_2,j_2}}$. Leveraging the split of different scenarios, we decompose the Hessian into a partition of square matrices.

Definition 3.2 (Hessian split). *We use $H_k^{(i_1,i_2)} \in \mathbb{R}^{d \times d}$ to represent the square matrix corresponding to the k-th case in Hessian computation. Notice that the j_1, j_2-th entry of $H_k^{(i_1,i_2)}$ is $\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_2}x_{i_2,j_2}}$. Then, the Hessian of the loss is a matrix partition consists of matrices of the above five cases. The formal representation can be found in Appendix D.1.*

The reason we introduce the Hessian split is that the square matrices of the same type share the similar formula. Therefore, we can compute the expression of each type (see detailed calculation in Section D) to derive $\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_2}x_{i_2,j_2}}$. This gives us the information of the Hessian of the loss function.

4 Main results

Now, we state the analysis of the correctness of our inversion attack strategy. Assuming the parameters are bounded, we verify the Hession of our loss function is Lipschitz continuous and PSD lower-bounded. Therefore, gradient-based and Hessian-based methods are used to solve the regularized regression model. We defer the proofs to the Appendix.

Properties of the Hessian We assume an unified upper bound for all parameters in our model, including the weight W, the value V, the output B, and the decision variable X.

Assumption 4.1 (Bounded Parameters, Informal version of Assumption F.1). *We assume $\|W\| \leq R, \|V\| \leq R, \|X\| \leq R, b_{i,j} \leq R^2$, where $\| \cdot \|$ is the matrix 2-norm and $R > 1$ is some constant.*

Next, we state the bounds for the Hessian of the loss function in terms of $\mathrm{poly}(n, d, R)$.

Theorem 4.2 (Properties of the Hessian, Informal version of Theorem G.12 and Theorem H.2). *We assume that Assumption 4.1 holds. Then, the Hessian of $L(X)$ is Lipschitz continuous with Lipschitz constant being $O(n^{3.5}d^{3.5}R^{10})$. Also, it has PSD lower bound: $L(X) \succeq -O(ndR^8) \cdot \mathbf{I}_{nd}$.*

Therefore, we define the regularization term to be $L_{\mathrm{reg}} := O(ndR^8) \cdot \| \mathrm{vec}(X)\|_2^2$ to have the PSD guarantee for our regression problem.

Convergence analysis With above properties of the loss function, we have the convergence results stated as follows. Theorem 4.3 shows the correctness of the gradient-based method. Theorem 4.3 shows the correctness of the Hessian-based method. The algorithm for approximating PSD matrices in Deng et al. (2022) can be applied to approximate the Hessian efficiently.

Theorem 4.3 (First-Order Main Result, Informal version of Theorem I.2). *We assume that Assumption 4.1 holds. Let X^* denote the optimal point of the regularized regression model defined in Definition 3.1. Then, for any accuracy parameter $\epsilon \in (0, 0.1)$, an algorithm based on the gradient-descent method can be employed to recover the initial data. It outputs a matrix $\widetilde{X} \in \mathbb{R}^{d \times n}$ satisfying $\|\widetilde{X} - X^*\|_F \leq \epsilon$. The algorithm runs $T = O(\mathrm{poly}(n, d, R) \cdot \log(\|X_0 - X^*\|_F/\epsilon))$ iterations, with execution time for each iteration being $\mathrm{poly}(n, d)$, where the degree of d depends on the current matrix computation time.*

Theorem 4.4 (Second-Order Main Result, Informal version of Theorem I.3). *We assume that Assumption 4.1 holds. Let X^* denote the optimal point of the regularized regression model defined in Definition 3.1. Suppose we choose an initial point X_0 such that $M \cdot \|X_0 - X^*\|_F \leq O(ndR^8)$ where $M = O(n^3d^3R^{10})$. Then, for any accuracy parameter $\epsilon \in (0, 0.1)$ and any failure probability $\delta \in (0, 0.1)$, an algorithm based on the approximation-Newton method can be employed to recover the initial data. It outputs a matrix $\widetilde{X} \in \mathbb{R}^{d \times n}$ satisfying $\|\widetilde{X} - X^*\|_F \leq \epsilon$ with a probability at least $1 - \delta$. The algorithm runs $T = O(\log(|X_0 - X^*|_F/\epsilon))$ iterations, with execution time for each iteration being $\mathrm{poly}(n, d, \log(1/\delta))$, where the degree of d depends on the current matrix computation time.*

These theorems show that we can utilize first-order method and second-order method to search an ϵ-optimal approximation to the real input data X within a preferable running time.

step	recovering text	loss
0	GrapeJUST once received cancer treatment at this hospital.	4.74
2500	precious quoted once received cancer treatment at this hospital.	4.61
5000	grass Tradable once received cancer treatment at this hospital.	4.50
6500	acrylic Bob once received cancer treatment at this hospital.	4.29
7500	Alan Bob once received cancer treatment at this hospital.	2.27

Table 1: Visualization of the results. Here, the original target text is **Alan Bob once received cancer treatment at this hospital.** We mask the sensitive data **Alan Bob** and run the gradient-descent inverse attack to recover. The blue-colored texts are the outputs in each iteration. The column on the right shows the value of the cross-entropy loss. It can be seen that the original data is leaked after 7500 steps, which echoes our convergence analysis.

5 EXPERIMENT

In this section, to verify the accuracy of our theory, we conducted a simple experiment to evaluate how our approach recovers data from the pre-trained weights in the LLM. In Section 5.1, we provide the setup and the design of our data-attack experiment. Next, we discuss our results in Section 5.2. Supplementary experimental details are provided in Appendix J.

5.1 EXPERIMENT DESIGN AND SETUP

We use the pre-trained language model GPT-2-small Radford et al. (2019). For the dataset, we utilize GPT-4 Achiam et al. (2023); Bubeck et al. (2023) to help us create hundreds of text data containing virtual information. This can be viewed as the toy or the synthetic dataset. Then, we use the synthetic dataset to fine-tune the pre-trained GPT-2-small with Adam optimizer Kingma & Ba (2014).

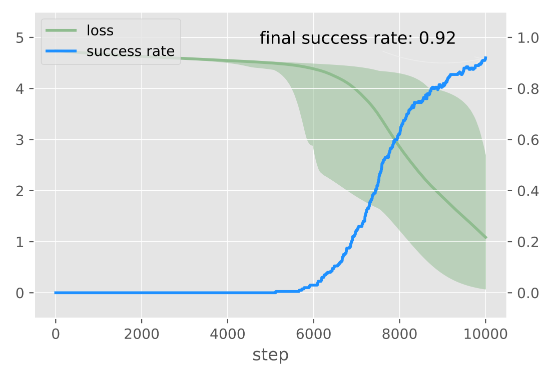


Figure 3: Training record of our inversion recovery attack. We state the maximum, mean, and minimum loss during 10000 updates. We also present the success rate of attack in 1000 repeated experiments.

For the recovery part, we first choose one text from the dataset and convert it into one-hot vectors through the model's vocabulary, denoted by $S^* \in \mathbb{R}^{n \times N}$ where N is the vocabulary size. Notice that GPT-2-small is trained to conduct next-token prediction by causal mask, namely, it uses the information of the first k words to predict the $(k+1)$-th word. Therefore, we split S^* to the masked part $S_1 \in \mathbb{R}^{m \times N}$ and the unmasked part $S_2 \in \mathbb{R}^{(n-m) \times N}$. Then, we use S_2 as part of the initial input and we introduce our inversion attack approach to recover S_1.

We initialize our recovery by a random matrix $X^0 \in \mathbb{R}^{m \times N}$ where each entry is sampled from $\mathcal{N}(0, 1)$. We compute $S_1^0 \in \mathbb{R}^{m \times N} := \mathsf{softmax}(X^0)$, and concatenate it with S_2 to form $S^0 \in \mathbb{R}^{n \times N} = \begin{bmatrix} S_1^0 \\ S_2^0 \end{bmatrix}$, then input it into the model. We denote the GPT-2-small model by a mapping $F : \mathbb{R}^{n \times N} \to \mathbb{R}^{n \times N}$. For any input matrix $A \in \mathbb{R}^{n \times N}$, the output of GPT-2-small $F(A) \in \mathbb{R}^{n \times N}$ will consist of row-wise soft-max vectors since we add a soft-max operation to the output of the last layer to compute the probability distribution. We use $S^t \in \mathbb{R}^{n \times N}$ to represent the matrix of soft-max vectors we recover at the t-th timestamp for integer $t \geq 0$ by minimizing the loss.

We define our problem as minimizing the cross-entropy loss which is calculated as $L(F(S^t), S^t) := \sum_{i=1}^{n-1} \sum_{j=1}^{N} -S^t_{i+1,j} \cdot \log(F(S^t)_{i,j})$.

Remark 5.1. *We use the cross-entropy loss here instead since it is commonly used in the training of current LLMs. Note that our approach to analyze the canonical softmax loss regression can be modified to show the correctness of the cross-entropy loss regression. Similar topics have been discussed in other LLM-related literature, e.g. Gao et al. (2023c).*

We use the gradient-descent method to conduct the attack. The update rule is defined as:

$$X_{t+1} \leftarrow X_t - \eta \nabla_{X_t} L(F(S^t), S^t),$$

where we use X_t to denote the recovering input at t-th timestamp for integer $t \geq 0$. Note that η denotes the learning rate. S^t is computed by X_t as we mentioned above.

The training involves Adam optimizer, and all the hyper-parameters are set to be defaults. Totally, we trained 10000 steps for the input recovery. All the experiments are repeated 1000 times to ensure reliability.

5.2 Results

We state our results of recovery in Figure 3. We recorded the mean, maximum, and minimum loss during the training. We also recorded the success rate at each stage in the 10000 updates. Notice that the success rate at the k-th update is computed by the count of successful experiments (i.e., the masked input data is recovered) at the k-th update divided by 1000, which is the repeated time. It's noteworthy that after 5000 steps, the success rate greatly increases, eventually, it demonstrates a high value of 0.92. This result verifies our attacking method has a high probability of recovery training, especially for private and sensitive data from open-source weights of language models.

Furthermore, we showcase one example of the recovery attacks in Table 1, where we create fake data "Alan Bob once received cancer treatment at this hospital.". Accordingly, the name "Alan Bob" in the context is private and masked. We cut these two words and converted the sentence " once received cancer treatment at this hospital." into one-hot vectors as S_2 in Section 5.1. Next, we run the inverse attack and record the output and loss value at each step. We use blue text to represent the text that is predicted by our algorithm. As we can see from Table 1, the recovering text is initially GrapeJUST with the cross-entropy loss 4.74 at the beginning. Then, at the 6500-th step of recovering, our algorithm outputs acrylic Bob, where the word "Bob" is successfully recovered. Finally, at the 7500-th step, our algorithm successfully recovers the target text Alan Bob.

6 Conclusion

In this study, we have presented a theoretical approach for conducting the inverse recovery on the input data using weights and outputs.

We propose the mathematical framework of the attention-inspired mechanism regression model. Our theoretical analysis part consists of the efficient calculation of the Hessian and the verification of its smoothness and strongly-convexity. With the aim of these properties, we introduce gradient-based and Hessian-based to do the inverse recovery. Then, we show the reliability of our proposed method by experiments on text reconstruction using GPT-2-small.

The insights gained from this research are intended to deepen our understanding and facilitate the development of more secure and robust transformer models. By doing so, we strive to foster responsible and ethical advancements in the field of deep learning. This work lays the groundwork for future research and development aimed at fortifying transformer technologies against potential threats and vulnerabilities.

References

Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altenschmidt, Sam Altman, Shyamal Anadkat, et al. Gpt-4 technical report. *arXiv preprint arXiv:2303.08774*, 2023.

Zeyuan Allen-Zhu, Yuanzhi Li, and Zhao Song. A convergence theory for deep learning via over-parameterization. In *International conference on machine learning*, pp. 242–252. PMLR, 2019a.

Zeyuan Allen-Zhu, Yuanzhi Li, and Zhao Song. On the convergence rate of training recurrent neural networks. *Advances in neural information processing systems*, 32, 2019b.

Josh Alman and Zhao Song. Fast attention requires bounded entries. In *NeurIPS*. arXiv preprint arXiv:2302.13214, 2023.

Josh Alman, Jiehao Liang, Zhao Song, Ruizhe Zhang, and Danyang Zhuo. Bypass exponential time preprocessing: Fast neural network training via weight-data correlation preprocessing. In *NeurIPS*. arXiv preprint arXiv:2211.14227, 2023.

Kurt M Anstreicher. The volumetric barrier for semidefinite programming. *Mathematics of Operations Research*, 2000.

Sanjeev Arora and Anirudh Goyal. A theory for emergence of complex skills in language models. *arXiv preprint arXiv:2307.15936*, 2023.

Sanjeev Arora, Simon Du, Wei Hu, Zhiyuan Li, and Ruosong Wang. Fine-grained analysis of optimization and generalization for overparameterized two-layer neural networks. In *International Conference on Machine Learning*, pp. 322–332. PMLR, 2019a.

Sanjeev Arora, Simon S Du, Wei Hu, Zhiyuan Li, Russ R Salakhutdinov, and Ruosong Wang. On exact computation with an infinitely wide neural net. *Advances in neural information processing systems*, 32, 2019b.

Jan van den Brand, Binghui Peng, Zhao Song, and Omri Weinstein. Training (overparametrized) neural networks in near-linear time. *arXiv preprint arXiv:2006.11648*, 2020.

Jan van den Brand, Zhao Song, and Tianyi Zhou. Algorithm and hardness for dynamic attention maintenance in large language models. *arXiv preprint arXiv:2304.02207*, 2023.

Hannah Brown, Katherine Lee, Fatemehsadat Mireshghallah, Reza Shokri, and Florian Tramèr. What does it mean for a language model to preserve privacy? In *Proceedings of the 2022 ACM Conference on Fairness, Accountability, and Transparency*, pp. 2280–2292, 2022.

Sébastien Bubeck, Varun Chandrasekaran, Ronen Eldan, Johannes Gehrke, Eric Horvitz, Ece Kamar, Peter Lee, Yin Tat Lee, Yuanzhi Li, Scott Lundberg, et al. Sparks of artificial general intelligence: Early experiments with gpt-4. *arXiv preprint arXiv:2303.12712*, 2023.

HanQin Cai, Yuchen Lou, Daniel Mckenzie, and Wotao Yin. A zeroth-order block coordinate descent algorithm for huge-scale black-box optimization. *arXiv preprint arXiv:2102.10707*, 2021.

Tianle Cai, Ruiqi Gao, Jikai Hou, Siyu Chen, Dong Wang, Di He, Zhihua Zhang, and Liwei Wang. Gram-gauss-newton method: Learning overparameterized neural networks for regression problems. *arXiv preprint arXiv:1905.11675*, 2019.

Yuan Cao and Quanquan Gu. Generalization bounds of stochastic gradient descent for wide and deep neural networks. *Advances in neural information processing systems*, 32, 2019.

Marco Cascella, Jonathan Montomoli, Valentina Bellini, and Elena Bignami. Evaluating the feasibility of chatgpt in healthcare: an analysis of multiple clinical and research scenarios. *Journal of Medical Systems*, 47(1):33, 2023.

ChatGPT. Optimizing language models for dialogue. *OpenAI Blog*, November 2022. URL https://openai.com/blog/chatgpt/.

Beidi Chen, Zichang Liu, Binghui Peng, Zhaozhuo Xu, Jonathan Lingjie Li, Tri Dao, Zhao Song, Anshumali Shrivastava, and Christopher Re. Mongoose: A learnable lsh framework for efficient neural network training. In *International Conference on Learning Representations*, 2021.

Heeyoul Choi, Kyunghyun Cho, and Yoshua Bengio. Fine-grained attention mechanism for neural machine translation. *Neurocomputing*, 284:171–176, 2018.

Timothy Chu, Zhao Song, and Chiwun Yang. How to protect copyright data in optimization of large language models? *arXiv preprint arXiv:2308.12247*, 2023a.

Timothy Chu, Zhao Song, and Chiwun Yang. Fine-tune language models to approximate unbiased in-context learning. *arXiv preprint arXiv:2310.03331*, 2023b.

Michael B Cohen, Yin Tat Lee, and Zhao Song. Solving linear programs in the current matrix multiplication time. In *STOC*, 2019.

Yichuan Deng, Zhao Song, and Omri Weinstein. Discrepancy minimization in input sparsity time. *arXiv preprint arXiv:2210.12468*, 2022.

Yichuan Deng, Zhihang Li, Sridhar Mahadevan, and Zhao Song. Zero-th order algorithm for softmax attention optimization. *arXiv preprint arXiv:2307.08352*, 2023a.

Yichuan Deng, Zhihang Li, and Zhao Song. Attention scheme inspired softmax regression. *arXiv preprint arXiv:2304.10411*, 2023b.

Yichuan Deng, Sridhar Mahadevan, and Zhao Song. Randomized and deterministic attention sparsification algorithms for over-parameterized feature dimension. *arxiv preprint: arxiv 2304.03426*, 2023c.

Yichuan Deng, Zhao Song, and Shenghao Xie. Convergence of two-layer regression with nonlinear units. *arXiv preprint arXiv:2308.08358*, 2023d.

Alexey Dosovitskiy and Thomas Brox. Inverting visual representations with convolutional networks. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 4829–4837, 2016.

Simon S Du, Xiyu Zhai, Barnabas Poczos, and Aarti Singh. Gradient descent provably optimizes over-parameterized neural networks. *arXiv preprint arXiv:1810.02054*, 2018.

Orhan Firat, Kyunghyun Cho, and Yoshua Bengio. Multi-way, multilingual neural machine translation with a shared attention mechanism. *arXiv preprint arXiv:1601.01073*, 2016.

Yeqi Gao, Sridhar Mahadevan, and Zhao Song. An over-parameterized exponential regression. *arXiv preprint arXiv:2303.16504*, 2023a.

Yeqi Gao, Zhao Song, and Shenghao Xie. In-context learning for attention scheme: from single softmax regression to multiple softmax regression via a tensor trick. *arXiv preprint arXiv:2307.02419*, 2023b.

Yeqi Gao, Zhao Song, and Shenghao Xie. In-context learning for attention scheme: from single softmax regression to multiple softmax regression via a tensor trick. *arXiv preprint arXiv:2307.02419*, 2023c.

Yeqi Gao, Zhao Song, and Xin Yang. Differentially private attention computation. *arXiv preprint arXiv:2305.04701*, 2023d.

Yeqi Gao, Zhao Song, Xin Yang, and Ruizhe Zhang. Fast quantum algorithm for attention computation. *arXiv preprint arXiv:2307.08045*, 2023e.

Yeqi Gao, Zhao Song, and Junze Yin. Gradientcoin: A peer-to-peer decentralized large language models. *arXiv preprint arXiv:2308.10502*, 2023f.

Ian Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio. Generative adversarial nets. *Advances in neural information processing systems*, 27, 2014.

Yuzhou Gu and Zhao Song. A faster small treewidth sdp solver. *arXiv preprint arXiv:2211.06033*, 2022.

Yuzhou Gu, Zhao Song, and Lichen Zhang. A nearly-linear time algorithm for structured support vector machines. *arXiv preprint arXiv:2307.07735*, 2023.

Xuanli He, Qiongkai Xu, Lingjuan Lyu, Fangzhao Wu, and Chenguang Wang. Protecting intellectual property of language generation apis with lexical watermark. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 36, pp. 10758–10766, 2022a.

Xuanli He, Qiongkai Xu, Yi Zeng, Lingjuan Lyu, Fangzhao Wu, Jiwei Li, and Ruoxi Jia. Cater: Intellectual property protection on text generation apis via conditional watermarks. *Advances in Neural Information Processing Systems*, 35:5431–5445, 2022b.

Briland Hitaj, Giuseppe Ateniese, and Fernando Perez-Cruz. Deep models under the gan: information leakage from collaborative deep learning. In *Proceedings of the 2017 ACM SIGSAC conference on computer and communications security*, pp. 603–618, 2017.

Baihe Huang, Xiaoxiao Li, Zhao Song, and Xin Yang. Fl-ntk: A neural tangent kernel-based framework for federated learning analysis. In *International Conference on Machine Learning*, pp. 4423–4434. PMLR, 2021a.

Baihe Huang, Shunhua Jiang, Zhao Song, Runzhou Tao, and Ruizhe Zhang. Solving sdp faster: A robust ipm framework and efficient implementation. In *2022 IEEE 63rd Annual Symposium on Foundations of Computer Science (FOCS)*, pp. 233–244. IEEE, 2022.

Yangsibo Huang, Zhao Song, Kai Li, and Sanjeev Arora. Instahide: Instance-hiding schemes for private distributed learning. In *International conference on machine learning*, pp. 4507–4518. PMLR, 2020.

Yangsibo Huang, Samyak Gupta, Zhao Song, Kai Li, and Sanjeev Arora. Evaluating gradient inversion attacks and defenses in federated learning. *Advances in Neural Information Processing Systems*, 34:7232–7241, 2021b.

Craig A Jensen, Russell D Reed, Robert Jackson Marks, Mohamed A El-Sharkawi, Jae-Byung Jung, Robert T Miyamoto, Gregory M Anderson, and Christian J Eggen. Inversion of feedforward neural networks: algorithms and applications. *Proceedings of the IEEE*, 87(9):1536–1549, 1999.

Ziwei Ji and Matus Telgarsky. Polylogarithmic width suffices for gradient descent to achieve arbitrarily small test error with shallow relu networks. *arXiv preprint arXiv:1909.12292*, 2019.

Shunhua Jiang, Zhao Song, Omri Weinstein, and Hengjie Zhang. Faster dynamic matrix inverse for faster lps. In *STOC*, 2021.

Praneeth Kacham, Vahab Mirrokni, and Peilin Zhong. Polysketchformer: Fast transformers via sketches for polynomial kernels. *arXiv preprint arXiv:2310.01655*, 2023.

Nikhil Kandpal, Eric Wallace, and Colin Raffel. Deduplicating training data mitigates privacy risks in language models. In *International Conference on Machine Learning*, pp. 10697–10707. PMLR, 2022.

Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.

John Kirchenbauer, Jonas Geiping, Yuxin Wen, Jonathan Katz, Ian Miers, and Tom Goldstein. A watermark for large language models. *arXiv preprint arXiv:2301.10226*, 2023.

Nikita Kitaev, Łukasz Kaiser, and Anselm Levskaya. Reformer: The efficient transformer. *arXiv preprint arXiv:2001.04451*, 2020.

Jason D Lee, Ruoqi Shen, Zhao Song, Mengdi Wang, et al. Generalized leverage score sampling for neural networks. *Advances in Neural Information Processing Systems*, 33:10775–10787, 2020.

Yin Tat Lee, Zhao Song, and Qiuyi Zhang. Solving empirical risk minimization in the current matrix multiplication time. In *Conference on Learning Theory (COLT)*, pp. 2140–2157. PMLR, 2019.

Shuai Li, Zhao Song, Yu Xia, Tong Yu, and Tianyi Zhou. The closeness of in-context learning and weight shifting for softmax regression. *arXiv preprint arXiv:2304.13276*, 2023a.

Yuanzhi Li and Yingyu Liang. Learning overparameterized neural networks via stochastic gradient descent on structured data. *Advances in neural information processing systems*, 31, 2018.

Yuchen Li, Yuanzhi Li, and Andrej Risteski. How do transformers learn topic structure: Towards a mechanistic understanding. *arXiv preprint arXiv:2303.04245*, 2023b.

Zhihang Li, Zhao Song, and Tianyi Zhou. Solving regularized exp, cosh and sinh regression problems. *arXiv preprint, 2303.15725*, 2023c.

Hong Liu, Zhiyuan Li, David Hall, Percy Liang, and Tengyu Ma. Sophia: A scalable stochastic second-order optimizer for language model pre-training. *arXiv preprint arXiv:2305.14342*, 2023.

Bao-Liang Lu, Hajime Kita, and Yoshikazu Nishikawa. Inverting feedforward neural networks using linear and nonlinear programming. *IEEE Transactions on Neural networks*, 10(6):1271–1290, 1999.

Aravindh Mahendran and Andrea Vedaldi. Understanding deep image representations by inverting them. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 5188–5196, 2015.

Sadhika Malladi, Tianyu Gao, Eshaan Nichani, Alex Damian, Jason D Lee, Danqi Chen, and Sanjeev Arora. Fine-tuning language models with just forward passes. *arXiv preprint arXiv:2305.17333*, 2023a.

Sadhika Malladi, Alexander Wettig, Dingli Yu, Danqi Chen, and Sanjeev Arora. A kernel-based view of language model fine-tuning. In *International Conference on Machine Learning*, pp. 23610–23641. PMLR, 2023b.

Louis Martin, Benjamin Muller, Pedro Javier Ortiz Suarez, Yoann Dupont, Laurent Romary, Eric Villemonte de La Clergerie, Djame Seddah, and Benoit Sagot. Camembert: a tasty french language model. *arXiv preprint arXiv:1911.03894*, 2019.

Richard McPherson, Reza Shokri, and Vitaly Shmatikov. Defeating image obfuscation with deep learning. *arXiv preprint arXiv:1609.00408*, 2016.

Luca Melis, Congzheng Song, Emiliano De Cristofaro, and Vitaly Shmatikov. Exploiting unintended feature leakage in collaborative learning. In *2019 IEEE symposium on security and privacy (SP)*, pp. 691–706. IEEE, 2019.

Alexander Munteanu, Simon Omlor, Zhao Song, and David Woodruff. Bounding the width of neural networks via coupled initialization a worst case analysis. In *International Conference on Machine Learning*, pp. 16083–16122. PMLR, 2022.

Usman Naseem, Imran Razzak, Katarzyna Musial, and Muhammad Imran. Transformer based deep intelligent contextual embedding for twitter sentiment analysis. *Future Generation Computer Systems*, 113:58–69, 2020.

OpenAI. Gpt-4 technical report. *arXiv preprint arXiv:2303.08774*, 2023.

Samet Oymak and Mahdi Soltanolkotabi. Toward moderate overparameterization: Global convergence guarantees for training shallow neural networks. *IEEE Journal on Selected Areas in Information Theory*, 1(1):84–105, 2020.

Xudong Pan, Mi Zhang, Shouling Ji, and Min Yang. Privacy risks of general-purpose language models. In *2020 IEEE Symposium on Security and Privacy (SP)*, pp. 1314–1331. IEEE, 2020.

Abhishek Panigrahi, Sadhika Malladi, Mengzhou Xia, and Sanjeev Arora. Trainable transformer in transformer. *arXiv preprint arXiv:2307.01189*, 2023a.

Abhishek Panigrahi, Nikunj Saunshi, Haoyu Zhao, and Sanjeev Arora. Task-specific skill localization in fine-tuned language models. *arXiv preprint arXiv:2302.06600*, 2023b.

Nicolas Papernot, Patrick McDaniel, Somesh Jha, Matt Fredrikson, Z Berkay Celik, and Ananthram Swami. The limitations of deep learning in adversarial settings. In *2016 IEEE European symposium on security and privacy (EuroS&P)*, pp. 372–387. IEEE, 2016.

Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, et al. Pytorch: An imperative style, high-performance deep learning library. *Advances in neural information processing systems*, 32, 2019.

Lianke Qin, Zhao Song, and Yuanyuan Yang. Efficient sgd neural network training via sublinear activated neuron identification. *arXiv preprint arXiv:2307.06565*, 2023.

Alec Radford, Jeffrey Wu, Rewon Child, David Luan, Dario Amodei, Ilya Sutskever, et al. Language models are unsupervised multitask learners. *OpenAI blog*, 1(8):9, 2019.

Rafael Rafailov, Archit Sharma, Eric Mitchell, Stefano Ermon, Christopher D.Manning, and Chelsea Finn. Direct preference optimization: Your language model is secretly a reward model. *arXiv preprint arXiv:2305.18290*, 2023.

Maria Rigaki and Sebastian Garcia. A survey of privacy attacks in machine learning. *ACM Computing Surveys*, 2020.

Clayton Sanford, Daniel Hsu, and Matus Telgarsky. Representational strengths and limitations of transformers. *arXiv preprint arXiv:2306.02896*, 2023.

Hanpu Shen, Cheng-Long Wang, Zihang Xiang, Yiming Ying, and Di Wang. Differentially private non-convex learning for multi-layer neural networks. *arXiv preprint arXiv:2310.08425*, 2023a.

Lingfeng Shen, Aayush Mishra, and Daniel Khashabi. Do pretrained transformers really learn in-context by gradient descent? *arXiv preprint arXiv:2310.08540*, 2023b.

Reza Shokri, Marco Stronati, Congzheng Song, and Vitaly Shmatikov. Membership inference attacks against machine learning models. In *2017 IEEE symposium on security and privacy (SP)*, pp. 3–18. IEEE, 2017.

Ritwik Sinha, Zhao Song, and Tianyi Zhou. A mathematical abstraction for balancing the trade-off between creativity and reality in large language models. *arXiv preprint arXiv:2306.02295*, 2023.

Charlie Snell, Ruiqi Zhong, Dan Klein, and Jacob Steinhardt. Approximating how single head attention learns. *arXiv preprint arXiv:2103.07601*, 2021.

Zhao Song and Xin Yang. Quadratic suffices for over-parametrization via matrix chernoff bound. *arXiv preprint arXiv:1906.03593*, 2019.

Zhao Song, Lichen Zhang, and Ruizhe Zhang. Training multi-layer over-parametrized neural network in subquadratic time. *arXiv preprint arXiv:2112.07628*, 2021.

Zhao Song, Junze Yin, and Lichen Zhang. Solving attention kernel regression problem via pre-conditioner. *arXiv preprint arXiv:2308.14304*, 2023.

Davoud Ataee Tarzanagh, Yingcong Li, Christos Thrampoulidis, and Samet Oymak. gsxs as support vector machines. *arXiv preprint arXiv:2308.16898*, 2023.

Yi Tay, Mostafa Dehghani, Samira Abnar, Yikang Shen, Dara Bahri, Philip Pham, Jinfeng Rao, Liu Yang, Sebastian Ruder, and Donald Metzler. Long range arena: A benchmark for efficient transformers. *arXiv preprint arXiv:2011.04006*, 2020.

Yi Tay, Dara Bahri, Donald Metzler, Da-Cheng Juan, Zhe Zhao, and Che Zheng. Synthesizer: Rethinking self-attention for transformer models. In *International conference on machine learning*, pp. 10183–10192. PMLR, 2021.

Mohd Usama, Belal Ahmad, Enmin Song, M Shamim Hossain, Mubarak Alrashoud, and Ghulam Muhammad. Attention-based sentiment analysis using convolutional and recurrent neural network. *Future Generation Computer Systems*, 113:571–578, 2020.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. *Advances in neural information processing systems*, 30, 2017.

Nikhil Vyas, Sham Kakade, and Boaz Barak. Provable copyright protection for generative models. *arXiv preprint arXiv:2302.10870*, 2023.

Zihan Wang, Jason Lee, and Qi Lei. Reconstructing training data from model gradient, provably. In *International Conference on Artificial Intelligence and Statistics*, pp. 6595–6612. PMLR, 2023.

Wenqi Wei, Ling Liu, Margaret Loper, Ka-Ho Chow, Mehmet Emre Gursoy, Stacey Truex, and Yanzhao Wu. A framework for evaluating gradient leakage attacks in federated learning. *arXiv preprint arXiv:2004.10397*, 2020.

Thomas Wolf, Lysandre Debut, Victor Sanh, Julien Chaumond, Clement Delangue, Anthony Moi, Pierric Cistac, Tim Rault, Rémi Louf, Morgan Funtowicz, et al. Huggingface's transformers: State-of-the-art natural language processing. *arXiv preprint arXiv:1910.03771*, 2019.

Shijie Wu, Ozan Irsoy, Steven Lu, Vadim Dabravolski, Mark Dredze, Sebastian Gehrmann, Prabhanjan Kambadur, David Rosenberg, and Gideon Mann. Bloomberggpt: A large language model for finance. *arXiv preprint arXiv:2303.17564*, 2023.

Mengzhou Xia, Tianyu Gao, Zhiyuan Zeng, and Danqi Chen. Sheared llama: Accelerating language model pre-training via structured pruning. *arXiv preprint arXiv:2310.06694*, 2023.

Zheng Xu, Yanxiang Zhang, Galen Andrew, Christopher A Choquette-Choo, Peter Kairouz, H Brendan McMahan, Jesse Rosenstock, and Yuanbo Zhang. Federated learning of gboard language models with differential privacy. *arXiv preprint arXiv:2305.18465*, 2023.

Hongxu Yin, Arun Mallya, Arash Vahdat, Jose M Alvarez, Jan Kautz, and Pavlo Molchanov. See through gradients: Image batch recovery via gradinversion. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 16337–16346, 2021.

Amir Zandieh, Insu Han, Majid Daliri, and Amin Karbasi. Kdeformer: Accelerating transformers via kernel density estimation. *arXiv preprint arXiv:2302.02451*, 2023.

Guodong Zhang, James Martens, and Roger B Grosse. Fast convergence of natural gradient descent for over-parameterized neural networks. *Advances in Neural Information Processing Systems*, 32, 2019.

Jingzhao Zhang, Sai Praneeth Karimireddy, Andreas Veit, Seungyeon Kim, Sashank Reddi, Sanjiv Kumar, and Suvrit Sra. Why are adaptive methods good for attention models? *Advances in Neural Information Processing Systems*, 33:15383–15393, 2020a.

Jingzhao Zhang, Sai Praneeth Karimireddy, Andreas Veit, Seungyeon Kim, Sashank Reddi, Sanjiv Kumar, and Suvrit Sra. Why are adaptive methods good for attention models? *Advances in Neural Information Processing Systems*, 33:15383–15393, 2020b.

Lichen Zhang. *Speeding up optimizations via data structures: Faster search, sample and maintenance*. PhD thesis, Master's thesis, Carnegie Mellon University, 2022.

Yi Zhang, Orestis Plevrakis, Simon S Du, Xingguo Li, Zhao Song, and Sanjeev Arora. Over-parameterized adversarial training: An analysis overcoming the curse of dimensionality. *Advances in Neural Information Processing Systems*, 33:679–688, 2020c.

Yuheng Zhang, Ruoxi Jia, Hengzhi Pei, Wenxiao Wang, Bo Li, and Dawn Song. The secret revealer: Generative model-inversion attacks against deep neural networks. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pp. 253–261, 2020d.

Bo Zhao, Konda Reddy Mopuri, and Hakan Bilen. idlg: Improved deep leakage from gradients. *arXiv preprint arXiv:2001.02610*, 2020.

Ligeng Zhu, Zhijian Liu, and Song Han. Deep leakage from gradients. *Advances in neural information processing systems*, 32, 2019.

Difan Zou and Quanquan Gu. An improved analysis of training over-parameterized deep neural networks. *Advances in neural information processing systems*, 32, 2019.

Roadmap. We arrange the appendix as follows. In Section A we provide details of computing the gradients. In Section B and Section C we provide detail of computing Hessian for two cases. In Section D we show how to split the Hessian matrix. In Section E we combine the results before and compute the Hessian for the loss function. In Section F we bound the basic functions to be used later. In Section G we provide proof for the Lipschitz property of the Hessian of the loss function. In Section H, we provide the proof for the PSD bound of the Hessian. In Section I, we provide the convergence analysis for our proposed methods. In Section J, we provide additional details for our experiment.

A GRADIENTS

Here in this section, we provide analysis for the gradient computation. In Section A.1 we state some facts to be used. In Section A.2 we provide some definitions. In Sections A.3, A.4, A.5, A.6, A.7, A.8 and A.9 we compute the gradient for the terms defined respectively. Finally in Section A.10 we compute the gradient for $L(X)$.

A.1 FACTS

Fact A.1 (Basic algebra)**.** *We have*

- $\langle u, v\rangle = \langle v, u\rangle = u^\top v = v^\top u$.
- $\langle u \circ v, w\rangle = \langle u \circ v \circ w, \mathbf{1}_n\rangle$
- $u^\top (v \circ w) = u^\top \operatorname{diag}(v) w$

Fact A.2 (Basic calculus rule)**.** *We have*

- $\frac{\mathrm{d}\langle f(x), g(x)\rangle}{\mathrm{d}t} = \langle \frac{\mathrm{d}f(x)}{\mathrm{d}t}, g(x)\rangle + \langle f(x), \frac{\mathrm{d}g(x)}{\mathrm{d}t}\rangle$ *(here t can be any variable)*
- $\frac{\mathrm{d}y^z}{\mathrm{d}x} = z \cdot y^{z-1} \frac{\mathrm{d}y}{\mathrm{d}x}$
- $u \cdot v = v \cdot u$
- $\frac{\mathrm{d}x}{\mathrm{d}x_j} = e_j$ *where e_j is a vector that only j-th entry is 1 and zero everywhere else.*
- *Let $x \in \mathbb{R}^d$, let $y \in \mathbb{R}$ be independent of x, we have* $\frac{\mathrm{d}x}{\mathrm{d}y} = \mathbf{0}_d$.
- *Let $f(x), g(x) \in \mathbb{R}$, we have* $\frac{\mathrm{d}(f(x)g(x))}{\mathrm{d}t} = \frac{\mathrm{d}f(x)}{\mathrm{d}t} g(x) + f(x) \frac{\mathrm{d}g(x)}{\mathrm{d}t}$
- *Let $x \in \mathbb{R}$,* $\frac{\mathrm{d}}{\mathrm{d}x} \exp(x) = \exp(x)$
- *Let $f(x) \in \mathbb{R}^n$, we have* $\frac{\mathrm{d}\exp(f(x))}{\mathrm{d}t} = \exp(f(x)) \circ \frac{\mathrm{d}f(x)}{\mathrm{d}t}$

A.2 DEFINITIONS

Definition A.3 (Simplified notations)**.** *We have following definitions*

- *We use $u(X)_{i_0,i_1}$ to denote the i_1-th entry of $u(X)_{i_0}$.*
- *We use $f(X)_{i_0,i_1}$ to denote the i_1-th entry of $f(X)_{i_0}$.*
- *We define $W_{j_1,*}$ to denote the j_1-th row of W. (In the proof, we treat $W_{j_1,*}$ as a column vector).*
- *We define W_{*,j_1} to denote the j_1-th column of W.*
- *We define w_{j_1,j_0} to denote the scalar equals to the entry in j_1-th row, j_0-th column of W.*
- *We define V_{*,j_1} to denote the j_1-th column of V.*
- *We define v_{j_1,j_0} to denote the scalar equals to the entry in j_1-th row, j_0-th column of V.*

- *We define X_{*,i_0} to denote the i_0-th column of X.*
- *We define x_{i_1,j_1} to denote the scalar equals to the entry in i_1***-th column,** *j_1***-th row** *of X.*

Definition A.4 (Exponential function u)**.** *If the following conditions hold*

- *Let $X \in \mathbb{R}^{d \times n}$*
- *Let $W \in \mathbb{R}^{d \times d}$*

For each $i_0 \in [n]$, we define $u(X)_{i_0} \in \mathbb{R}^n$ as follows

$$u(X)_{i_0} = \exp(X^\top W X_{*,i_0})$$

Definition A.5 (Sum function of softmax α)**.** *If the following conditions hold*

- *Let $X \in \mathbb{R}^{d \times n}$*
- *Let $u(X)_{i_0}$ be defined as Definition A.4*

We define $\alpha(X)_{i_0} \in \mathbb{R}$ for all $i_0 \in [n]$ as follows

$$\alpha(X)_{i_0} = \langle u(X)_{i_0}, \mathbf{1}_n \rangle$$

Definition A.6 (Softmax probability function f)**.** *If the following conditions hold*

- *Let $X \in \mathbb{R}^{d \times n}$*
- *Let $u(X)_{i_0}$ be defined as Definition A.4*
- *Let $\alpha(X)_{i_0}$ be defined as Definition A.5*

We define $f(X)_{i_0} \in \mathbb{R}^n$ for each $i_0 \in [n]$ as follows

$$f(X)_{i_0} := \alpha(X)_{i_0}^{-1} u(X)_{i_0}$$

Definition A.7 (Value function h)**.** *If the following conditions hold*

- *Let $X \in \mathbb{R}^{d \times n}$*
- *Let $V \in \mathbb{R}^{d \times d}$*

We define $h(X)_{j_0} \in \mathbb{R}^n$ for each $j_0 \in [n]$ as follows

$$h(X)_{j_0} := X^\top V_{*,j_0}$$

Definition A.8 (One-unit loss function c)**.** *If the following conditions hold*

- *Let $f(X)_{i_0}$ be defined as Definition A.6*
- *Let $h(X)_{j_0}$ be defined as Definition A.7*

We define $c(X) \in \mathbb{R}^{n \times d}$ as follows

$$c(X)_{i_0,j_0} := \langle f(X)_{i_0}, h(X)_{j_0} \rangle - b_{i_0,j_0}, \forall i_0 \in [n], j_0 \in [d]$$

Definition A.9 (Overall function L)**.** *If the following conditions hold*

- *Let $c(X)_{i_0,j_0}$ be defined as Definition A.8*

We define $L(X) \in \mathbb{R}$ as follows

$$L(X) := \sum_{i_0=1}^{n} \sum_{j_0=1}^{d} (c(X)_{i_0,j_0})^2$$

A.3 Gradient for each column of $X^\top W X_{*,i_0}$

Lemma A.10. *We have*

- **Part 1.** *Let* $i_0 = i_1 \in [n]$, $j_1 \in [d]$

$$\underbrace{\frac{\mathrm{d}X^\top W X_{*,i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} = \underbrace{e_{i_0}}_{n\times 1} \cdot \underbrace{\langle W_{j_1,*}, X_{*,i_0}\rangle}_{\mathrm{scalar}} + \underbrace{X^\top}_{n\times d} \underbrace{W_{*,j_1}}_{d\times 1}$$

- **Part 2** *Let* $i_0 \neq i_1 \in [n]$, $j_1 \in [d]$

$$\underbrace{\frac{\mathrm{d}X^\top W X_{*,i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} = \underbrace{e_{i_1}}_{n\times 1} \cdot \underbrace{\langle W_{j_1,*}, X_{*,i_0}\rangle}_{\mathrm{scalar}}$$

Proof. **Proof of Part 1.**

$$\begin{aligned}
\underbrace{\frac{\mathrm{d}X^\top W X_{*,i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} &= \underbrace{\frac{\mathrm{d}X^\top}{\mathrm{d}X_{i_1,j_1}}}_{n\times d} \underbrace{W}_{d\times d} \underbrace{X_{*,i_0}}_{d\times 1} + \underbrace{X^\top}_{n\times d} \underbrace{W}_{d\times d} \underbrace{\frac{\mathrm{d}X_{*,i_0}}{\mathrm{d}X_{i_1,j_1}}}_{d\times 1} \\
&= \underbrace{e_{i_1}}_{n\times 1} \underbrace{e_{j_1}^\top}_{1\times d} \underbrace{W}_{d\times d} \underbrace{X_{*,i_0}}_{d\times 1} + \underbrace{X^\top}_{n\times d} \underbrace{W}_{d\times d} \underbrace{e_{j_1}}_{d\times 1} \\
&= \underbrace{e_{i_1}}_{n\times 1} \cdot \underbrace{\langle W_{j_1,*}, X_{*,i_0}\rangle}_{\mathrm{scalar}} + \underbrace{X^\top}_{n\times d} \underbrace{W_{*,j_1}}_{d\times 1} \\
&= \underbrace{e_{i_0}}_{n\times 1} \cdot \underbrace{\langle W_{j_1,*}, X_{*,i_0}\rangle}_{\mathrm{scalar}} + \underbrace{X^\top}_{n\times d} \underbrace{W_{*,j_1}}_{d\times 1}
\end{aligned}$$

where the 1st step follows from Fact A.2, the 2nd step follows from simple derivative rule, the 3rd is simple algebra, the 4th step ie because $i_0 = i_1$.

Proof of Part 2

$$\begin{aligned}
\underbrace{\frac{\mathrm{d}X^\top W X_{*,i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} &= \underbrace{\frac{\mathrm{d}X^\top}{\mathrm{d}x_{i_1,j_1}}}_{n\times d} \underbrace{W}_{d\times d} \underbrace{X_{*,i_0}}_{d\times 1} + \underbrace{X^\top}_{n\times d} \underbrace{W}_{d\times d} \underbrace{\frac{\mathrm{d}X_{*,i_0}}{\mathrm{d}x_{i_1,j_1}}}_{d\times 1} \\
&= \underbrace{e_{i_1}}_{n\times 1} \underbrace{e_{j_1}^\top}_{1\times d} \underbrace{W}_{d\times d} \underbrace{X_{*,i_0}}_{d\times 1} + \underbrace{X^\top}_{n\times d} \underbrace{W}_{d\times d} \underbrace{\mathbf{0}_d}_{d\times 1} \\
&= \underbrace{e_{i_1}}_{n\times 1} \cdot \underbrace{\langle W_{j_1,*}, X_{*,i_0}\rangle}_{\mathrm{scalar}}
\end{aligned}$$

where the 1st step follows from Fact A.2, the 2nd step follows from simple derivative rule, the 3rd is simple algebra. □

A.4 Gradient for $u(X)_{i_0}$

Lemma A.11. *Under following conditions*

- *Let* $u(X)_{i_0}$ *be defined as Definition A.4*

We have

- **Part 1.** *For each* $i_0 = i_1 \in [n]$, $j_1 \in [d]$

$$\underbrace{\frac{\mathrm{d}u(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} = u(X)_{i_0} \circ (e_{i_0} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle + X^\top W_{*,j_1})$$

- **Part 2** *For each* $i_0 \neq i_1 \in [n]$, $j_1 \in [d]$
$$\underbrace{\frac{\mathrm{d}u(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} = \underbrace{u(X)_{i_0}}_{n\times 1} \circ (e_{i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle)$$

Proof.

Proof of Part 1

$$\begin{aligned}
\underbrace{\frac{\mathrm{d}u(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} &= \underbrace{\frac{\mathrm{d}\exp(X^\top W X_{*,i_0})}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} \\
&= \exp(\underbrace{X^\top}_{n\times d} \underbrace{W}_{d\times d} \underbrace{X_{*,i_0}}_{d\times 1}) \circ \underbrace{\frac{\mathrm{d}X^\top W X_{*,i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} \\
&= \underbrace{u(X)_{i_0}}_{n\times 1} \circ \underbrace{\frac{\mathrm{d}X^\top W X_{*,i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} \\
&= \underbrace{u(X)_{i_0}}_{n\times 1} \circ (\underbrace{e_{i_0}}_{n\times 1} \cdot \underbrace{\langle W_{j_1,*}, X_{*,i_0} \rangle}_{\mathrm{scalar}} + \underbrace{X^\top}_{n\times d} \underbrace{W_{*,j_1}}_{d\times 1})
\end{aligned}$$

where the 1st step and the 3rd step follow from Definition of $u(X)_{i_0}$ (see Definition A.4), the 2nd step follows from Fact A.2, the 4th step follows by Lemma A.10.

Proof of Part 2

$$\begin{aligned}
\underbrace{\frac{\mathrm{d}u(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} &= \underbrace{\frac{\mathrm{d}\exp(X^\top W X_{*,i_0})}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} \\
&= \exp(\underbrace{X^\top}_{n\times d} \underbrace{W}_{d\times d} \underbrace{X_{*,i_0}}_{d\times 1}) \circ \underbrace{\frac{\mathrm{d}X^\top W X_{*,i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} \\
&= \underbrace{u(X)_{i_0}}_{n\times 1} \circ \underbrace{\frac{\mathrm{d}X^\top W X_{*,i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} \\
&= \underbrace{u(X)_{i_0}}_{n\times 1} \circ (\underbrace{e_{i_1}}_{n\times 1} \cdot \underbrace{\langle W_{j_1,*}, X_{*,i_0} \rangle}_{\mathrm{scalar}})
\end{aligned}$$

where the 1st step and the 3rd step follow from Definition of $u(X)_{i_0}$ (see Definition A.4), the 2nd step follows from Fact A.2, the 4th step follows by Lemma A.10.

□

A.5 Gradient Computation for $\alpha(X)_{i_0}$

Lemma A.12 (A generalization of Lemma 5.6 in Deng et al. (2023b))**.** *If the following conditions hold*

- *Let* $\alpha(X)_{i_0}$ *be defined as Definition A.5*

Then, we have

- **Part 1.** *For each* $i_0 = i_1 \in [n]$, $j_1 \in [d]$
$$\underbrace{\frac{\mathrm{d}\alpha(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{\mathrm{scalar}} = u(X)_{i_0,i_0} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + \langle u(X)_{i_0}, X^\top W_{*,j_1} \rangle$$

- **Part 2.** *For each* $i_0 \neq i_1 \in [n]$, $j_1 \in [d]$

$$\underbrace{\frac{\mathrm{d}\alpha(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} = u(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$

Proof. **Proof of Part 1.**

$$\begin{aligned}
\underbrace{\frac{\mathrm{d}\alpha(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} = & \underbrace{\frac{\mathrm{d}\langle u(X)_{i_0}, \mathbf{1}_n \rangle}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} \\
= & \langle \underbrace{\frac{\mathrm{d}u(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n \times 1}, \underbrace{\mathbf{1}_n}_{n \times 1} \rangle \\
= & \langle \underbrace{u(X)_{i_0}}_{n \times 1} \circ (e_{i_0} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + X^\top W_{*,j_1}), \underbrace{\mathbf{1}_n}_{n \times 1} \rangle \\
= & \langle \underbrace{u(X)_{i_0}}_{n \times 1} \circ e_{i_0}, \mathbf{1}_n \rangle \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + \langle u(X)_{i_0} \circ (X^\top W_{*,j_1}), \underbrace{\mathbf{1}_n}_{n \times 1} \rangle \\
= & \langle \underbrace{u(X)_{i_0}}_{n \times 1}, e_{i_0} \rangle \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + \langle u(X)_{i_0}, X^\top W_{*,j_1} \rangle \\
= & u(X)_{i_0,i_0} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + \langle u(X)_{i_0}, X^\top W_{*,j_1} \rangle
\end{aligned}$$

where the 1st step follows from the definition of $\alpha(X)_{i_0}$ (see Definition A.5), the 2nd step follows from Fact A.2, the 3rd step follows from Lemma A.11, the 4th step is rearrangement, the 5th step is derived by Fact A.1, the last step is by the definition of $U(X)_{i_0,i_0}$.

Proof of Part 2.

$$\begin{aligned}
\underbrace{\frac{\mathrm{d}\alpha(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} = & \underbrace{\frac{\mathrm{d}\langle u(X)_{i_0}, \mathbf{1}_n \rangle}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} \\
= & \langle \underbrace{\frac{\mathrm{d}u(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n \times 1}, \underbrace{\mathbf{1}_n}_{n \times 1} \rangle \\
= & \langle \underbrace{u(X)_{i_0}}_{n \times 1} \circ (e_{i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle), \underbrace{\mathbf{1}_n}_{n \times 1} \rangle \\
= & \langle \underbrace{u(X)_{i_0}}_{n \times 1} \circ e_{i_1}, \underbrace{\mathbf{1}_n}_{n \times 1} \rangle \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle \\
= & \underbrace{u(X)_{i_0,i_1}}_{\text{scalar}} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle
\end{aligned}$$

where the 1st step follows from the definition of $\alpha(X)_{i_0}$ (see Definition A.5), the 2nd step follows from Fact A.2, the 3rd step follows from Lemma A.11, the 4th step is rearrangement, the 5th step is derived by Fact A.1.

□

A.6 GRADIENT COMPUTATION FOR $\alpha(X)_{i_0}^{-1}$

Lemma A.13 (A generalization of Lemma 5.6 in Deng et al. (2023b)). *If the following conditions hold*

- *Let $\alpha(X)_{i_0}$ be defined as Definition A.5*

we have

- **Part 1.** *For* $i_0 = i_1 \in [n]$, $j_1 \in [d]$

$$\underbrace{\frac{\mathrm{d}\alpha(X)_{i_0}^{-1}}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} = -\alpha(X)_{i_0}^{-1} \cdot (f(X)_{i_0,i_0} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle + \langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle\rangle))$$

- **Part 2.** *For* $i_0 \neq i_1 \in [n]$, $j_1 \in [d]$

$$\underbrace{\frac{\mathrm{d}\alpha(X)_{i_0}^{-1}}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} = -\alpha(X)_{i_0}^{-1} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle$$

Proof. **Proof of Part 1.**

$$\begin{aligned}\underbrace{\frac{\mathrm{d}\alpha(X)_{i_0}^{-1}}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} &= \underbrace{-1}_{\text{scalar}} \cdot \underbrace{(\alpha(X)_{i_0})^{-2}}_{\text{scalar}} \cdot \underbrace{\frac{\mathrm{d}(\alpha(X)_{i_0})}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} \\ &= -\underbrace{(\alpha(X)_{i_0})^{-2}}_{\text{scalar}} \cdot (u(X)_{i_0,i_0} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle + \langle u(X)_{i_0}, X^\top W_{*,j_1}\rangle) \\ &= -\alpha(X)_{i_0}^{-1} \cdot (f(X)_{i_0,i_0} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle + \langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle)\end{aligned}$$

where the 1st step follows from Fact A.2, the 2nd step follows by Lemma A.12.

Proof of Part 2.

$$\begin{aligned}\underbrace{\frac{\mathrm{d}\alpha(X)_{i_0}^{-1}}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} &= \underbrace{-1}_{\text{scalar}} \cdot \underbrace{(\alpha(X)_{i_0})^{-2}}_{\text{scalar}} \cdot \underbrace{\frac{\mathrm{d}(\alpha(X)_{i_0})}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} \\ &= -\underbrace{(\alpha(X)_{i_0})^{-2}}_{\text{scalar}} \cdot u(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\ &= -\alpha(X)_{i_0}^{-1} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle\end{aligned}$$

where the 1st step follows from Fact A.2, the 2nd step follows from result from Lemma A.12.

□

A.7 GRADIENT FOR $f(X)_{i_0}$

Lemma A.14. *If the following conditions hold*

- *Let* $f(X)_{i_0}$ *be defined as Definition A.6*

Then, we have

- **Part 1.** *For all* $i_0 = i_1 \in [n]$, $j_1 \in [d]$

$$\begin{aligned}\underbrace{\frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} = &- \underbrace{f(X)_{i_0}}_{n\times 1} \cdot \underbrace{(f(X)_{i_0,i_0} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle + \langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle)}_{\text{scalar}} \\ &+ \underbrace{f(X)_{i_0} \circ (e_{i_0} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle + X^\top W_{*,j_1})}_{n\times 1}\end{aligned}$$

- **Part 2.** *For all* $i_0 \neq i_1 \in [n]$, $j_1 \in [d]$

$$\underbrace{\frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} = -\underbrace{f(X)_{i_0}}_{n\times 1} \cdot \underbrace{f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle}_{\text{scalar}}$$

$$+ \underbrace{f(X)_{i_0} \circ (e_{i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle)}_{n \times 1}$$

Proof. **Proof of Part 1.**

$$\begin{aligned}
\underbrace{\frac{\mathrm{d} f(X)_{i_0}}{\mathrm{d} x_{i_1,j_1}}}_{n \times 1} &= \underbrace{\frac{\mathrm{d} \alpha(X)_{i_0}^{-1} u(X)_{i_0}}{\mathrm{d} x_{i_1,j_1}}}_{n \times 1} \\
&= \underbrace{u(X)_{i_0}}_{n \times 1} \cdot \underbrace{\frac{\mathrm{d}}{\mathrm{d} x_{i_1,j_1}} \alpha(X)_{i_0}^{-1}}_{\text{scalar}} + \underbrace{\alpha(X)_{i_0}^{-1}}_{\text{scalar}} \cdot \underbrace{\frac{\mathrm{d}}{\mathrm{d} x_{i_1,j_1}} u(X)_{i_0}}_{n \times 1} \\
&= - \underbrace{u(X)_{i_0}}_{n \times 1} \cdot \underbrace{(\alpha(X)_{i_0})^{-1} \cdot (f(X)_{i_0,i_0} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + \langle f(X)_{i_0}, X^\top W_{*,j_1} \rangle)}_{\text{scalar}} \\
&\quad + \underbrace{\alpha(X)_{i_0}^{-1}}_{\text{scalar}} \cdot \underbrace{\frac{\mathrm{d}}{\mathrm{d} x_{i_1,j_1}} u(X)_{i_0}}_{n \times 1} \\
&= - \underbrace{u(X)_{i_0}}_{n \times 1} \cdot \underbrace{(\alpha(X)_{i_0})^{-1} \cdot (f(X)_{i_0,i_0} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + \langle f(X)_{i_0}, X^\top W_{*,j_1} \rangle)}_{\text{scalar}} \\
&\quad + \underbrace{\alpha(X)_{i_0}^{-1}}_{\text{scalar}} \cdot \underbrace{(u(X)_{i_0} \circ (e_{i_0} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + X^\top W_{*,j_1}))}_{n \times 1} \\
&= - \underbrace{f(X)_{i_0}}_{n \times 1} \cdot \underbrace{(f(X)_{i_0,i_0} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + \langle f(X)_{i_0}, X^\top W_{*,j_1} \rangle)}_{\text{scalar}} \\
&\quad + \underbrace{f(X)_{i_0} \circ (e_{i_0} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + X^\top W_{*,j_1})}_{n \times 1}
\end{aligned}$$

where the 1st step follows from the definition of $f(X)_{i_0}$ (see Definition A.6), the 2nd step follows from Fact A.2, the 3rd step follows from Lemma A.13, the 4th step follows from result from Lemma A.11, the 5th step from the definition of $f(X)_{i_0}$ (see Definition A.6).

Proof of Part 2.

$$\begin{aligned}
\underbrace{\frac{\mathrm{d} f(X)_{i_0}}{\mathrm{d} x_{i_1,j_1}}}_{n \times 1} &= \underbrace{\frac{\mathrm{d} \alpha(X)_{i_0}^{-1} u(X)_{i_0}}{\mathrm{d} x_{i_1,j_1}}}_{n \times 1} \\
&= \underbrace{u(X)_{i_0}}_{n \times 1} \cdot \underbrace{\frac{\mathrm{d}}{\mathrm{d} x_{i_1,j_1}} \alpha(X)_{i_0}^{-1}}_{\text{scalar}} + \underbrace{\alpha(X)_{i_0}^{-1}}_{\text{scalar}} \cdot \underbrace{\frac{\mathrm{d}}{\mathrm{d} x_{i_1,j_1}} u(X)_{i_0}}_{n \times 1} \\
&= - \underbrace{u(X)_{i_0}}_{n \times 1} \cdot \underbrace{(\alpha(X)_{i_0})^{-2} \cdot u(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle}_{\text{scalar}} \\
&\quad + \underbrace{\alpha(X)_{i_0}^{-1}}_{\text{scalar}} \cdot \underbrace{\frac{\mathrm{d}}{\mathrm{d} x_{i_1,j_1}} u(X)_{i_0}}_{n \times 1} \\
&= - \underbrace{u(X)_{i_0}}_{n \times 1} \cdot \underbrace{(\alpha(X)_{i_0})^{-2} \cdot u(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle}_{\text{scalar}} \\
&\quad + \underbrace{\alpha(X)_{i_0}^{-1}}_{\text{scalar}} \cdot \underbrace{(u(X)_{i_0} \circ (e_{i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle))}_{n \times 1} \\
&= - \underbrace{f(X)_{i_0}}_{n \times 1} \cdot \underbrace{f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle}_{\text{scalar}} \\
&\quad + e_{i_1} \cdot \underbrace{f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle)}_{\text{scalar}}
\end{aligned}$$

where the 1st step follows from the definition of $f(X)_{i_0}$ (see Definition A.6), the 2nd step follows from Fact A.2, the 3rd step follows from Lemma A.13, the 4th step follows from result from Lemma A.11, the 5th step from the definition of $f(X)_{i_0}$ (see Definition A.6). □

A.8 GRADIENT FOR $h(X)_{j_0}$

Lemma A.15. *If the following conditions hold*

- *Let $h(X)_{j_0}$ be defined as Definition A.7*

Then, for all $i_1 \in [n]$, $j_0, j_1 \in [d]$, we have

$$\underbrace{\frac{\mathrm{d}h(X)_{j_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} = e_{i_1} \cdot v_{j_1,j_0}$$

Proof.

$$\begin{aligned}
\underbrace{\frac{\mathrm{d}h(X)_{j_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} &= \underbrace{\frac{\mathrm{d}X^\top V_{*,j_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1} \\
&= \underbrace{\frac{\mathrm{d}X^\top}{\mathrm{d}x_{i_1,j_1}}}_{n\times d} \cdot \underbrace{V_{*,j_0}}_{d\times 1} \\
&= \underbrace{e_{i_1}}_{n\times 1} \cdot \underbrace{e_{j_1}^\top}_{1\times d} \cdot \underbrace{V_{*,j_0}}_{d\times 1} \\
&= \underbrace{e_{i_1}}_{n\times 1} \cdot \underbrace{v_{j_1,j_0}}_{\text{scalar}}
\end{aligned}$$

where the first step is by definition of $h(X)_{j_0}$ (see Definition A.7), the 2nd and the 3rd step are by differentiation rules, the 4th step is by simple algebra. □

A.9 GRADIENT FOR $c(X)_{i_0,j_0}$

Lemma A.16. *If the following conditions hold*

- *Let $c(X)_{i_0}$ be defined as Definition A.8*
- *Let $s(X)_{i_0,j_0} := \langle f(X)_{i_0}, h(X)_{j_0}\rangle$*

Then, we have

- **Part 1.** *For all $i_0 = i_1 \in [n]$, $j_0, j_1 \in [d]$*

$$\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}} = C_1(X) + C_2(X) + C_3(X) + C_4(X) + C_5(X)$$

  where we have definitions:

  - $C_1(X) := -s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle$
  - $C_2(X) := -s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle$
  - $C_3(X) := f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle$
  - $C_4(X) := \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle$
  - $C_5(X) := f(X)_{i_0,i_0} \cdot v_{j_1,j_0}$

- **Part 2.** *For all* $i_0 \neq i_1 \in [n]$, $j_0, j_1 \in [d]$

$$\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}} = C_6(X) + C_7(X) + C_8(X)$$

where we have definitions:

  - $C_6(X) := -s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$
    - *This is corresponding to* $C_1(X)$
  - $C_7(X) := f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$
    - *This is corresponding to* $C_3(X)$
  - $C_8(X) := f(X)_{i_0,i_1} \cdot v_{j_1,j_0}$
    - *This is corresponding to* $C_5(X)$

Proof. **Proof of Part 1**

$$\begin{aligned}
\underbrace{\frac{\mathrm{d}c(X)_{i_0,j_1}}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} &= \underbrace{\frac{\mathrm{d}(\langle f(X)_{i_0}, h(X)_{j_0}\rangle - b_{i_0,j_0})}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} \\
&= \underbrace{\frac{\mathrm{d}\langle f(X)_{i_0}, h(X)_{j_0}\rangle}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} \\
&= \langle \underbrace{\frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1}, \underbrace{h(X)_{j_0}}_{n\times 1}\rangle + \langle \underbrace{f(X)_{i_0}}_{n\times 1}, \underbrace{\frac{\mathrm{d}h(X)_{j_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1}\rangle \\
&= \langle \underbrace{\frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}}_{n\times 1}, \underbrace{h(X)_{j_0}}_{n\times 1}\rangle + \langle \underbrace{f(X)_{i_0}}_{n\times 1}, \underbrace{e_{i_1}}_{n\times 1} \cdot \underbrace{v_{j_1,j_0}}_{\text{scalar}}\rangle \\
&= \langle -\underbrace{f(X)_{i_0}}_{n\times 1} \cdot \underbrace{(f(X)_{i_0,i_0} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle + \langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle)}_{\text{scalar}} \\
&\quad + \underbrace{f(X)_{i_0} \circ (e_{i_0} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle + X^\top W_{*,j_1})}_{n\times 1}, \underbrace{h(X)_{j_0}}_{n\times 1}\rangle + \langle \underbrace{f(X)_{i_0}}_{n\times 1}, \underbrace{e_{i_1}}_{n\times 1} \cdot \underbrace{v_{j_1,j_0}}_{\text{scalar}}\rangle \\
&= -s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&\quad - s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle \\
&\quad + f(X)_{i_0,i_0} h(X)_{j_0,i_0} \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&\quad + \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle \\
&\quad + f(X)_{i_0,i_1} v_{j_1,j_0} \\
&:= C_1(X) + C_2(X) + C_3(X) + C_4(X) + C_5(X)
\end{aligned}$$

where the first step is by definition of $c(X)_{i_0,j_0}$ (see Definition A.8), the 2nd step is because b_{i_0,j_0} is independent of X, the 3rd step is by Fact A.2, the 4th step uses Lemma A.15, the 5th step uses Lemma A.14, the 6th and 8th step are rearrangement of terms, the 7th step holds by the definition of $f(X)_{i_0}$ (see Definition A.6).

Proof of Part 2

$$\begin{aligned}
\underbrace{\frac{\mathrm{d}c(X)_{i_0,j_1}}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} &= \underbrace{\frac{\mathrm{d}(\langle f(X)_{i_0}, h(X)_{j_0}\rangle - b_{i_0,j_0})}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}} \\
&= \underbrace{\frac{\mathrm{d}\langle f(X)_{i_0}, h(X)_{j_0}\rangle}{\mathrm{d}x_{i_1,j_1}}}_{\text{scalar}}
\end{aligned}$$

$$
\begin{aligned}
&= \langle \underbrace{\frac{\mathrm{d} f(X)_{i_0}}{\mathrm{d} x_{i_1,j_1}}}_{n\times 1}, \underbrace{h(X)_{j_0}}_{n\times 1}\rangle + \langle \underbrace{f(X)_{i_0}}_{n\times 1}, \underbrace{\frac{\mathrm{d} h(X)_{j_0}}{\mathrm{d} x_{i_1,j_1}}}_{n\times 1}\rangle \\
&= \langle \underbrace{\frac{\mathrm{d} f(X)_{i_0}}{\mathrm{d} x_{i_1,j_1}}}_{n\times 1}, \underbrace{h(X)_{j_0}}_{n\times 1}\rangle + \langle \underbrace{f(X)_{i_0}}_{n\times 1}, \underbrace{e_{i_1}}_{n\times 1} \cdot \underbrace{v_{j_1,j_0}}_{\text{scalar}}\rangle \\
&= \langle -\underbrace{(\alpha(X)_{i_0})^{-1}}_{\text{scalar}} \cdot \underbrace{f(X)_{i_0}}_{n\times 1} \cdot \underbrace{u(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle}_{\text{scalar}} \\
&\quad + \underbrace{f(X)_{i_0} \circ (e_{i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle)}_{n\times 1}, \underbrace{h(X)_{j_0}}_{n\times 1}\rangle + \langle \underbrace{f(X)_{i_0}}_{n\times 1}, \underbrace{e_{i_1}}_{n\times 1} \cdot \underbrace{v_{j_1,j_0}}_{\text{scalar}}\rangle \\
&= -\underbrace{(\alpha(X)_{i_0})^{-1} \cdot \langle f(X)_{i_0}, h(X)_{j_0}\rangle \cdot u(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle}_{\text{scalar}} \\
&\quad + \underbrace{\langle f(X)_{i_0} \circ e_{i_1}, h(X)_{j_0}\rangle \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle}_{\text{scalar}} \\
&\quad + \langle \underbrace{f(X)_{i_0}}_{n\times 1}, \underbrace{e_{i_1}}_{n\times 1} \cdot \underbrace{v_{j_1,j_0}}_{\text{scalar}}\rangle \\
&= -s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&\quad + f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&\quad + f(X)_{i_0,i_1} \cdot v_{j_1,j_0} \\
&:= C_6(X) + C_7(X) + C_8(X)
\end{aligned}
$$

where the first step is by definition of $c(X)_{i_0,j_0}$ (see Definition A.8), the 2nd step is because b_{i_0,j_0} is independent of X, the 3rd step is by Fact A.2, the 4th step uses Lemma A.15, the 5th step uses Lemma A.14, the 6th and 7th step are rearrangement of terms. □

A.10 Gradient for $L(X)$

Lemma A.17. *If the following holds*

- *Let $L(X)$ be defined as Definition A.9*

For $i_1 \in [n]$, $j_1 \in [d]$, we have

$$\frac{\mathrm{d} L(X)}{\mathrm{d} x_{i_1,j_1}} = \sum_{i_0=1}^{n} \sum_{j_0=1}^{d} c(X)_{i_0,j_0} \cdot \frac{\mathrm{d} c(X)_{i_0,j_0}}{\mathrm{d} x_{i_1,j_1}}$$

Proof. The result directly follows by chain rule. □

B Hessian case 1: $i_0 = i_1$

Here in this section, we provide Hessian analysis for the first case. In Sections B.1, B.2, B.3, B.4, B.5, B.6 and B.8, we calculate the derivative for several important terms. In Section B.9, B.10, B.11, B.12 and B.13 we calculate derivative for C_1, C_2, C_3, C_4 and C_5 respectively. Finally in Section B.14 we calculate derivative of $\frac{c(X)_{i_0,j_0}}{\mathrm{d} x_{i_1,j_1} \mathrm{d}_{i_2,j_2}}$.

Now, we list some simplified notations which will be used in following sections.

Definition B.1. *We have following definitions to simplify the expression.*

- $s(X)_{i,j} := \langle f(X)_i, h(X)_j\rangle$
- $w(X)_{i,j} := \langle W_{j,*}, X_{*,i}\rangle$
- $z(X)_{i,j} := \langle f(X)_i, X^\top W_{*,j}\rangle$

- $z(X)_i := WX \cdot f(X)_i$
- $w(X)_{i,*} := WX_{*,i}$

B.1 Derivative of Scalar Function $w(X)_{i_0,j_1}$

Lemma B.2. *We have*

- **Part 1** *For* $i_0 = i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$
$$\frac{\mathrm{d}w(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} = w_{j_1,j_2}$$
- **Part 2** *For* $i_0 = i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$
$$\frac{\mathrm{d}w(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} = 0$$

Proof. **Proof of Part 1**
$$\begin{aligned}\frac{\mathrm{d}w(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} &= \langle W_{j_1,*}, \frac{\mathrm{d}X_{*,i_0}}{\mathrm{d}x_{i_2,j_2}}\rangle \\ &= \langle W_{j_1,*}, e_{j_2}\rangle \\ &= w_{j_1,j_2}\end{aligned}$$
where the first step and the 2nd step are by Fact A.2, the 3rd step is simple algebra.

Proof of Part 2
$$\begin{aligned}\frac{\mathrm{d}w(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} &= \langle W_{j_1,*}, \frac{\mathrm{d}X_{*,i_0}}{\mathrm{d}x_{i_2,j_2}}\rangle \\ &= \langle W_{j_1,*}, \mathbf{0}_d\rangle \\ &= 0\end{aligned}$$
where the first step is by Fact A.2, the 2nd step is because $i_0 \neq i_2$. □

B.2 Derivative of Vector Function $X^\top W_{*,j_1}$

Lemma B.3. *We have*

- **Part 1** *For* $i_0 = i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$
$$\frac{\mathrm{d}X^\top W_{*,j_1}}{\mathrm{d}x_{i_2,j_2}} = e_{i_0} \cdot w_{j_2,j_1}$$
- **Part 2** *For* $i_0 = i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$
$$\frac{\mathrm{d}X^\top W_{*,j_1}}{\mathrm{d}x_{i_2,j_2}} = e_{i_2} \cdot w_{j_2,j_1}$$

Proof. **Proof of Part 1**
$$\begin{aligned}\frac{\mathrm{d}X^\top W_{*,j_1}}{\mathrm{d}x_{i_2,j_2}} &= \frac{\mathrm{d}X^\top}{\mathrm{d}x_{i_2,j_2}} \cdot W_{*,j_1} \\ &= e_{i_2}e_{j_2}^\top \cdot W_{*,j_1} \\ &= e_{i_2} \cdot w_{j_2,j_1} \\ &= e_{i_0} \cdot w_{j_2,j_1}\end{aligned}$$
where the first step and the 2nd step are by Fact A.2, the 3rd step is simple algebra, the 4th step holds since $i_0 = i_2$.

Proof of Part 2

$$\begin{aligned}\frac{\mathrm{d}X^\top W_{*,j_1}}{\mathrm{d}x_{i_2,j_2}} &= \frac{\mathrm{d}X^\top}{\mathrm{d}x_{i_2,j_2}} \cdot W_{*,j_1} \\ &= e_{i_2} e_{j_2}^\top \cdot W_{*,j_1} \\ &= e_{i_2} \cdot w_{j_2,j_1}\end{aligned}$$

where the first step and the 2nd step are by Fact A.2, the 3rd step is simple algebra. □

B.3 Derivative of Scalar Function $f(X)_{i_0,i_0}$

Lemma B.4. *If the following holds:*

- *Let $f(X)_{i_0}$ be defined as Definition A.6*

We have

- **Part 1** *For $i_0 = i_2 \in [n]$, $j_1, j_2 \in [d]$*

$$\begin{aligned}\frac{\mathrm{d}f(X)_{i_0,i_0}}{\mathrm{d}x_{i_2,j_2}} =& - f(X)_{i_0,i_0} \cdot (f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle f(X)_{i_0}, X^\top W_{*,j_2}\rangle) \\ &+ f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0}\rangle\end{aligned}$$

- **Part 2** *For $i_0 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*

$$\frac{\mathrm{d}f(X)_{i_0,i_0}}{\mathrm{d}x_{i_2,j_2}} = -f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2}$$

Proof. **Proof of Part 1**

$$\begin{aligned}\frac{\mathrm{d}f(X)_{i_0,i_0}}{\mathrm{d}x_{i_2,j_2}} =& (-(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0} \cdot (u(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle u(X)_{i_0}, X^\top W_{*,j_2}\rangle) \\ &+ f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2} + X^\top W_{*,j_2}))_{i_0} \\ =& - (\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0,i_0} \cdot (u(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle u(X)_{i_0}, X^\top W_{*,j_2}\rangle) \\ &+ (f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2}))_{i_0} + (f(X)_{i_0} \circ (X^\top W_{*,j_2}))_{i_0} \\ =& - (\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0,i_0} \cdot (u(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle u(X)_{i_0}, X^\top W_{*,j_2}\rangle) \\ &+ f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + f(X)_{i_0,i_0} \cdot \langle W_{*,j_2}, X_{*,i_0}\rangle \\ =& - f(X)_{i_0,i_0} \cdot (f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle f(X)_{i_0}, X^\top W_{*,j_2}\rangle) \\ &+ f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + f(X)_{i_0,i_0} \cdot \langle W_{*,j_2}, X_{*,i_0}\rangle\end{aligned}$$

where the first step uses Lemma A.14 for $i_0 = i_2$, the following steps are taking the i_0-th entry of $f(X)_{i_0}$, the last step is by the definition of $f(X)_{i_0}$ (see Definition A.6).

Proof of Part 2

$$\begin{aligned}\frac{\mathrm{d}f(X)_{i_0,i_0}}{\mathrm{d}x_{i_2,j_2}} =& (-(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0} \cdot u(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \\ &+ f(X)_{i_0} \circ (e_{i_2} \cdot w(X)_{i_0,j_2}))_{i_0} \\ =& - (\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0,i_0} \cdot u(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \\ &+ (f(X)_{i_0} \circ (e_{i_2} \cdot w(X)_{i_0,j_2}))_{i_0} \\ =& - (\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0,i_0} \cdot u(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \\ =& - f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2}\end{aligned}$$

where the first step uses Lemma A.14 for $i_0 \neq i_2$, the 2nd step is taking the i_0-th entry of $f(X)_{i_0}$, the 3rd step is because $i_0 \neq i_2$, the last step is by the definition of $f(X)_{i_0}$ (see Definition A.6). □

B.4 DERIVATIVE OF SCALAR FUNCTION $h(X)_{j_0,i_0}$

Lemma B.5. *If the following holds:*

- *Let* $h(X)_{j_0}$ *be defined as Definition A.7*

We have

- **Part 1** *For* $i_0 = i_2 \in [n]$, $j_1, j_2 \in [d]$
$$\frac{\mathrm{d}h(X)_{j_0,i_0}}{\mathrm{d}x_{i_2,j_2}} = v_{j_2,j_0}$$
- **Part 2** *For* $i_0 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$
$$\frac{\mathrm{d}h(X)_{j_0,i_0}}{\mathrm{d}x_{i_2,j_2}} = 0$$

Proof. **Proof of Part 1**
$$\begin{aligned}\frac{\mathrm{d}h(X)_{j_0,i_0}}{\mathrm{d}x_{i_2,j_2}} &= (e_{i_2} \cdot v_{j_2,j_0})_{i_0}\\ &= v_{j_2,j_0}\end{aligned}$$
where the first step is by Lemma A.15, the 2nd step is because $i_0 = i_2$.

Proof of Part 2
$$\begin{aligned}\frac{\mathrm{d}h(X)_{j_0,i_0}}{\mathrm{d}x_{i_2,j_2}} &= (e_{i_2} \cdot v_{j_2,j_0})_{i_0}\\ &= 0\end{aligned}$$
where the first step is by Lemma A.15, the 2nd step is because $i_0 \neq i_2$. ☐

B.5 DERIVATIVE OF SCALAR FUNCTION $z(X)_{i_0,j_1}$

Lemma B.6. *If the following holds:*

- *Let* $f(X)_{i_0}$ *be defined as Definition A.6*
- *Let* $z(X)_{i_0,j_1} := \langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle$
- *Let* $w(X)_{i_0,j_1} = \langle W_{j_1,*}, X_{*,i_0}\rangle$

We have

- **Part 1** *For* $i_0 = i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$
$$\begin{aligned}&\frac{\mathrm{d}z(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}}\\ =&-z(X)_{i_0,j_1} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2}\\ &-z(X)_{i_0,j_1} \cdot z(X)_{i_0,j_2}\\ &+f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0}\rangle \cdot w(X)_{i_0,j_2}\\ &+\langle f(X)_{i_0} \circ X^\top W_{*,j_2}, X^\top W_{*,j_1}\rangle\\ &+f(X)_{i_0,i_0} \cdot w_{j_2,j_1}\end{aligned}$$
- **Part 2** *For* $i_0 = i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$
$$\begin{aligned}&\frac{\mathrm{d}\langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle}{\mathrm{d}x_{i_2,j_2}}\\ =&-z(X)_{i_0,j_1} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2}\\ &+f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \cdot \langle W_{*,j_1}, X_{*,i_0}\rangle\\ &+f(X)_{i_0,i_0} \cdot w_{j_2,j_1}\end{aligned}$$

Proof. **Proof of Part 1**

$$
\begin{aligned}
& \frac{\mathrm{d}\langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle}{\mathrm{d}x_{i_2,j_2}} \\
= & \langle \frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_2,j_2}}, X^\top W_{*,j_1}\rangle + \langle f(X)_{i_0}, \frac{\mathrm{d}X^\top W_{*,j_1}}{\mathrm{d}x_{i_2,j_2}}\rangle \\
= & \langle \frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_2,j_2}}, X^\top W_{*,j_1}\rangle + \langle f(X)_{i_0}, e_{i_0} \cdot w_{j_2,j_1}\rangle \\
= & \langle \frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_2,j_2}}, X^\top W_{*,j_1}\rangle + f(X)_{i_0,i_0} \cdot w_{j_2,j_1} \\
= & \langle -(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0} \cdot (u(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle u(X)_{i_0}, X^\top W_{*,j_2}\rangle) \\
& + f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2} + X^\top W_{*,j_2}), X^\top W_{*,j_1}\rangle + f(X)_{i_0,i_0} \cdot w_{j_2,j_1} \\
= & \langle -f(X)_{i_0} \cdot (f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle f(X)_{i_0}, X^\top W_{*,j_2}\rangle) \\
& + f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2} + X^\top W_{*,j_2}), X^\top W_{*,j_1}\rangle + f(X)_{i_0,i_0} \cdot w_{j_2,j_1} \\
= & - z(X)_{i_0,j_1} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \\
& - z(X)_{i_0,j_1} \cdot z(X)_{i_0,j_2} \\
& + f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0}\rangle \cdot w(X)_{i_0,j_2} \\
& + \langle f(X)_{i_0} \circ X^\top W_{*,j_2}, X^\top W_{*,j_1}\rangle \\
& + f(X)_{i_0,i_0} \cdot w_{j_2,j_1}
\end{aligned}
$$

where the 1st step is by Fact A.2, the 2nd step uses Lemma B.3, the 3rd step is taking the i_0-th entry of $f(X)_{i_0}$, the 4th step uses Lemma A.14, the 5th step is by the definition of $f(X)_{i_0}$ (see Definition A.6).

Proof of Part 2

$$
\begin{aligned}
& \frac{\mathrm{d}\langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle}{\mathrm{d}x_{i_2,j_2}} \\
= & \langle \frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_2,j_2}}, X^\top W_{*,j_1}\rangle + \langle f(X)_{i_0}, \frac{\mathrm{d}X^\top W_{*,j_1}}{\mathrm{d}x_{i_2,j_2}}\rangle \\
= & \langle \frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_2,j_2}}, X^\top W_{*,j_1}\rangle + \langle f(X)_{i_0}, e_{i_2} \cdot w_{j_2,j_1}\rangle \\
= & \langle \frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_2,j_2}}, X^\top W_{*,j_1}\rangle + f(X)_{i_0,i_2} \cdot w_{j_2,j_1} \\
= & \langle -(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0} \cdot u(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \\
& + f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2}), X^\top W_{*,j_1}\rangle + f(X)_{i_0,i_0} \cdot w_{j_2,j_1} \\
= & \langle -f(X)_{i_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \\
& + f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2}), X^\top W_{*,j_1}\rangle + f(X)_{i_0,i_0} \cdot w_{j_2,j_1} \\
= & - z(X)_{i_0,j_1} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \\
& + f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \cdot \langle W_{*,j_1}, X_{*,i_0}\rangle \\
& + f(X)_{i_0,i_0} \cdot w_{j_2,j_1}
\end{aligned}
$$

where the 1st step is by Fact A.2, the 2nd step uses Lemma B.3, the 3rd step is taking the i_0-th entry of $f(X)_{i_0}$, the 4th step uses Lemma A.14, the last step is by the definition of $f(X)_{i_0}$ (see Definition A.6). □

B.6 DERIVATIVE OF SCALAR FUNCTION $f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0}$

Lemma B.7. *If the following holds:*

- *Let $f(X)_{i_0}$ be defined as Definition A.6*

- *Let $h(X)_{j_0}$ be defined as Definition A.7*

We have

- **Part 1** *For $i_0 = i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$*
$$\frac{\mathrm{d} f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0}}{\mathrm{d} x_{i_2,j_2}}$$
$$= (-f(X)_{i_0,i_0} \cdot (f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle f(X)_{i_0}, X^\top W_{*,j_2} \rangle) + f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0} \rangle) \cdot h(X)_{j_0,i_0} + f(X)_{i_0,i_0} \cdot v_{j_2,j_0}$$

- **Part 2** *For $i_0 = i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*
$$\frac{\mathrm{d} f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0}}{\mathrm{d} x_{i_2,j_2}} = -f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot h(X)_{j_0,i_0}$$

Proof. **Proof of Part 1**
$$\frac{\mathrm{d} f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0}}{\mathrm{d} x_{i_2,j_2}}$$
$$= \frac{\mathrm{d} f(X)_{i_0,i_0}}{\mathrm{d} x_{i_2,j_2}} \cdot h(X)_{j_0,i_0} + f(X)_{i_0,i_0} \cdot \frac{\mathrm{d} h(X)_{j_0,i_0}}{\mathrm{d} x_{i_2,j_2}}$$
$$= \frac{\mathrm{d} f(X)_{i_0,i_0}}{\mathrm{d} x_{i_2,j_2}} \cdot h(X)_{j_0,i_0} + f(X)_{i_0,i_0} \cdot v_{j_2,j_0}$$
$$= (-(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0,i_0} \cdot (u(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle u(X)_{i_0}, X^\top W_{*,j_2} \rangle) + f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0} \rangle) \cdot h(X)_{j_0,i_0} + f(X)_{i_0,i_0} \cdot v_{j_2,j_0}$$
$$= (-f(X)_{i_0,i_0} \cdot (f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle f(X)_{i_0}, X^\top W_{*,j_2} \rangle) + f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0} \rangle) \cdot h(X)_{j_0,i_0} + f(X)_{i_0,i_0} \cdot v_{j_2,j_0}$$
where the fist step is by Fact A.2, the 2nd step calls Lemma B.5, the 3rd step uses Lemma B.4, the last step is by the definition of $f(X)_{i_0}$ (see Definition A.6).

Proof of Part 2
$$\frac{\mathrm{d} f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0}}{\mathrm{d} x_{i_2,j_2}}$$
$$= \frac{\mathrm{d} f(X)_{i_0,i_0}}{\mathrm{d} x_{i_2,j_2}} \cdot h(X)_{j_0,i_0} + f(X)_{i_0,i_0} \cdot \frac{\mathrm{d} h(X)_{j_0,i_0}}{\mathrm{d} x_{i_2,j_2}}$$
$$= -(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0,i_0} \cdot u(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot h(X)_{j_0,i_0}$$
$$= -f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot h(X)_{j_0,i_0}$$
where the fist step is by Fact A.2, the 2nd step calls Lemma B.5, the 3rd step uses Lemma B.4, the last step is by the definition of $f(X)_{i_0}$ (see Definition A.6). ☐

B.7 Derivative of Scalar Function $f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1}$

Lemma B.8. *If the following holds:*

- *Let $f(X)_{i_0}$ be defined as Definition A.6*

We have

- **Part 1** *For $i_0 = i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$*
$$\frac{\mathrm{d} f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1}}{\mathrm{d} x_{i_2,j_2}}$$
$$= (f(X)_{i_0,i_0} \cdot (f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle f(X)_{i_0}, X^\top W_{*,j_2} \rangle) + f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0} \rangle) \cdot w(X)_{i_0,j_1} + f(X)_{i_0,i_0} \cdot w_{j_1,j_2}$$

- **Part 2** *For* $i_0 = i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$
$$\frac{\mathrm{d} f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1}}{\mathrm{d} x_{i_2,j_2}} = -f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1}$$

Proof. **Proof of Part 1**

$$\begin{aligned}
& \frac{\mathrm{d} f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1}}{\mathrm{d} x_{i_2,j_2}} \\
= & \frac{\mathrm{d} f(X)_{i_0,i_0}}{\mathrm{d} x_{i_2,j_2}} \cdot w(X)_{i_0,j_1} + f(X)_{i_0,i_0} \cdot \frac{\mathrm{d} w(X)_{i_0,j_1}}{\mathrm{d} x_{i_2,j_2}} \\
= & \frac{\mathrm{d} f(X)_{i_0,i_0}}{\mathrm{d} x_{i_2,j_2}} \cdot w(X)_{i_0,j_1} + f(X)_{i_0,i_0} \cdot w_{j_1,j_2} \\
= & (-(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0,i_0} \cdot (u(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle u(X)_{i_0}, X^\top W_{*,j_2} \rangle) \\
& + f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0} \rangle) \cdot w(X)_{i_0,j_1} + f(X)_{i_0,i_0} \cdot w_{j_1,j_2} \\
= & (-f(X)_{i_0,i_0} \cdot (f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle f(X)_{i_0}, X^\top W_{*,j_2} \rangle) \\
& + f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0} \rangle) \cdot w(X)_{i_0,j_1} + f(X)_{i_0,i_0} \cdot w_{j_1,j_2}
\end{aligned}$$

where step 1 is by Fact A.2, the 2nd step calls Lemma B.2, the 3rd step uses Lemma B.4, the last step is by the definition of $f(X)_{i_0}$ (see Definition A.6).

Proof of Part 2

$$\begin{aligned}
& \frac{\mathrm{d} f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1}}{\mathrm{d} x_{i_2,j_2}} \\
= & \frac{\mathrm{d} f(X)_{i_0,i_0}}{\mathrm{d} x_{i_2,j_2}} \cdot w(X)_{i_0,j_1} + f(X)_{i_0,i_0} \cdot \frac{\mathrm{d} w(X)_{i_0,j_1}}{\mathrm{d} x_{i_2,j_2}} \\
= & \frac{\mathrm{d} f(X)_{i_0,i_0}}{\mathrm{d} x_{i_2,j_2}} \cdot w(X)_{i_0,j_1} \\
= & -(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0,i_0} \cdot u(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
= & -f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1}
\end{aligned}$$

where step 1 is by Fact A.2, the 2nd step calls Lemma B.2, the 3rd step uses Lemma B.4, the last step is by the definition of $f(X)_{i_0}$ (see Definition A.6). ☐

B.8 DERIVATIVE OF VECTOR FUNCTION $f(X)_{i_0} \circ (X^\top W_{*,j_1})$

Lemma B.9. *If the following holds:*

- *Let* $f(X)_{i_0}$ *be defined as Definition A.6*

We have

- **Part 1** *For* $i_0 = i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$
$$\begin{aligned}
& \frac{\mathrm{d} f(X)_{i_0} \circ (X^\top W_{*,j_1})}{\mathrm{d} x_{i_2,j_2}} \\
= & (-f(X)_{i_0} \cdot (f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle f(X)_{i_0}, X^\top W_{*,j_2} \rangle) \\
& + f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2} + X^\top W_{*,j_2})) \circ (X^\top W_{*,j_1}) + f(X)_{i_0} \circ (e_{i_0} \cdot w_{j_2,j_1})
\end{aligned}$$

- **Part 2** *For* $i_0 = i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$
$$\begin{aligned}
& \frac{\mathrm{d} f(X)_{i_0} \circ (X^\top W_{*,j_1})}{\mathrm{d} x_{i_2,j_2}} \\
= & (-f(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \\
& + f(X)_{i_0} \circ (e_{i_2} \cdot w(X)_{i_0,j_2})) \circ (X^\top W_{*,j_1}) + f(X)_{i_0} \circ (e_{i_2} \cdot w_{j_2,j_1})
\end{aligned}$$

Table 2: C_1 Part 1 Summary

ID	Term	Symmetric?	Table Name
1	$+2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0}^2 \cdot w(X)_{i_0,j_1} \cdot w(X)_{i_0,j_2}$	Yes	N/A
2	$-f(X)_{i_0,i_0}^2 \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1}$	Yes	N/A
3	$-f(X)_{i_0,i_0} \cdot \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), h(X)_{j_0} \rangle \cdot w(X)_{i_0,j_1}$	No	Table 5: 1
4	$-f(X)_{i_0,i_0}^2 \cdot v_{j_2,j_0} \cdot w(X)_{i_0,j_1}$	No	Table 6: 1
5	$-s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1}$	Yes	N/A
6	$-s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot \langle W_{*,j_2}, X_{*,i_0} \rangle \cdot w(X)_{i_0,j_1}$	No	Table 3: 7
7	$-s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w_{j_1,j_2}$	No	Table 3: 9
8	$2f(X)_{i_0,i_0} \cdot s(X)_{i_0,j_0} \cdot z(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1}$	No	Table 3: 1

Proof. **Proof of Part 1**

$$\begin{aligned}
&\frac{\mathrm{d}f(X)_{i_0} \circ (X^\top W_{*,j_1})}{\mathrm{d}x_{i_2,j_2}} \\
=& \frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_2,j_2}} \circ (X^\top W_{*,j_1}) + f(X)_{i_0} \circ \frac{\mathrm{d}X^\top W_{*,j_1}}{\mathrm{d}x_{i_2,j_2}} \\
=& \frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_2,j_2}} \circ (X^\top W_{*,j_1}) + f(X)_{i_0} \circ (e_{i_0} \cdot w_{j_2,j_1}) \\
=& (-(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0} \cdot (u(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle u(X)_{i_0}, X^\top W_{*,j_2} \rangle) \\
&+ f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2} + X^\top W_{*,j_2})) \circ (X^\top W_{*,j_1}) + f(X)_{i_0} \circ (e_{i_0} \cdot w_{j_2,j_1}) \\
=& (-f(X)_{i_0} \cdot (f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle f(X)_{i_0}, X^\top W_{*,j_2} \rangle) \\
&+ f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2} + X^\top W_{*,j_2})) \circ (X^\top W_{*,j_1}) + f(X)_{i_0} \circ (e_{i_0} \cdot w_{j_2,j_1})
\end{aligned}$$

where the 1st step is by Fact A.2, the 2nd step uses Lemma B.3, the 3rd step uses Lemma A.14, the last step is by the definition of $f(X)_{i_0}$ (see Definition A.6).

Proof of Part 2

$$\begin{aligned}
&\frac{\mathrm{d}f(X)_{i_0} \circ (X^\top W_{*,j_1})}{\mathrm{d}x_{i_2,j_2}} \\
=& \frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_2,j_2}} \circ (X^\top W_{*,j_1}) + f(X)_{i_0} \circ \frac{\mathrm{d}X^\top W_{*,j_1}}{\mathrm{d}x_{i_2,j_2}} \\
=& \frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_2,j_2}} \circ (X^\top W_{*,j_1}) + f(X)_{i_0} \circ (e_{i_2} \cdot w_{j_2,j_1}) \\
=& -((\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0} \cdot u(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \\
&+ f(X)_{i_0} \circ (e_{i_2} \cdot w(X)_{i_0,j_2})) \circ (X^\top W_{*,j_1}) + f(X)_{i_0} \circ (e_{i_2} \cdot w_{j_2,j_1}) \\
=& (-f(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \\
&+ f(X)_{i_0} \circ (e_{i_2} \cdot w(X)_{i_0,j_2})) \circ (X^\top W_{*,j_1}) + f(X)_{i_0} \circ (e_{i_2} \cdot w_{j_2,j_1})
\end{aligned}$$

where the 1st step is by Fact A.2, the 2nd step uses Lemma B.3, the 3rd step uses Lemma A.14, the last step is by the definition of $f(X)_{i_0}$ (see Definition A.6). □

B.9 Derivative of $C_1(X)$

Lemma B.10. *If the following holds:*

- *Let $C_1(X) \in \mathbb{R}$ be defined as in Lemma A.16*
- *Let $z(X)_{i_0,j_1} = \langle f(X)_{i_0}, X^\top W_{*,j_1} \rangle$*
- *Let $w(X)_{i_0,j_1} = \langle W_{j_1,*}, X_{*,i_0} \rangle$*

We have

- **Part 1** *For* $i_0 = i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$

$$\begin{aligned}
&\frac{\mathrm{d}C_1(X)}{\mathrm{d}x_{i_2,j_2}} \\
= & + 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0}^2 \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
& + 2f(X)_{i_0,i_0} \cdot s(X)_{i_0,j_0} \cdot z(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
& - f(X)_{i_0,i_0}^2 \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
& - f(X)_{i_0,i_0} \cdot \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), h(X)_{j_0} \rangle \cdot w(X)_{i_0,j_1} \\
& - f(X)_{i_0,i_0}^2 \cdot v_{j_2,j_0} \cdot w(X)_{i_0,j_1} \\
& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot \langle W_{*,j_2}, X_{*,i_0} \rangle \cdot w(X)_{i_0,j_1} \\
& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w_{j_1,j_2}
\end{aligned}$$

- **Part 2** *For* $i_0 = i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$

$$\begin{aligned}
&\frac{\mathrm{d}C_1(X)}{\mathrm{d}x_{i_2,j_2}} \\
&= s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
&\quad - f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w(X)_{i_0,j_2} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
&\quad - f(X)_{i_0,i_2} \cdot v_{j_2,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
&\quad + s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1}
\end{aligned}$$

Proof. **Proof of Part 1**

$$\begin{aligned}
&\frac{\mathrm{d}C_1(X)}{\mathrm{d}x_{i_2,j_2}} \\
= & \frac{\mathrm{d} - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} \\
= & - \frac{\mathrm{d}s(X)_{i_0,j_0}}{\mathrm{d}x_{i_2,j_2}} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
& - s(X)_{i_0,j_0} \cdot \frac{\mathrm{d}f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} \\
= & - \frac{\mathrm{d}s(X)_{i_0,j_0}}{\mathrm{d}x_{i_2,j_2}} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
& - s(X)_{i_0,j_0} \cdot ((-(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0,i_0} \cdot (u(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle u(X)_{i_0}, X^\top W_{*,j_2} \rangle) \\
& + f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0} \rangle) \cdot w(X)_{i_0,j_1} + f(X)_{i_0,i_0} \cdot w_{j_1,j_2}) \\
= & - (-s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} - s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0}, X^\top W_{*,j_2} \rangle \\
& + f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \\
& + \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), h(X)_{j_0} \rangle + f(X)_{i_0,i_2} \cdot v_{j_2,j_0}) \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
& - s(X)_{i_0,j_0} \cdot ((-f(X)_{i_0,i_0} \cdot (f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle f(X)_{i_0}, X^\top W_{*,j_2} \rangle) \\
& + f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0} \rangle) \cdot w(X)_{i_0,j_1} + f(X)_{i_0,i_0} \cdot w_{j_1,j_2}) \\
= & \, 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0}^2 \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
& + 2s(X)_{i_0,j_0} \cdot Z(X)_{i_0,j_2} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
& - f(X)_{i_0,i_0}^2 \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
& - f(X)_{i_0,i_0} \cdot \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), h(X)_{j_0} \rangle \cdot w(X)_{i_0,j_1}
\end{aligned}$$

Table 3: C_2 Part 1 Summary

ID	Term	Symmetric Terms	Table Name
1	$2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1}$	No	Table 2: 9
2	$s(X)_{i_0,j_0} \cdot z(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1}$	Yes	N/A
3	$-f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1}$	No	Table 4: 3
4	$-\langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), h(X)_{j_0} \rangle \cdot z(X)_{i_0,j_1}$	No	Table 5: 2
5	$-f(X)_{i_0,i_0} \cdot v_{j_2,j_0} \cdot z(X)_{i_0,j_1}$	No	Table 6: 2
6	$+s(X)_{i_0,j_0} \cdot z(X)_{i_0,j_1} \cdot f(X)_{i_0,i_0} \cdot z(X)_{i_0,j_2}$	Yes	N/A
7	$-s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0} \rangle \cdot w(X)_{i_0,j_2}$	No	Table 2: 6
8	$-s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), X^\top W_{*,j_1} \rangle$	Yes	N/A
9	$-s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w_{j_2,j_1}$	No	Table 2: 7

$$
\begin{aligned}
&- f(X)_{i_0,i_0}^2 \cdot v_{j_2,j_0} \cdot w(X)_{i_0,j_1} \\
&- s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0} \rangle \cdot w(X)_{i_0,j_1} \\
&- s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w_{j_1,j_2}
\end{aligned}
$$

where the first step is by definition of $C_1(X)$ (see Lemma A.16), the 2nd step is by Fact A.2, the 3rd step is by Lemma B.8, the 4th step is because Lemma A.16, the 5th step is a rearrangement.

Proof of Part 2

$$
\begin{aligned}
&\frac{\mathrm{d}C_1(X)}{\mathrm{d}x_{i_2,j_2}} \\
= &\frac{\mathrm{d} - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} \\
= &- \frac{\mathrm{d}s(X)_{i_0,j_0}}{\mathrm{d}x_{i_2,j_2}} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
&- s(X)_{i_0,j_0} \cdot \frac{\mathrm{d}f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} \\
= &- \frac{\mathrm{d}s(X)_{i_0,j_0}}{\mathrm{d}x_{i_2,j_2}} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
&+ s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
= &- (-s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} + f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w(X)_{i_0,j_2} \\
&+ f(X)_{i_0,i_2} \cdot v_{j_2,j_0}) \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
&+ s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
= &s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
&- f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w(X)_{i_0,j_2} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
&- f(X)_{i_0,i_2} \cdot v_{j_2,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
&+ s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1}
\end{aligned}
$$

where the first step is by definition of $C_1(X)$ (see Lemma A.16), the 2nd step is by Fact A.2, the 3rd step is by Lemma B.8, the 4th step is because Lemma A.16, the 5th step is a rearrangement. □

B.10 Derivative of $C_2(X)$

Lemma B.11. *If the following holds:*

- *Let $C_2(X)$ be defined as in Lemma A.16*
- *We define $z(X)_{i_0,j_1} := \langle f(X)_{i_0}, X^\top W_{*,j_1} \rangle$.*

We have

- **Part 1** *For* $i_0 = i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$

$$\begin{aligned}
&\frac{\mathrm{d}C_2(X)}{\mathrm{d}x_{i_2,j_2}} \\
= & + 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
& + s(X)_{i_0,j_0} \cdot z(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
& - f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
& - \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), h(X)_{j_0} \rangle \cdot z(X)_{i_0,j_1} \\
& - f(X)_{i_0,i_0} \cdot v_{j_2,j_0} \cdot z(X)_{i_0,j_1} \\
& + s(X)_{i_0,j_0} \cdot z(X)_{i_0,j_1} \cdot f(X)_{i_0,i_0} \cdot z(X)_{i_0,j_2} \\
& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0} \rangle \cdot w(X)_{i_0,j_2} \\
& - s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), X^\top W_{*,j_1} \rangle \\
& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w_{j_2,j_1}
\end{aligned}$$

- **Part 2** *For* $i_0 = i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$

$$\begin{aligned}
&\frac{\mathrm{d}C_2(X)}{\mathrm{d}x_{i_2,j_2}} \\
= & + s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
& - f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
& - f(X)_{i_0,i_2} \cdot v_{j_2,j_0} \cdot z(X)_{i_0,j_1} \\
& + s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0}, X^\top W_{*,j_1} \rangle \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \\
& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0} \rangle \cdot w(X)_{i_0,j_2} \\
& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w_{j_2,j_1}
\end{aligned}$$

Proof. **Proof of Part 1**

$$\begin{aligned}
&\frac{\mathrm{d} - C_2(X)}{\mathrm{d}x_{i_2,j_2}} \\
= & \frac{\mathrm{d}s(X)_{i_0,j_0} \cdot z(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} \\
= & \frac{\mathrm{d}s(X)_{i_0,j_0}}{\mathrm{d}x_{i_2,j_2}} \cdot z(X)_{i_0,j_1} + s(X)_{i_0,j_0} \cdot \frac{\mathrm{d}z(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} \\
= & \frac{\mathrm{d}s(X)_{i_0,j_0}}{\mathrm{d}x_{i_2,j_2}} \cdot z(X)_{i_0,j_1} \\
& + s(X)_{i_0,j_0} \cdot (\langle -(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0} \cdot (u(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle u(X)_{i_0}, X^\top W_{*,j_2} \rangle) \\
& + f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2} + X^\top W_{*,j_2}), X^\top W_{*,j_1} \rangle + f(X)_{i_0,i_0} \cdot w_{j_2,j_1}) \\
= & (-s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} - s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0}, X^\top W_{*,j_2} \rangle \\
& + f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \\
& + \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), h(X)_{j_0} \rangle + f(X)_{i_0,i_2} \cdot v_{j_2,j_0}) \cdot z(X)_{i_0,j_1} \\
& + s(X)_{i_0,j_0} \cdot (\langle -(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0} \cdot (u(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle u(X)_{i_0}, X^\top W_{*,j_2} \rangle) \\
& + f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2} + X^\top W_{*,j_2}), X^\top W_{*,j_1} \rangle + f(X)_{i_0,i_0} \cdot w_{j_2,j_1}) \\
= & - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
& - s(X)_{i_0,j_0} \cdot z(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
& + f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
& + \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), h(X)_{j_0} \rangle \cdot z(X)_{i_0,j_1} \\
& + f(X)_{i_0,i_2} \cdot v_{j_2,j_0} \cdot z(X)_{i_0,j_1} \\
& - s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0}, X^\top W_{*,j_1} \rangle \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2}
\end{aligned}$$

Table 4: C_3 Part 1 Summary

ID	Term	Symmetric Terms	Table Name
1	$-f(X)_{i_0,i_0}^2 \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1}$	Yes	N/A
2	$f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1}$	Yes	N/A
3	$-f(X)_{i_0,i_0} \cdot z(X)_{i_0,j_2} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1}$	No	Table 3: 3
4	$f(X)_{i_0,i_0} \cdot \langle W_{*,j_2}, X_{*,i_0}\rangle \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1}$	No	Table 5: 3
5	$f(X)_{i_0,i_0} \cdot v_{j_2,j_0} \cdot w(X)_{i_0,j_1}$	No	Table 6: 3
6	$f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0} \cdot w_{j_1,j_2}$	No	Table 5: 5

$$
\begin{aligned}
& - s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle \cdot f(X)_{i_0,i_0} \cdot \langle f(X)_{i_0}, X^\top W_{*,j_2}\rangle \\
& + s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0}\rangle \cdot w(X)_{i_0,j_2} \\
& + s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), X^\top W_{*,j_1}\rangle \\
& + s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w_{j_2,j_1}
\end{aligned}
$$

where the first step is by definition of $C_2(X)$ (see Lemma A.16), the 2nd step is by Fact A.2, the 3rd step is by Lemma B.6, the 4th step is because Lemma A.16, the 5th step is a rearrangement.

Proof of Part 2

$$
\begin{aligned}
& \frac{\mathrm{d} - C_2(X)}{\mathrm{d}x_{i_2,j_2}} \\
= & \frac{\mathrm{d}s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle}{\mathrm{d}x_{i_2,j_2}} \\
= & \frac{\mathrm{d}s(X)_{i_0,j_0}}{\mathrm{d}x_{i_2,j_2}} \cdot z(X)_{i_0,j_1} + s(X)_{i_0,j_0} \cdot \frac{\mathrm{d}\langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle}{\mathrm{d}x_{i_2,j_2}} \\
= & \frac{\mathrm{d}s(X)_{i_0,j_0}}{\mathrm{d}x_{i_2,j_2}} \cdot z(X)_{i_0,j_1} \\
& + s(X)_{i_0,j_0} \cdot (\langle -(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0} \cdot u(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \\
& + f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2}), X^\top W_{*,j_1}\rangle + f(X)_{i_0,i_0} \cdot w_{j_2,j_1}) \\
= & (-s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} + f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w(X)_{i_0,j_2} \\
& + f(X)_{i_0,i_2} \cdot v_{j_2,j_0}) \cdot z(X)_{i_0,j_1} \\
& + s(X)_{i_0,j_0} \cdot (\langle -(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0} \cdot u(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \\
& + f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2}), X^\top W_{*,j_1}\rangle + f(X)_{i_0,i_0} \cdot w_{j_2,j_1}) \\
= & - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
& + f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
& + f(X)_{i_0,i_2} \cdot v_{j_2,j_0} \cdot z(X)_{i_0,j_1} \\
& - s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0}, X^\top W_{*,j_1}\rangle \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \\
& + s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0}\rangle \cdot w(X)_{i_0,j_2} \\
& + s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w_{j_2,j_1}
\end{aligned}
$$

where the first step is by definition of $C_2(X)$ (see Lemma A.16), the 2nd step is by Fact A.2, the 3rd step is by Lemma B.6, the 4th step is because Lemma A.16, the 5th step is a rearrangement. □

B.11 Derivative of $C_3(X)$

Lemma B.12. *If the following holds:*

- *Let $C_3(X)$ be defined as in Lemma A.16*

We have

- **Part 1** *For* $i_0 = i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$

$$\begin{aligned} &\frac{\mathrm{d}C_3(X)}{\mathrm{d}x_{i_2,j_2}} \\ = & - f(X)_{i_0,i_0}^2 \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\ & - f(X)_{i_0,i_0} \cdot z(X)_{i_0,j_2} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1} \\ & + f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1} \\ & + f(X)_{i_0,i_0} \cdot \langle W_{*,j_2}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1} \\ & + f(X)_{i_0,i_0} \cdot v_{j_2,j_0} \cdot w(X)_{i_0,j_1} \\ & + f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0} \cdot w_{j_1,j_2} \end{aligned}$$

- **Part 2** *For* $i_0 = i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$

$$\begin{aligned} &\frac{\mathrm{d}C_3(X)}{\mathrm{d}x_{i_2,j_2}} \\ = & - f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1} \end{aligned}$$

Proof. **Proof of Part 1**

$$\begin{aligned} &\frac{\mathrm{d}C_3(X)}{\mathrm{d}x_{i_2,j_2}} \\ = & \frac{\mathrm{d}f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} \\ = & \frac{\mathrm{d}f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0}}{\mathrm{d}x_{i_2,j_2}} \cdot w(X)_{i_0,j_1} + f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0} \cdot \frac{\mathrm{d}w(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} \\ = & \frac{\mathrm{d}f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0}}{\mathrm{d}x_{i_2,j_2}} \cdot w(X)_{i_0,j_1} + f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0} \cdot w_{j_1,j_2} \\ = & ((-f(X)_{i_0,i_0} \cdot (f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle f(X)_{i_0}, X^\top W_{*,j_2} \rangle) \\ & + f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0} \rangle) \cdot h(X)_{j_0,i_0} + f(X)_{i_0,i_0} \cdot v_{j_2,j_0}) \cdot w(X)_{i_0,j_1} \\ & + f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0} \cdot w_{j_1,j_2} \\ = & - f(X)_{i_0,i_0}^2 \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\ & - f(X)_{i_0,i_0} \cdot Z(X)_{i_0,j_2} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1} \\ & + f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1} \\ & + f(X)_{i_0,i_0} \cdot v_{j_2,j_0} \cdot w(X)_{i_0,j_1} \\ & + f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0} \cdot w_{j_1,j_2} \end{aligned}$$

where the first step is by definition of $C_3(X)$ (see Lemma A.16), the 2nd step is by Fact A.2, the 3rd step is by Lemma B.2, the 4th step is because Lemma B.7, the 5th step is a rearrangement.

Proof of Part 2

$$\begin{aligned} &\frac{\mathrm{d}C_3(X)}{\mathrm{d}x_{i_2,j_2}} \\ = & \frac{\mathrm{d}f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} \\ = & \frac{\mathrm{d}f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0}}{\mathrm{d}x_{i_2,j_2}} \cdot w(X)_{i_0,j_1} + f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0} \cdot \frac{\mathrm{d}w(X)_{i_0,j_1}}{\mathrm{d}x_{i_2,j_2}} \\ = & \frac{\mathrm{d}f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0}}{\mathrm{d}x_{i_2,j_2}} \cdot w(X)_{i_0,j_1} \\ = & - f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1} \end{aligned}$$

where the first step is by definition of $C_3(X)$ (see Lemma A.16), the 2nd step is by Fact A.2, the 3rd step is by Lemma B.2, the 4th step is because Lemma B.7, the 5th step is a rearrangement.

□

Table 5: C_4 Part 1 Summary

ID	Term	Symmetric?	Table Name
1	$-\langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2}$	No	Table 2: 3
2	$-\langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle \cdot Z(X)_{i_0,j_2}$	No	Table 3: 4
3	$f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0}\rangle \cdot w(X)_{i_0,j_2}$	No	Table 4: 4
4	$\langle f(X)_{i_0} \circ (X^\top W_{*,j_2}) \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle$	Yes	N/A
5	$f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w_{j_2,j_1}$	No	Table 4: 6
6	$f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0}\rangle \cdot v_{j_2,j_0}$	No	Table 6:4

B.12 Derivative of $C_4(X)$

Lemma B.13. *If the following holds:*

- *Let $C_4(X)$ be defined as in Lemma A.16*

We have

- **Part 1** *For $i_0 = i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$*

$$\begin{aligned} &\frac{\mathrm{d}C_4(X)}{\mathrm{d}x_{i_2,j_2}} \\ = &-\langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \\ &-\langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle \cdot Z(X)_{i_0,j_2} \\ &+ f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0}\rangle \cdot w(X)_{i_0,j_2} \\ &+ \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}) \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle \\ &+ f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w_{j_2,j_1} \\ &+ f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0}\rangle \cdot v_{j_2,j_0} \end{aligned}$$

- **Part 2** *For $i_0 = i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*

$$\begin{aligned} &\frac{\mathrm{d}C_4(X)}{\mathrm{d}x_{i_2,j_2}} \\ = &-\langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \\ &+ f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot \langle W_{*,j_1}, X_{*,i_2}\rangle \cdot w(X)_{i_0,j_2} \\ &+ f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w_{j_2,j_1} \\ &+ f(X)_{i_0,i_2} \cdot \langle W_{*,j_1}, X_{*,i_2}\rangle \cdot v_{j_2,j_0} \end{aligned}$$

Proof. **Proof of Part 1**

$$\begin{aligned} &\frac{\mathrm{d}C_4(X)}{\mathrm{d}x_{i_2,j_2}} \\ = &\frac{\mathrm{d}\langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle}{\mathrm{d}x_{i_2,j_2}} \\ = &\langle \frac{\mathrm{d}f(X)_{i_0} \circ (X^\top W_{*,j_1})}{\mathrm{d}x_{i_2,j_2}}, h(X)_{j_0}\rangle + \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), \frac{\mathrm{d}h(X)_{j_0}}{\mathrm{d}x_{i_2,j_2}}\rangle \\ = &\langle \frac{\mathrm{d}f(X)_{i_0} \circ (X^\top W_{*,j_1})}{\mathrm{d}x_{i_2,j_2}}, h(X)_{j_0}\rangle + \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), e_{i_2} \cdot v_{j_2,j_0}\rangle \\ = &\langle (-f(X)_{i_0} \cdot (f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle f(X)_{i_0}, X^\top W_{*,j_2}\rangle) \\ &+ f(X)_{i_0} \circ (e_{i_0} \cdot w(X)_{i_0,j_2} + X^\top W_{*,j_2})) \circ (X^\top W_{*,j_1}) + f(X)_{i_0} \circ (e_{i_0} \cdot w_{j_2,j_1}), h(X)_{j_0}\rangle \end{aligned}$$

Table 6: C_5 Part 1 Summary

Term	Symmetric Terms	Table Name
$-f(X)_{i_0,i_0}^2 \cdot w(X)_{i_0,j_2} \cdot v_{j_1,j_0}$	No	$C_1(X)$: 4
$-f(X)_{i_0,i_0} \cdot z(X)_{i_0,j_2} \cdot v_{j_1,j_0}$	No	Table 3: 5
$f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \cdot v_{j_1,j_0}$	No	Table 4:5
$f(X)_{i_0,i_0} \cdot \langle W_{*,j_2}, X_{*,i_0}\rangle \cdot v_{j_1,j_0}$	No	Table 5: 6

$$\begin{aligned}
& + \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), e_{i_0} \cdot v_{j_2,j_0}\rangle \\
= & - \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \\
& - \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle \cdot \langle f(X)_{i_0}, X^\top W_{*,j_2}\rangle \\
& + f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0}\rangle \cdot w(X)_{i_0,j_2} \\
& + \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}) \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle \\
& + f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w_{j_2,j_1} \\
& + f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0}\rangle \cdot v_{j_2,j_0}
\end{aligned}$$

where the first step is by definition of $C_4(X)$ (see Lemma A.16), the 2nd step is by Fact A.2, the 3rd step is by Lemma A.15, the 4th step is because Lemma B.9, the 5th step is a rearrangement.

Proof of Part 2

$$\begin{aligned}
& \frac{\mathrm{d}C_4(X)}{\mathrm{d}x_{i_2,j_2}} \\
= & \frac{\mathrm{d}\langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle}{\mathrm{d}x_{i_2,j_2}} \\
= & \langle \frac{\mathrm{d}f(X)_{i_0} \circ (X^\top W_{*,j_1})}{\mathrm{d}x_{i_2,j_2}}, h(X)_{j_0}\rangle + \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), \frac{\mathrm{d}h(X)_{j_0}}{\mathrm{d}x_{i_2,j_2}}\rangle \\
= & \langle \frac{\mathrm{d}f(X)_{i_0} \circ (X^\top W_{*,j_1})}{\mathrm{d}x_{i_2,j_2}}, h(X)_{j_0}\rangle + \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), e_{i_2} \cdot v_{j_2,j_0}\rangle \\
= & \langle -(f(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \\
& + f(X)_{i_0} \circ (e_{i_2} \cdot w(X)_{i_0,j_2})) \circ (X^\top W_{*,j_1}) + f(X)_{i_0} \circ (e_{i_2} \cdot w_{j_2,j_1}), h(X)_{j_0}\rangle \\
& + \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), e_{i_2} \cdot v_{j_2,j_0}\rangle \\
= & - \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0}\rangle \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \\
& + f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot \langle W_{*,j_1}, X_{*,i_2}\rangle \cdot w(X)_{i_0,j_2} \\
& + f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w_{j_2,j_1} \\
& + f(X)_{i_0,i_2} \cdot \langle W_{*,j_1}, X_{*,i_2}\rangle \cdot v_{j_2,j_0}
\end{aligned}$$

where the first step is by definition of $C_4(X)$ (see Lemma A.16), the 2nd step is by Fact A.2, the 3rd step is by Lemma A.15, the 4th step is because Lemma B.9, the 5th step is a rearrangement.

□

B.13 DERIVATIVE OF $C_5(X)$

Lemma B.14. *If the following holds:*

- *Let $C_5(X)$ be defined as in Lemma A.16*

We have

- **Part 1** *For $i_0 = i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$*

$$\frac{\mathrm{d}C_5(X)}{\mathrm{d}x_{i_2,j_2}} = -f(X)_{i_0,i_0}^2 \cdot w(X)_{i_0,j_2} \cdot v_{j_1,j_0}$$

$$- f(X)_{i_0,i_0} \cdot z(X)_{i_0,j_2} \cdot v_{j_1,j_0}$$
$$+ f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \cdot v_{j_1,j_0}$$
$$+ f(X)_{i_0,i_0} \cdot \langle W_{*,j_2}, X_{*,i_0} \rangle \cdot v_{j_1,j_0}$$

- **Part 2** *For* $i_0 = i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$

$$\frac{\mathrm{d} C_5(X)}{\mathrm{d} x_{i_2,j_2}} = - f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot v_{j_1,j_0}$$

Proof. **Proof of Part 1**

$$\begin{aligned}
& \frac{\mathrm{d} C_5(X)}{\mathrm{d} x_{i_2,j_2}} \\
= & \frac{\mathrm{d} f(X)_{i_0,i_0} \cdot v_{j_1,j_0}}{\mathrm{d} x_{i_2,j_2}} \\
= & \frac{\mathrm{d} f(X)_{i_0,i_0}}{\mathrm{d} x_{i_2,j_2}} \cdot v_{j_1,j_0} \\
= & (-f(X)_{i_0,i_0} \cdot (f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} + \langle f(X)_{i_0}, X^\top W_{*,j_2} \rangle) \\
& + f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0} \rangle) \cdot v_{j_1,j_0} \\
= & - f(X)_{i_0,i_0}^2 \cdot w(X)_{i_0,j_2} \cdot v_{j_1,j_0} \\
& - f(X)_{i_0,i_0} \cdot \langle f(X)_{i_0}, X^\top W_{*,j_2} \rangle \cdot v_{j_1,j_0} \\
& + f(X)_{i_0,i_0} \cdot \langle W_{j_2,*} + W_{*,j_2}, X_{*,i_0} \rangle \cdot v_{j_1,j_0}
\end{aligned}$$

where the first step is by definition of $C_5(X)$ (see Lemma A.16), the 2nd step is by Fact A.2, the 3rd step is by Lemma B.4, the 4th step is a rearrangement.

Proof of Part 2

$$\begin{aligned}
& \frac{\mathrm{d} C_5(X)}{\mathrm{d} x_{i_2,j_2}} \\
= & \frac{\mathrm{d} f(X)_{i_0,i_0} \cdot v_{j_1,j_0}}{\mathrm{d} x_{i_2,j_2}} \\
= & \frac{\mathrm{d} f(X)_{i_0,i_0}}{\mathrm{d} x_{i_2,j_2}} \cdot v_{j_1,j_0} \\
= & - f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot v_{j_1,j_0}
\end{aligned}$$

where the first step is by definition of $C_5(X)$ (see Lemma A.16), the 2nd step is by Fact A.2, the 3rd step is by Lemma B.4. ☐

B.14 Derivative of $\frac{c(X)_{i_0,j_0}}{\mathrm{d} x_{i_1,j_1}}$

Lemma B.15. *If the following holds:*

- *Let* $c(X)_{i_0,j_0}$ *be defined as in Definition A.8*

We have

- **Part 1** *For* $i_0 = i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$

$$\frac{\mathrm{d} c(X)_{i_0,j_0}}{\mathrm{d} x_{i_1,j_1} x_{i_2,j_2}} = \sum_{i=1}^{21} D_i(X)$$

where we have following definitions

$$D_1(X) := 2 s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0}^2 \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1}$$
$$D_2(X) := 2 f(X)_{i_0,i_0} \cdot s(X)_{i_0,j_0} \cdot z(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1}$$

$$
\begin{aligned}
& + 2f(X)_{i_0,i_0} \cdot s(X)_{i_0,j_0} \cdot z(X)_{i_0,j_1} \cdot w(X)_{i_0,j_2} \\
D_3(X) :=& - f(X)_{i_0,i_0}^2 \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
D_4(X) :=& - f(X)_{i_0,i_0} \cdot \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), h(X)_{j_0} \rangle \cdot w(X)_{i_0,j_1} \\
& - f(X)_{i_0,i_0} \cdot \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0} \rangle \cdot w(X)_{i_0,j_2} \\
D_5(X) :=& - f(X)_{i_0,i_0}^2 \cdot v_{j_2,j_0} \cdot w(X)_{i_0,j_1} - f(X)_{i_0,i_0}^2 \cdot v_{j_1,j_0} \cdot w(X)_{i_0,j_2} \\
D_6(X) :=& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
D_7(X) :=& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot \langle W_{*,j_2}, X_{*,i_0} \rangle \cdot w(X)_{i_0,j_1} \\
& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0} \rangle \cdot w(X)_{i_0,j_2} \\
D_8(X) :=& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w_{j_1,j_2} - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w_{j_2,j_1} \\
D_9(X) :=& s(X)_{i_0,j_0} \cdot z(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
D_{10}(X) :=& - f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
& - f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1} \cdot z(X)_{i_0,j_2} \\
D_{11}(X) :=& - \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), h(X)_{j_0} \rangle \cdot z(X)_{i_0,j_1} \\
& - \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0} \rangle \cdot z(X)_{i_0,j_2} \\
D_{12}(X) :=& - f(X)_{i_0,i_0} \cdot v_{j_2,j_0} \cdot z(X)_{i_0,j_1} - f(X)_{i_0,i_0} \cdot v_{j_1,j_0} \cdot z(X)_{i_0,j_2} \\
D_{13}(X) :=& s(X)_{i_0,j_0} \cdot z(X)_{i_0,j_1} \cdot f(X)_{i_0,i_0} \cdot z(X)_{i_0,j_2} \\
D_{14}(X) :=& - s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}), X^\top W_{*,j_1} \rangle \\
D_{15}(X) :=& - f(X)_{i_0,i_0}^2 \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
D_{16}(X) :=& f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1} \\
D_{17}(X) :=& f(X)_{i_0,i_0} \cdot \langle W_{*,j_2}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1} \\
& + f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_2} \\
D_{18}(X) :=& f(X)_{i_0,i_0} \cdot v_{j_2,j_0} \cdot w(X)_{i_0,j_1} + f(X)_{i_0,i_0} \cdot v_{j_1,j_0} \cdot w(X)_{i_0,j_2} \\
D_{19}(X) :=& f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0} \cdot w_{j_1,j_2} + f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0} \cdot w_{j_2,j_1} \\
D_{20}(X) :=& \langle f(X)_{i_0} \circ (X^\top W_{*,j_2}) \circ (X^\top W_{*,j_1}), h(X)_{j_0} \rangle \\
D_{21}(X) :=& f(X)_{i_0,i_0} \cdot \langle W_{*,j_2}, X_{*,i_0} \rangle \cdot v_{j_1,j_0} + f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0} \rangle \cdot v_{j_2,j_0}
\end{aligned}
$$

- **Part 2** *For* $i_0 = i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$

$$
\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1} x_{i_2,j_2}} = \sum_{i=1}^{15} E_i(X)
$$

where we have following definitions

$$
\begin{aligned}
E_1(X) :=& 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
E_2(X) :=& - 2f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w(X)_{i_0,j_2} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
E_3(X) :=& - f(X)_{i_0,i_2} \cdot v_{j_2,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1} \\
E_4(X) :=& s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
E_5(X) :=& - f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w(X)_{i_0,j_2} \cdot z(X)_{i_0,j_1} \\
E_6(X) :=& - f(X)_{i_0,i_2} \cdot v_{j_2,j_0} \cdot z(X)_{i_0,j_1} \\
E_7(X) :=& s(X)_{i_0,j_0} \cdot \langle f(X)_{i_0}, X^\top W_{*,j_1} \rangle \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_2} \\
E_8(X) :=& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot \langle W_{*,j_1}, X_{*,i_0} \rangle \cdot w(X)_{i_0,j_2} \\
E_9(X) :=& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w_{j_2,j_1} \\
E_{10}(X) :=& - f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,j_1} \\
E_{11}(X) :=& - \langle f(X)_{i_0} \circ (X^\top W_{*,j_1}), h(X)_{j_0} \rangle \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \\
E_{12}(X) :=& f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot \langle W_{*,j_1}, X_{*,i_2} \rangle \cdot w(X)_{i_0,j_2} \\
E_{13}(X) :=& f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w_{j_2,j_1} \\
E_{14}(X) :=& f(X)_{i_0,i_2} \cdot \langle W_{*,j_1}, X_{*,i_2} \rangle \cdot v_{j_2,j_0}
\end{aligned}
$$

$$E_{15}(X) := -f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot v_{j_1,j_0}$$

Proof. The proof is a combination of derivatives of $C_i(X)$ in this section.

Notice that the symmetricity for **Part 1** is verified by tables in this section. □

C HESSIAN CASE 2: $i_0 \neq i_1$

In this section, we focus on the second case of Hessian. In Sections C.1, C.2, C.3, C.4 and C.5, we calculated derivative of some important terms. In Sections C.6, C.7 and C.8 we calculate derivative of C_6, C_7 and C_8 respectively. And in Section C.9 we calculate the derivative of $\frac{\mathrm{d}c(X)_{i_0,j_1}}{\mathrm{d}x_{i_1,j_1}}$.

C.1 DERIVATIVE OF SCALAR FUNCTION $f(X)_{i_0,i_1}$

Lemma C.1. *If the following holds:*

- *Let $f(X)_{i_0}$ be defined as Definition A.6*
- *For $i_0 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*

We have

- **Part 1.** *For $i_0 \neq i_2, i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$*
$$\begin{aligned}\frac{\mathrm{d}f(X)_{i_0,i_1}}{\mathrm{d}x_{i_2,j_2}} = &-f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2}\\ &+ f(X)_{i_0,i_1} \cdot w(X)_{i_0,j_2}\end{aligned}$$
- **Part 2.** *For $i_0 \neq i_2, i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*
$$\frac{\mathrm{d}f(X)_{i_0,i_1}}{\mathrm{d}x_{i_2,j_2}} = -f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2}$$

Proof. **Proof of Part 1**

$$\begin{aligned}\frac{\mathrm{d}f(X)_{i_0,i_1}}{\mathrm{d}x_{i_2,j_2}} &= (-(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0} \cdot u(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle\\ &\quad + f(X)_{i_0} \circ (e_{i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle))_{i_1}\\ &= -(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0,i_1} \cdot u(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle\\ &\quad + f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle\\ &= -f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2}\\ &\quad + f(X)_{i_0,i_1} \cdot w(X)_{i_0,j_2}\end{aligned}$$

where the first step follows from Part 1 of Lemma A.14, the second step follows from simple algebra, the first step follows from Definition A.6.

Proof of Part 2

$$\begin{aligned}\frac{\mathrm{d}f(X)_{i_0,i_1}}{\mathrm{d}x_{i_2,j_2}} &= (-(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0} \cdot u(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle\\ &\quad + f(X)_{i_0} \circ (e_{i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle))_{i_1}\\ &= -(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0,i_1} \cdot u(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle\\ &= -f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2}\end{aligned}$$

where the first step follows from Part 1 of Lemma A.14, the second step follows from simple algebra, the first step follows from Definition A.6. □

C.2 Derivative of scalar function $h(X)_{j_0,i_1}$

Lemma C.2. *If the following holds:*

- *Let $h(X)_{j_0}$ be defined as Definition A.7*
- *For $i_0 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*

We have

- **Part 1.** *For $i_0 \neq i_2, i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$*
$$\frac{\mathrm{d}h(X)_{j_0,i_1}}{\mathrm{d}x_{i_2,j_2}} = v_{j_2,j_0}$$
- **Part 2.** *For $i_0 \neq i_2, i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*
$$\frac{\mathrm{d}h(X)_{j_0,i_1}}{\mathrm{d}x_{i_2,j_2}} = 0$$

Proof. **Proof of Part 1.**

$$\begin{aligned}\frac{\mathrm{d}h(X)_{j_0,i_1}}{\mathrm{d}x_{i_2,j_2}} &= (e_{i_2} \cdot v_{j_2,j_0})_{i_1} \\ &= v_{j_2,j_0}\end{aligned}$$

where the first step follows from Lemma A.7, the second step follows from $i_1 = i_2$.

Proof of Part 1.

$$\begin{aligned}\frac{\mathrm{d}h(X)_{j_0,i_1}}{\mathrm{d}x_{i_2,j_2}} &= (e_{i_2} \cdot v_{j_2,j_0})_{i_1} \\ &= 0\end{aligned}$$

where the first step follows from Lemma A.7, the second step follows from $i_1 \neq i_2$. □

C.3 Derivative of scalar function $\langle f(X)_{i_0}, h(X)_{j_0}\rangle$

Lemma C.3. *If the following holds:*

- *Let $f(X)_{i_0}$ be defined as Definition A.6*
- *Let $h(X)_{j_0}$ be defined as Definition A.7*
- *For $i_0 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*

We have

$$\begin{aligned}\frac{\mathrm{d}\langle f(X)_{i_0}, h(X)_{j_0}\rangle}{\mathrm{d}x_{i_2,j_2}} = &\langle -f(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \\ &+ f(X)_{i_0} \circ (e_{i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle), h(X)_{j_0}\rangle + f(X)_{i_0,i_2} \cdot v_{j_2,j_0}\end{aligned}$$

Proof.

$$\begin{aligned}\frac{\mathrm{d}\langle f(X)_{i_0}, h(X)_{j_0}\rangle}{\mathrm{d}x_{i_2,j_2}} &= \langle \frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_2,j_2}}, h(X)_{j_0}\rangle + \langle f(X)_{i_0}, \frac{\mathrm{d}h(X)_{j_0}}{\mathrm{d}x_{i_2,j_2}}\rangle \\ &= \langle -(\alpha(X)_{i_0})^{-1} \cdot f(X)_{i_0} \cdot u(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \\ &\quad + f(X)_{i_0} \circ (e_{i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle), h(X)_{j_0}\rangle + \langle f(X)_{i_0}, \frac{\mathrm{d}h(X)_{j_0}}{\mathrm{d}x_{i_2,j_2}}\rangle \\ &= \langle -f(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle\end{aligned}$$

$$+ f(X)_{i_0} \circ (e_{i_2} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle), h(X)_{j_0} \rangle + \langle f(X)_{i_0}, \frac{\mathrm{d}h(X)_{j_0}}{\mathrm{d}x_{i_2,j_2}} \rangle$$
$$= \langle -f(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle$$
$$+ f(X)_{i_0} \circ (e_{i_2} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle), h(X)_{j_0} \rangle + \langle f(X)_{i_0}, e_{i_2} \cdot v_{j_2,j_0} \rangle$$
$$= \langle -f(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle$$
$$+ f(X)_{i_0} \circ (e_{i_2} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle), h(X)_{j_0} \rangle + f(X)_{i_0,i_2} \cdot v_{j_2,j_0}$$

where the first step follows from simple differential rule, the second step follows from Lemma A.14, the third step follows from simple algebra and Definition A.6, the fourth step follows from Lemma A.15, the last step follows from simple algebra. □

C.4 Derivative of scalar function $f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$

Lemma C.4. *If the following holds:*

- *Let $f(X)_{i_0}$ be defined as Definition A.6*
- *For $i_0 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*

We have

- **Part 1.** *For $i_0 \neq i_2, i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$*
$$\frac{\mathrm{d}f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle}{\mathrm{d}x_{i_2,j_2}}$$
$$= (-f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$
- **Part 2.** *For $i_0 \neq i_2, i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*
$$\frac{\mathrm{d}f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle}{\mathrm{d}x_{i_2,j_2}}$$
$$= - f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$

Proof. **Proof of Part 1**

$$\frac{\mathrm{d}f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle}{\mathrm{d}x_{i_2,j_2}}$$
$$= \frac{\mathrm{d}f(X)_{i_0,i_1}}{\mathrm{d}x_{i_2,j_2}} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + \frac{\mathrm{d}\langle W_{j_1,*}, X_{*,i_0} \rangle}{\mathrm{d}x_{i_2,j_2}} \cdot f(X)_{i_0,i_1}$$
$$= (-f(X)_{i_0,i_2} f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$
$$+ \frac{\mathrm{d}\langle W_{j_1,*}, X_{*,i_0} \rangle}{\mathrm{d}x_{i_2,j_2}} \cdot f(X)_{i_0,i_1}$$
$$= (-f(X)_{i_0,i_2} f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + \mathbf{0}_d \cdot f(X)_{i_0,i_1}$$
$$= (-f(X)_{i_0,i_2} f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$

where the first step follows from simple differential rule, the second step follows from Lemma C.1, the third step follows from $i_0 \neq i_2$, the last step follows from simple algebra.

Proof of Part 2

$$\frac{\mathrm{d}f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle}{\mathrm{d}x_{i_2,j_2}}$$
$$= \frac{\mathrm{d}f(X)_{i_0,i_1}}{\mathrm{d}x_{i_2,j_2}} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + \frac{\mathrm{d}\langle W_{j_1,*}, X_{*,i_0} \rangle}{\mathrm{d}x_{i_2,j_2}} \cdot f(X)_{i_0,i_1}$$
$$= (-f(X)_{i_0,i_2} f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$
$$+ \frac{\mathrm{d}\langle W_{j_1,*}, X_{*,i_0} \rangle}{\mathrm{d}x_{i_2,j_2}} \cdot f(X)_{i_0,i_1}$$

$$= (-f(X)_{i_0,i_2} f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + \mathbf{0}_d \cdot f(X)_{i_0,i_1}$$
$$= -f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$

where the first step follows from simple differential rule, the second step follows from Lemma C.1, the third step follows from $i_0 \neq i_2$, the last step follows from simple algebra. □

C.5 DERIVATIVE OF SCALAR FUNCTION $f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1}$

Lemma C.5. *If the following holds:*

- *Let $f(X)_{i_0}$ be defined as Definition A.6*
- *Let $h(X)_{j_0}$ be defined as Definition A.7*

We have

- **Part 1** *For $i_0 \neq i_2, i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$*
$$\frac{\mathrm{d} f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1}}{\mathrm{d} x_{i_2,j_2}}$$
$$= (-f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_1} + v_{j_2,j_0} \cdot f(X)_{i_0,i_1}$$
- **Part 2** *For $i_0 \neq i_2, i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*
$$\frac{\mathrm{d} f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0}}{\mathrm{d} x_{i_2,j_2}}$$
$$= -f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_1}$$

Proof. **Proof of Part 1.**

$$\begin{aligned}\frac{\mathrm{d} f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1}}{\mathrm{d} x_{i_2,j_2}} &= \frac{\mathrm{d} f(X)_{i_0,i_1}}{\mathrm{d} x_{i_2,j_2}} \cdot h(X)_{j_0,i_1} + \frac{\mathrm{d} h(X)_{j_0,i_1}}{\mathrm{d} x_{i_2,j_2}} \cdot f(X)_{i_0,i_1} \\ &= (-f(X)_{i_0,i_2} f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_1} \\ &\quad + \frac{\mathrm{d} h(X)_{j_0,i_1}}{\mathrm{d} x_{i_2,j_2}} \cdot f(X)_{i_0,i_1} \\ &= (-f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_1} \\ &\quad + v_{j_2,j_0} \cdot f(X)_{i_0,i_1}\end{aligned}$$

where the first step follows from simple differential rule, the second step follows from Lemma C.1, the third step follows from Part 1 of Lemma C.2.

Proof of Part 2.

$$\begin{aligned}\frac{\mathrm{d} f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1}}{\mathrm{d} x_{i_2,j_2}} &= \frac{\mathrm{d} f(X)_{i_0,i_1}}{\mathrm{d} x_{i_2,j_2}} \cdot h(X)_{j_0,i_1} + \frac{\mathrm{d} h(X)_{j_0,i_1}}{\mathrm{d} x_{i_2,j_2}} \cdot f(X)_{i_0,i_1} \\ &= -f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_1} \\ &\quad + \frac{\mathrm{d} h(X)_{j_0,i_1}}{\mathrm{d} x_{i_2,j_2}} \cdot f(X)_{i_0,i_1} \\ &= -f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_1}\end{aligned}$$

where the first step follows from simple differential rule, the second step follows from Lemma C.1, the third step follows from Part 2 of Lemma C.2. □

C.6 DERIVATIVE OF $C_6(X)$

Lemma C.6. *If the following holds:*

- *Let $C_6(X) \in \mathbb{R}$ be defined as in Lemma A.16*
- *For $i_0 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*

We have

- **Part 1** *For $i_0 \neq i_2, i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$*

$$\begin{aligned}
&\frac{\mathrm{d}C_6(X)}{\mathrm{d}x_{i_2,j_2}} \\
=& -(\langle -f(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \\
&+ f(X)_{i_0} \circ (e_{i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle), h(X)_{j_0}\rangle + f(X)_{i_0,i_2} \cdot v_{j_2,j_0}) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&+ (-\langle f(X)_{i_0}, h(X)_{j_0}\rangle) \cdot (-f(X)_{i_0,i_2} f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle
\end{aligned}$$

- **Part 2** *For $i_0 \neq i_2, i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*

$$\begin{aligned}
&\frac{\mathrm{d}C_6(X)}{\mathrm{d}x_{i_2,j_2}} \\
=& -(\langle -f(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \\
&+ f(X)_{i_0} \circ (e_{i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle), h(X)_{j_0}\rangle + f(X)_{i_0,i_2} \cdot v_{j_2,j_0}) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&+ \langle f(X)_{i_0}, h(X)_{j_0}\rangle \cdot f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle
\end{aligned}$$

Proof. **Proof of Part 1**

$$\begin{aligned}
&\frac{\mathrm{d}C_6(X)}{\mathrm{d}x_{i_2,j_2}} \\
=& \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(-\langle f(X)_{i_0}, h(X)_{j_0}\rangle \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle) \\
=& \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(-\langle f(X)_{i_0}, h(X)_{j_0}\rangle) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&+ (-\langle f(X)_{i_0}, h(X)_{j_0}\rangle) \cdot \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle) \\
=& \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(-\langle f(X)_{i_0}, h(X)_{j_0}\rangle) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&+ (-\langle f(X)_{i_0}, h(X)_{j_0}\rangle) \cdot (-f(X)_{i_0,i_2} f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
=& -(\langle -f(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \\
&+ f(X)_{i_0} \circ (e_{i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle), h(X)_{j_0}\rangle + f(X)_{i_0,i_2} \cdot v_{j_2,j_0}) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&+ (-\langle f(X)_{i_0}, h(X)_{j_0}\rangle) \cdot (-f(X)_{i_0,i_2} f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle
\end{aligned}$$

where the first step follows from Lemma A.16, the second step follows from simple differential rule, the third step follows from Lemma C.4, last step follows from Lemma C.3.

Proof of Part 2

$$\begin{aligned}
&\frac{\mathrm{d}C_6(X)}{\mathrm{d}x_{i_2,j_2}} \\
=& \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(-\langle f(X)_{i_0}, h(X)_{j_0}\rangle \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle) \\
=& \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(-\langle f(X)_{i_0}, h(X)_{j_0}\rangle) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&+ (-\langle f(X)_{i_0}, h(X)_{j_0}\rangle) \cdot \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle) \\
=& \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(-\langle f(X)_{i_0}, h(X)_{j_0}\rangle) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle
\end{aligned}$$

$$+ \langle f(X)_{i_0}, h(X)_{j_0} \rangle) \cdot f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$
$$= -(\langle -f(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle$$
$$+ f(X)_{i_0} \circ (e_{i_2} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle), h(X)_{j_0} \rangle + f(X)_{i_0,i_2} \cdot v_{j_2,j_0}) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$
$$+ \langle f(X)_{i_0}, h(X)_{j_0} \rangle \cdot f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$

where the first step follows from Lemma A.16, the second step follows from simple differential rule, the third step follows from Lemma C.4, last step follows from Lemma C.3. □

C.7 Derivative of $C_7(X)$

Lemma C.7. *If the following holds:*

- *Let $C_7(X) \in \mathbb{R}$ be defined as in Lemma A.16*

We have

- **Part 1.** *For $i_0 \neq i_2, i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$*

$$\frac{\mathrm{d}C_7(X)}{\mathrm{d}x_{i_2,j_2}} = (-f(X)_{i_0,i_2} + 1) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + v_{j_2,j_0} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$

- **Part 2.** *For $i_0 \neq i_2, i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*

$$\frac{\mathrm{d}C_7(X)}{\mathrm{d}x_{i_2,j_2}} = -f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$

Proof. **Proof of Part 1.**

$$\frac{\mathrm{d}C_7(X)}{\mathrm{d}x_{i_2,j_2}}$$
$$= \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle)$$
$$= \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1}) \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1} \cdot \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(\langle W_{j_1,*}, X_{*,i_0} \rangle)$$
$$= (-f(X)_{i_0,i_2} + 1) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$
$$+ v_{j_2,j_0} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$
$$+ f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1} \cdot \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(\langle W_{j_1,*}, X_{*,i_0} \rangle)$$
$$= (-f(X)_{i_0,i_2} + 1) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0} \rangle \cdot h(X)_{j_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$
$$+ v_{j_2,j_0} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle$$

where the first step follows from Lemma A.16, the second step follows from differential rule, the third step follows from Part 1 of Lemma C.3, the fourth step follows from $i_0 \neq i_2$.

Proof of Part 2.

$$\frac{\mathrm{d}C_7(X)}{\mathrm{d}x_{i_2,j_2}}$$
$$= \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle)$$
$$= \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1}) \cdot \langle W_{j_1,*}, X_{*,i_0} \rangle + f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1} \cdot \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(\langle W_{j_1,*}, X_{*,i_0} \rangle)$$

$$
\begin{aligned}
&= -f(X)_{i_0,i_2} f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot h(X)_{j_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&\quad + f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1} \cdot \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(\langle W_{j_1,*}, X_{*,i_0}\rangle) \\
&= -f(X)_{i_0,i_2} f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot h(X)_{j_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&\quad + f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1} \cdot \mathbf{0}_d \\
&= -f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot h(X)_{j_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle
\end{aligned}
$$

where the first step follows from Lemma A.16, the second step follows from differential rule, the third step follows from Part 2 of Lemma C.3, the fourth step follows from $i_0 \neq i_2$, the last step follows from simple algebra. □

C.8 DERIVATIVE OF $C_8(X)$

Lemma C.8. *If the following holds:*

- *Let $C_8(X) \in \mathbb{R}$ be defined as in Lemma A.16*
- *For $i_0 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*

We have

- **Part 1.** *For $i_0 \neq i_2, i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$*

$$
\begin{aligned}
&\frac{\mathrm{d}C_8(X)}{\mathrm{d}x_{i_2,j_2}} \\
&= (-f(X)_{i_0,i_2} f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot v_{j_1,j_0}
\end{aligned}
$$

- **Part 2.** *For $i_0 \neq i_2, i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$*

$$
\begin{aligned}
&\frac{\mathrm{d}C_8(X)}{\mathrm{d}x_{i_2,j_2}} \\
&= -f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot v_{j_1,j_0}
\end{aligned}
$$

Proof. **Proof of Part 1**

$$
\begin{aligned}
\frac{\mathrm{d}C_8(X)}{\mathrm{d}x_{i_2,j_2}} &= \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}} f(X)_{i_0,i_1} \cdot v_{j_1,j_0} \\
&= (-f(X)_{i_0,i_2} f(X)_{i_0,i_1} + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot v_{j_1,j_0}
\end{aligned}
$$

where the first step follows from Lemma A.16, the second step follows from differential rule and Lemma C.1.

Proof of Part 2

$$
\begin{aligned}
\frac{\mathrm{d}C_8(X)}{\mathrm{d}x_{i_2,j_2}} &= \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}} f(X)_{i_0,i_1} \cdot v_{j_1,j_0} \\
&= -f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot v_{j_1,j_0}
\end{aligned}
$$

where the first step follows from Lemma A.16, the second step follows from differential rule and Lemma C.1. □

C.9 DERIVATIVE OF $\frac{\mathrm{d}c(X)_{i_0,j_1}}{\mathrm{d}x_{i_1,j_1}}$

Lemma C.9. *If the following holds:*

- *Let $c(X)_{i_0,j_1} \in \mathbb{R}$ be defined as in Lemma A.16 and Definition A.8*

We have

- **Part 1** *For* $i_0 \neq i_2, i_1 = i_2 \in [n]$, $j_1, j_2 \in [d]$

$$\frac{\mathrm{d}c(X)}{\mathrm{d}x_{i_1,j_1}, \mathrm{d}x_{i_2,j_2}} = \sum_{i=1}^{6} F_i(X)$$

where we have following definitions

$$\begin{aligned}
F_1(X) &= 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1}^2 \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
F_2(X) &= -f(X)_{i_0,i_1}^2 \cdot h(X)_{j_0,i_1} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
F_3(X) &= -f(X)_{i_0,i_1}^2 \cdot v_{j_2,j_0} \cdot w(X)_{i_0,j_1} - f(X)_{i_0,i_1}^2 \cdot v_{j_1,j_0} \cdot w(X)_{i_0,j_2} \\
F_4(X) &= -s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1} \cdot w(X)_{i_0,j_1} \cdot w(X)_{i_0,j_2} \\
F_5(X) &= f(X)_{i_0,i_1} \cdot w(X)_{i_0,j_1} \cdot w(X)_{i_0,j_2} \cdot h(X)_{j_0,i_1} \\
F_6(X) &= v_{j_2,j_0} \cdot f(X)_{i_0,i_1} \cdot w(X)_{i_0,j_1} + v_{j_1,j_0} \cdot f(X)_{i_0,i_1} \cdot w(X)_{i_0,j_2}
\end{aligned}$$

- **Part 2** *For* $i_0 \neq i_2, i_1 \neq i_2 \in [n]$, $j_1, j_2 \in [d]$

$$\frac{\mathrm{d}c(X)}{\mathrm{d}x_{i_1,j_1}, \mathrm{d}x_{i_2,j_2}} = \sum_{i=1}^{3} G_i(X)$$

where we have following definitions

$$\begin{aligned}
G_1(X) &= 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
G_2(X) &= -f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \cdot (h(X)_{j_0,i_2} + h(X)_{j_0,i_1}) \\
G_3(X) &= -f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot (v_{j_2,j_0} \cdot w(X)_{i_0,j_1} + v_{j_1,j_0} \cdot w(X)_{i_0,j_2})
\end{aligned}$$

Proof. **Proof of Part 1.**

$$\begin{aligned}
& \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}, \mathrm{d}x_{i_2,j_2}} \\
= & \frac{\mathrm{d}C_6}{\mathrm{d}x_{i_2,j_2}} + \frac{\mathrm{d}C_7}{\mathrm{d}x_{i_2,j_2}} + \frac{\mathrm{d}C_8}{\mathrm{d}x_{i_2,j_2}} \\
= & -(\langle -f(X)_{i_0} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle + f(X)_{i_0} \circ (e_{i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle), h(X)_{j_0}\rangle \\
& + f(X)_{i_0,i_1} \cdot v_{j_2,j_0}) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
& + (-\langle f(X)_{i_0}, h(X)_{j_0}\rangle) \cdot (-f(X)_{i_0,i_1}^2 + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
& (-f(X)_{i_0,i_2} + 1) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot h(X)_{j_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
& + v_{j_2,j_0} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
& + (-f(X)_{i_0,i_1}^2 + f(X)_{i_0,i_1}) \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot v_{j_1,j_0} \\
= & 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1}^2 \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
& - 2f(X)_{i_0,i_1}^2 \cdot h(X)_{j_0,i_1} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
& - f(X)_{i_0,i_1}^2 \cdot v_{j_2,j_0} \cdot w(X)_{i_0,j_1} - f(X)_{i_0,i_1}^2 \cdot v_{j_1,j_0} \cdot w(X)_{i_0,j_2} \\
& - s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1} \cdot w(X)_{i_0,j_1} \cdot w(X)_{i_0,j_2} \\
& + f(X)_{i_0,i_1} \cdot w(X)_{i_0,j_1} \cdot w(X)_{i_0,j_2} \cdot h(X)_{j_0,i_1} \\
& + v_{j_2,j_0} \cdot f(X)_{i_0,i_1} \cdot w(X)_{i_0,j_1} + v_{j_1,j_0} \cdot f(X)_{i_0,i_1} \cdot w(X)_{i_0,j_2}
\end{aligned}$$

where the first step follows from Lemma A.16, the second step follows from previous results in this section, the last step is a rearrangement.

Proof of Part 2.

$$\begin{aligned}
& \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}, \mathrm{d}x_{i_2,j_2}} \\
= & \frac{\mathrm{d}C_6}{\mathrm{d}x_{i_2,j_2}} + \frac{\mathrm{d}C_7}{\mathrm{d}x_{i_2,j_2}} + \frac{\mathrm{d}C_8}{\mathrm{d}x_{i_2,j_2}}
\end{aligned}$$

$$
\begin{aligned}
&= -(\langle -f(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \\
&\quad + f(X)_{i_0} \circ (e_{i_2} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle), h(X)_{j_0}\rangle + f(X)_{i_0,i_2} \cdot v_{j_2,j_0}) \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&\quad + \langle f(X)_{i_0}, h(X)_{j_0}\rangle \cdot f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&\quad - f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot h(X)_{j_0,i_1} \cdot \langle W_{j_1,*}, X_{*,i_0}\rangle \\
&\quad - f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_1} \cdot \langle W_{j_2,*}, X_{*,i_0}\rangle \cdot v_{j_1,j_0} \\
&= 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
&\quad - f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w(X)_{i_0,j_2} \cdot w(X)_{i_0,j_1} \\
&\quad - f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,j_1} \cdot w(X)_{i_0,j_2} \cdot h(X)_{j_0,i_1} \\
&\quad - f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot v_{j_2,j_0} \cdot w(X)_{i_0,j_1} - f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot v_{j_1,j_0} \cdot w(X)_{i_0,j_2}
\end{aligned}
$$

where the first step follows from Lemma A.16, the second step follows from Lemma C.6, the third step follows from Part 2 of Lemma C.7, the last step follows from Lemma C.8.

Notice that, by our construction, **Part 1** should be symmetric w.r.t. j_1, j_2, **Part 2** should be symmetric w.r.t. i_1, i_2, which are all satisfied. □

D HESSIAN REFORMULATION

In this section, we provide a reformulation of Hessian formula, which simplifies our calculation and analysis. In Section D.1 we show the way we split the Hessian. In Section D.2 we show the decomposition when $i_0 = i_1 = i_2$.

D.1 HESSIAN SPLIT

Definition D.1 (Hessian of functions of matrix)**.** *We define the Hessian of $c(X)_{i_0,j_0}$ by considering its Hessian with respect to $x = \mathrm{vec}(X)$. This means that, $\nabla^2 c(X)_{i_0,j_0}$ is a $nd \times nd$ matrix with its $(i_1 \cdot j_1, i_2 \cdot j_2)$-th entry being*

$$
\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_2} x_{i_2,j_2}}
$$

Definition D.2 (Hessian split)**.** *We split the hessian of $c(X)_{i_0,j_0}$ into following cases*

- *Part 1: $i_0 = i_1 = i_2$: $H_1^{(i_1,i_2)}$*
- *Part 2: $i_0 = i_1$, $i_0 \neq i_2$: $H_2^{(i_1,i_2)}$*
- *Part 3: $i_0 \neq i_1$, $i_0 = i_2$: $H_3^{(i_1,i_2)}$*
- *Part 4: $i_0 \neq i_1$, $i_0 \neq i_2$, $i_1 = i_2$: $H_4^{(i_1,i_2)}$*
- *Part 5: $i_0 \neq i_1$, $i_0 \neq i_2$, $i_1 \neq i_2$: $H_5^{(i_1,i_2)}$*

In above, $H_i^{(i_1,i_2)}$ is a $d \times d$ matrix with its j_1, j_2-th entry being

$$
\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_2} x_{i_2,j_2}}
$$

Utilizing above definitions, we split the Hessian to a $n \times n$ partition with its i_1, i_2-th component being $H_i(i_1, i_2)$ based on above definition.

Definition D.3. *We define $\nabla^2 c(X)_{i_0,j_0}$ to be as following*

$$\begin{bmatrix} H_4^{(1,1)} & H_5^{(1,2)} & H_5^{(1,3)} & \cdots & H_5^{(1,i_0-1)} & H_3^{(1,i_0)} & H_5^{(1,i_0+1)} & \cdots & H_5^{(1,n)} \\ H_5^{(2,1)} & H_4^{(2,2)} & H_5^{(2,3)} & \cdots & H_5^{(2,i_0-1)} & H_3^{(2,i_0)} & H_5^{(2,i_0+1)} & \cdots & H_5^{(2,n)} \\ H_5^{(3,1)} & H_5^{(3,2)} & H_4^{(3,3)} & \cdots & H_5^{(3,i_0-1)} & H_3^{(3,i_0)} & H_5^{(3,i_0+1)} & \cdots & H_5^{(3,n)} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ H_2^{(i_0,1)} & H_2^{(i_0,2)} & H_2^{(i_0,3)} & \cdots & H_2^{(i_0,i_0-1)} & H_1^{(i_0,i_0)} & H_2^{(i_0,i_0+1)} & \cdots & H_2^{(i_0,n)} \\ H_5^{(i_0+1,1)} & H_5^{(i_0+1,2)} & H_5^{(i_0+1,3)} & \cdots & H_5^{(i_0+1,i_0-1)} & H_3^{(i_0+1,i_0)} & H_4^{(i_0+1,i_0+1)} & \cdots & H_5^{(i_0+1,n)} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ H_5^{(n,1)} & H_5^{(n,2)} & H_5^{(n,3)} & \cdots & H_5^{(n,i_0-1)} & H_3^{(n,i_0)} & H_5^{(n,i_0+1)} & \cdots & H_4^{(n,n)} \end{bmatrix}$$

D.2 DECOMPOSITION HESSIAN : PART 1

Lemma D.4 (Helpful lemma)**.** *Under following conditions*

- *Let* $z(X)_{i_0} := W^\top X \cdot f(X)_{i_0}$
- *Let* $w(X)_{i_0,*} := WX_{*,i_0}$

we have

- *Part 1:* $w(X)_{i_0,j_1} = e_{j_1}^\top \cdot w(X)_{i_0,*}$
- *Part 2:* $z(X)_{i_0,j_1} = e_{j_1}^\top \cdot z(X)_{i_0}$

Proof. **Proof of Part 1**

$$\begin{aligned} w(X)_{i_0,j_1} &= \langle W_{j_1,*}, X_{*,i_0} \rangle \\ &= W_{j_1,*}^\top X_{*,i_0} \\ &= e_{j_1}^\top \cdot WX_{*,i_0} \\ &= e_{j_1}^\top \cdot w(X)_{i_0,*} \end{aligned}$$

where the first step is by the definition of $w(X)_{i_0,j_1}$ the 2nd and 3rd step are from linear algebra facts, the 4th step is by the definition of $w(X)_{i_0,*}$.

Proof of Part 2

$$\begin{aligned} z(X)_{i_0,j_1} &= \langle f(X)i_0, X^\top W_{*,j_1} \rangle \\ &= (X^\top W_{*,j_1})^\top f(X)_{i_0} \\ &= W_{*,j_1}^\top X \cdot f(X)_{i_0} \\ &= e_{j_1}^\top \cdot W^\top X \cdot f(X)_{i_0} \\ &= e_{j_1}^\top \cdot z(X)_{i_0} \end{aligned}$$

where the first step is by the definition of $w(X)_{i_0,j_1}$ the 2nd, 3rd, and the 4th step are from linear algebra facts, the 5th step is by the definition of $w(X)_{i_0,*}$. □

Lemma D.5. *Under following conditions*

- *Let $D_i(X)$ be defined as Lemma B.15*
- *Let* $z(X)_{i_0} := W^\top X \cdot f(X)_{i_0}$
- *Let* $w(X)_{i_0,*} := WX_{*,i_0}$

we have

$$D_1(X) = e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0}^2 \cdot w(X)_{i_0,*}^\top \cdot e_{j_2}$$

$$\begin{aligned}
D_2(X) = & e_{j_1}^\top \cdot (w(X)_{i_0,*} \cdot 2f(X)_{i_0,i_0} \cdot s(X)_{i_0,j_0} \cdot z(X)_{i_0}^\top \\
& + z(X)_{i_0} \cdot 2f(X)_{i_0,i_0} \cdot s(X)_{i_0,j_0} \cdot w(X)_{i_0,*}^\top) \cdot e_{j_2} \\
D_3(X) = & - e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot f(X)_{i_0,i_0}^2 \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
D_4(X) = & - e_{j_1}^\top \cdot W^\top \cdot f(X)_{i_0,i_0} \cdot X \cdot \mathrm{diag}(f(X)_{i_0}) \cdot h(X)_{j_0} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
& - e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot f(X)_{i_0,i_0} \cdot h(X)_{j_0}^\top \cdot \mathrm{diag}(f(X)_{i_0}) \cdot X^\top \cdot W \cdot e_{j_2} \\
D_5(X) = & - e_{j_1}^\top \cdot (w(X)_{i_0,*} \cdot f(X)_{i_0,i_0}^2 \cdot V_{*,j_0}^\top + V_{*,j_0} \cdot f(X)_{i_0,i_0}^2 \cdot w(X)_{i_0,*}^\top) \cdot e_{j_2} \\
D_6(X) = & - e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
D_7(X) = & - e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot X_{*,i_0}^\top \cdot W \cdot e_{j_2} \\
& - e_{j_1}^\top \cdot W^\top \cdot X_{*,i_0} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
D_8(X) = & e_{j_1}^\top \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot (W^\top - W) \cdot e_{j_2} \\
D_9(X) = & e_{j_1}^\top \cdot z(X)_{i_0} \cdot s(X)_{i_0,j_0} \cdot z(X)_{i_0}^\top \cdot e_{j_2} \\
D_{10}(X) = & - e_{j_1}^\top \cdot (z(X)_{i_0} \cdot f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,*}^\top \\
& + w(X)_{i_0,*} \cdot f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot z(X)_{i_0}^\top) \cdot e_{j_2} \\
D_{11}(X) = & - e_{j_1}^\top \cdot (z(X)_{i_0} \cdot h(X)_{j_0}^\top \cdot \mathrm{diag}(f(X)_{i_0}) \cdot X^\top \cdot W \\
& + W^\top \cdot X \cdot \mathrm{diag}(f(X)_{i_0}) \cdot h(X)_{j_0} \cdot z(X)_{i_0}^\top) \cdot e_{j_2} \\
D_{12}(X) = & - e_{j_1}^\top \cdot (z(X)_{i_0} \cdot f(X)_{i_0,i_0} \cdot V_{*,j_0}^\top + V_{*,j_0} \cdot f(X)_{i_0,i_0} \cdot z(X)_{i_0}^\top) \cdot e_{j_2} \\
D_{13}(X) = & e_{j_1}^\top \cdot z(X)_{i_0} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot z(X)_{i_0}^\top \cdot e_{j_2} \\
D_{14}(X) = & - e_{j_1}^\top \cdot W^\top \cdot X \cdot s(X)_{i_0,j_0} \cdot \mathrm{diag}(f(X)_{i_0}) \cdot X^\top \cdot W \cdot e_{j_2} \\
D_{15}(X) = & - e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot f(X)_{i_0,i_0}^2 \cdot h(X)_{j_0,i_0} \cdot \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
D_{16}(X) = & e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
D_{17}(X) = & e_{j_1}^\top \cdot (w(X)_{i_0,*} \cdot f(X)_{i_0,i_0} \cdot X_{*,i_0}^\top \cdot h(X)_{j_0,i_0} \cdot W \\
& + W^\top \cdot X_{*,i_0} \cdot f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0}) \cdot e_{j_2} \\
D_{18}(X) = & e_{j_1}^\top \cdot (w(X)_{i_0,*} f(X)_{i_0,i_0} \cdot V_{j_2,*}^\top + V_{j_1,*}^\top \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top) \cdot e_{j_2} \\
D_{19}(X) = & e_{j_1}^\top \cdot f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0} \cdot (W + W^\top) \cdot e_{j_2} \\
D_{20}(X) := & e_{j_1}^\top \cdot W^\top \cdot X \cdot \mathrm{diag}(f(X)_{i_0}) \cdot \mathrm{diag}(h(X)_{j_0}) \cdot X^\top \cdot W \cdot e_{j_2} \\
D_{21}(X) := & e_{j_1}^\top \cdot (W^\top \cdot X_{*,i_0} \cdot f(X)_{i_0,i_0} \cdot V_{*,j_0}^\top + V_{*,j_0} \cdot f(X)_{i_0,i_0} \cdot X_{*,i_0}^\top \cdot W) \cdot e_{j_2}
\end{aligned}$$

Proof. This lemma is followed by Lemma D.4 and linear algebra facts. □

Based on above auxiliary lemma, we have following definition.

Definition D.6. *Under following conditions*

- *Let* $z(X)_{i_0} := W^\top X \cdot f(X)_{i_0}$
- *Let* $w(X)_{i_0,*} := W X_{*,i_0}$

We present the **Case 1** *component of Hessian* $c(X)_{i_0,j_0}$ *to be*

$$H_1^{(i_0,i_0)}(X) := B(X)$$

where we have

$$\begin{aligned}
B(X) := & \sum_{i=1}^{21} B_i(X) \\
B_1(X) := & w(X)_{i_0,*} \cdot 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0}^2 \cdot w(X)_{i_0,*}^\top
\end{aligned}$$

$$B_2(X) := w(X)_{i_0,*} \cdot 2f(X)_{i_0,i_0} \cdot s(X)_{i_0,j_0} \cdot z(X)_{i_0}^\top + z(X)_{i_0} \cdot 2f(X)_{i_0,i_0} \cdot s(X)_{i_0,j_0} \cdot w(X)_{i_0,*}^\top$$

$$B_3(X) := -w(X)_{i_0,*} \cdot f(X)_{i_0,i_0}^2 \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,*}^\top$$

$$B_4(X) := -W^\top \cdot f(X)_{i_0,i_0} \cdot X \cdot \mathrm{diag}(f(X)_{i_0}) \cdot h(X)_{j_0} \cdot w(X)_{i_0,*}^\top - w(X)_{i_0,*} \cdot f(X)_{i_0,i_0} \cdot h(X)_{j_0}^\top \cdot \mathrm{diag}(f(X)_{i_0}) \cdot X^\top \cdot W$$

$$B_5(X) := -w(X)_{i_0,*} \cdot f(X)_{i_0,i_0}^2 \cdot V_{*,j_0}^\top - V_{*,j_0} \cdot f(X)_{i_0,i_0}^2 \cdot w(X)_{i_0,*}^\top$$

$$B_6(X) := -w(X)_{i_0,*} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top$$

$$B_7(X) := -w(X)_{i_0,*} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot X_{*,i_0}^\top \cdot W - W^\top \cdot X_{*,i_0} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top$$

$$B_8(X) := s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot (W^\top - W)$$

$$B_9(X) := z(X)_{i_0} \cdot s(X)_{i_0,j_0} \cdot z(X)_{i_0}^\top$$

$$B_{10}(X) := -z(X)_{i_0} \cdot f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,*}^\top - w(X)_{i_0,*} \cdot f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot z(X)_{i_0}^\top$$

$$B_{11}(X) := -z(X)_{i_0} \cdot (h(X)_{j_0}^\top \cdot \mathrm{diag}(f(X)_{i_0}) \cdot X^\top \cdot W - W^\top \cdot X \cdot \mathrm{diag}(f(X)_{i_0}) \cdot h(X)_{j_0} \cdot z(X)_{i_0}^\top$$

$$B_{12}(X) := -z(X)_{i_0} \cdot f(X)_{i_0,i_0} \cdot V_{*,j_0}^\top + V_{*,j_0} \cdot f(X)_{i_0,i_0} \cdot z(X)_{i_0}^\top$$

$$B_{13}(X) := z(X)_{i_0} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot z(X)_{i_0}^\top$$

$$B_{14}(X) := -W^\top \cdot X \cdot s(X)_{i_0,j_0} \cdot \mathrm{diag}(f(X)_{i_0}) \cdot X^\top \cdot W$$

$$B_{15}(X) := -w(X)_{i_0,*} \cdot f(X)_{i_0,i_0}^2 \cdot h(X)_{j_0,i_0} \cdot \cdot w(X)_{i_0,*}^\top$$

$$B_{16}(X) := w(X)_{i_0,*} \cdot f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot \cdot w(X)_{i_0,*}^\top$$

$$B_{17}(X) := w(X)_{i_0,*} \cdot f(X)_{i_0,i_0} \cdot X_{*,i_0}^\top \cdot h(X)_{j_0,i_0} \cdot W + W^\top \cdot X_{*,i_0} \cdot f(X)_{i_0,i_0} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0}$$

$$B_{18}(X) := w(X)_{i_0,*} \cdot f(X)_{i_0,i_0} \cdot V_{j_2,*}^\top + V_{j_1,*}^\top \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top$$

$$B_{19}(X) := f(X)_{i_0,i_0} \cdot h(X)_{i_0,i_0} \cdot (W + W^\top)$$

$$B_{20}(X) := W^\top \cdot X \cdot \mathrm{diag}(f(X)_{i_0}) \cdot \mathrm{diag}(h(X)_{j_0}) \cdot X^\top$$

$$B_{21}(X) := W^\top \cdot X_{*,i_0} \cdot f(X)_{i_0,i_0} \cdot V_{*,j_0}^\top + V_{*,j_0} \cdot f(X)_{i_0,i_0} \cdot X_{*,i_0}^\top \cdot W$$

D.3 Decomposition Hessian: Part 2 and Part 3

Lemma D.7. *Under following conditions*

- *Let $E_i(X)$ be defined as Lemma B.15*
- *Let $z(X)_{i_0} := W^\top X \cdot f(X)_{i_0}$*
- *Let $w(X)_{i_0,*} := W X_{*,i_0}$*

we have

$$E_1(X) = e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2}$$

$$E_2(X) = -e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot 2f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2}$$

$$E_3(X) = -e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_0} \cdot V_{*,j_0}^\top \cdot e_{j_2}$$

$$E_4(X) = e_{j_1}^\top \cdot z(X)_{i_0} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2}$$

$$E_5(X) = -e_{j_1}^\top \cdot z(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2}$$

$$E_6(X) = -e_{j_1}^\top \cdot z(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot V_{*,j_0}^\top \cdot e_{j_2}$$

$$\begin{aligned}
E_7(X) &= e_{j_1}^\top \cdot z(X)_{i_0} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
E_8(X) &= -e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
E_9(X) &= -e_{j_1}^\top \cdot W^\top \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot e_{j_2} \\
E_{10}(X) &= -e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
E_{11}(X) &= -e_{j_1}^\top \cdot W^\top \cdot X \cdot \mathrm{diag}(f(X)_{i_0}) \cdot h(X)_{j_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
E_{12}(X) &= e_{j_1}^\top \cdot W^\top \cdot X_{*,i_2} \cdot f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
E_{13}(X) &= e_{j_1}^\top \cdot W^\top f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot e_{j_2} \\
E_{14}(X) &= e_{j_1}^\top \cdot W^\top \cdot X_{*,i_2} \cdot f(X)_{i_0,i_2} \cdot V_{*,j_0}^\top \cdot e_{j_2} \\
E_{15}(X) &= -e_{j_1}^\top \cdot V_{*,j_0} \cdot f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2}
\end{aligned}$$

Proof. This lemma is followed by Lemma D.4 and linear algebra facts. □

Based on above auxiliary lemma, we have following definition.

Definition D.8. *Under following conditions*

- *Let* $z(X)_{i_0} := W^\top X \cdot f(X)_{i_0}$
- *Let* $w(X)_{i_0,*} := W X_{*,i_0}$

We present the **Case 2** *component of Hessian* $c(X)_{i_0,j_0}$ *to be*

$$H_2^{(i_0,i_2)}(X) := J(X)$$

where we have

$$\begin{aligned}
J(X) &:= \sum_{i=1}^{15} J_i(X) \\
J_1(X) &:= w(X)_{i_0,*} \cdot 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top \\
J_2(X) &:= -w(X)_{i_0,*} \cdot 2f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top \\
J_3(X) &:= -w(X)_{i_0,*} \cdot f(X)_{i_0,i_2} \cdot f(X)_{i_0,i_0} \cdot V_{*,j_0}^\top \\
J_4(X) &:= z(X)_{i_0} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,*}^\top \\
J_5(X) &:= -z(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w(X)_{i_0,*}^\top \\
J_6(X) &:= -z(X)_{i_0} \cdot f(X)_{i_0,i_2} \cdot V_{*,j_0}^\top \\
J_7(X) &:= z(X)_{i_0} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top \\
J_8(X) &:= -w(X)_{i_0,*} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,*}^\top \\
J_9(X) &:= -W^\top \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \\
J_{10}(X) &:= -w(X)_{i_0,*} \cdot f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_0} \cdot w(X)_{i_0,*}^\top \\
J_{11}(X) &:= -W^\top \cdot X \cdot \mathrm{diag}(f(X)_{i_0}) \cdot h(X)_{j_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,*}^\top \\
J_{12}(X) &:= W^\top \cdot X_{*,i_2} \cdot f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \cdot w(X)_{i_0,*}^\top \\
J_{13}(X) &:= W^\top f(X)_{i_0,i_2} \cdot h(X)_{j_0,i_2} \\
J_{14}(X) &:= W^\top \cdot X_{*,i_2} \cdot f(X)_{i_0,i_2} \cdot V_{*,j_0}^\top \\
J_{15}(X) &:= -V_{*,j_0} \cdot f(X)_{i_0,i_0} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,*}^\top
\end{aligned}$$

Next, we define the third case by the symmetricity of Hessian.

Definition D.9. *We present the* **Case 3** *component of Hessian* $c(X)_{i_0,j_0}$ *to be*

$$H_3^{(i,i_0)}(X) := H_2^{(i_0,i)}(X)$$

D.4 Decomposition Hessian : Part 4

Lemma D.10. *Under following conditions*

- *Let $F_i(X)$ be defined as Lemma C.9*
- *Let $z(X)_{i_0} := W^\top X \cdot f(X)_{i_0}$*
- *Let $w(X)_{i_0,*} := W X_{*,i_0}$*

we have

$$\begin{aligned}
F_1(X) &= e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1}^2 \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
F_2(X) &= -e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot f(X)_{i_0,i_1}^2 \cdot h(X)_{j_0,i_1} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
F_3(X) &= -e_{j_1}^\top \cdot (w(X)_{i_0,*} \cdot f(X)_{i_0,i_1}^2 \cdot V_{*,j_0}^\top + V_{*,j_0} \cdot f(X)_{i_0,i_1}^2 \cdot w(X)_{i_0,*}^\top) \cdot e_{j_2} \\
F_4(X) &= -e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
F_5(X) &= e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2} \\
F_6(X) &= e_{j_1}^\top \cdot (w(X)_{i_0,*} \cdot f(X)_{i_0,i_1} \cdot V_{*,j_0}^\top + V_{*,j_0} \cdot f(X)_{i_0,i_1} \cdot w(X)_{i_0,*}^\top) \cdot e_{j_2}
\end{aligned}$$

Proof. This lemma is followed by Lemma D.4 and linear algebra facts. □

Based on above auxiliary lemma, we have following definition.

Definition D.11. *Under following conditions*

- *Let $z(X)_{i_0} := W^\top X \cdot f(X)_{i_0}$*
- *Let $w(X)_{i_0,*} := W X_{*,i_0}$*

We present the **Case 4** *component of Hessian $c(X)_{i_0,j_0}$ to be*

$$H_4^{(i_1,i_1)}(X) := K(X)$$

where we have

$$\begin{aligned}
K(X) &:= \sum_{i=1}^{6} K_i(X) \\
K_1(X) &:= w(X)_{i_0,*} \cdot 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1}^2 \cdot w(X)_{i_0,*}^\top \\
K_2(X) &:= -w(X)_{i_0,*} \cdot f(X)_{i_0,i_1}^2 \cdot h(X)_{j_0,i_1} \cdot w(X)_{i_0,*}^\top \\
K_3(X) &:= -w(X)_{i_0,*} \cdot f(X)_{i_0,i_1}^2 \cdot V_{*,j_0}^\top - V_{*,j_0} \cdot f(X)_{i_0,i_1}^2 \cdot w(X)_{i_0,*}^\top \\
K_4(X) &:= -w(X)_{i_0,*} \cdot s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1} \cdot w(X)_{i_0,*}^\top \\
K_5(X) &:= w(X)_{i_0,*} \cdot f(X)_{i_0,i_1} \cdot h(X)_{j_0,i_1} \cdot w(X)_{i_0,*}^\top \\
K_6(X) &:= w(X)_{i_0,*} \cdot f(X)_{i_0,i_1} \cdot V_{*,j_0}^\top + V_{*,j_0} \cdot f(X)_{i_0,i_1} \cdot w(X)_{i_0,*}^\top
\end{aligned}$$

D.5 Decomposition Hessian : Part 5

Lemma D.12. *Under following conditions*

- *Let $G_i(X)$ be defined as Lemma C.9*
- *Let $z(X)_{i_0} := W^\top X \cdot f(X)_{i_0}$*
- *Let $w(X)_{i_0,*} := W X_{*,i_0}$*

we have

$$G_1(X) = e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,*}^\top \cdot e_{j_2}$$

$$G_2(X) = -e_{j_1}^\top \cdot w(X)_{i_0,*} \cdot f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot (h(X)_{j_0,i_2} + h(X)_{j_0,i_1}) \cdot w(X)_{i_0,*}^\top \cdot e_{j_2}$$
$$G_3(X) = -e_{j_1}^\top \cdot f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot (w(X)_{i_0,*} \cdot V_{*,j_0}^\top + V_{*,j_0} \cdot w(X)_{*,j_2}) \cdot e_{j_2}$$

Proof. This lemma is followed by Lemma D.4 and linear algebra facts. □

Based on above auxiliary lemma, we have following definition.

Definition D.13. *Under following conditions*

- *Let* $z(X)_{i_0} := W^\top X \cdot f(X)_{i_0}$
- *Let* $w(X)_{i_0,*} := WX_{*,i_0}$

We present the **Case 5** *component of Hessian* $c(X)_{i_0,j_0}$ *to be*

$$H_5^{(i_1,i_2)}(X) := N(X)$$

where we have

$$N(X) := \sum_{i=1}^{3} N_i(X)$$
$$N_1(X) := w(X)_{i_0,*} \cdot 2s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot w(X)_{i_0,*}^\top$$
$$N_2(X) := -w(X)_{i_0,*} \cdot f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot (h(X)_{j_0,i_2} + h(X)_{j_0,i_1}) \cdot w(X)_{i_0,*}^\top$$
$$N_3(X) := -f(X)_{i_0,i_1} \cdot f(X)_{i_0,i_2} \cdot (w(X)_{i_0,*} \cdot V_{*,j_0}^\top + V_{*,j_0} \cdot w(X)_{*,j_2}^\top)$$

E HESSIAN OF LOSS FUNCTION

In this section, we provide the Hessian of our loss function.

Lemma E.1 (A single entry)**.** *Under following conditions*

- *Let* $L(X)$ *be defined as Definition A.9*

we have

$$\frac{\mathrm{d}L(X)}{\mathrm{d}x_{i_1,j_1}x_{i_2,j_2}} = \sum_{i_0=1}^{n}\sum_{j_0=1}^{d} \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}} \cdot \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_2}} + c(X)_{i_0,j_0} \cdot \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}x_{i_2,j_2}}$$

Proof. **Proof of Part 1:** $i_1 = i_2$

$$\frac{\mathrm{d}L(X)}{\mathrm{d}x_{i_1,j_1}x_{i_2,j_2}} = \frac{\mathrm{d}}{\mathrm{d}x_{i_2,j_2}}(\sum_{i_0=1}^{n}\sum_{j_0=1}^{d} c(X)_{i_0,j_0} \cdot \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}})$$
$$= \sum_{i_0=1}^{n}\sum_{j_0=1}^{d} \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}} \cdot \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_2,j_2}} + c(X)_{i_0,j_0} \cdot \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}x_{i_2,j_2}}$$

where the first step is given by chain rule, and the 2nd step are given by product rule. □

Lemma E.2 (Matrix Representation of Hessian)**.** *Under following conditions*

- *Let* $c(X)_{i_0,j_0}$ *be defined as Definition A.8*
- *Let* $L(X)$ *be defined as Definition A.9*

we have

$$\nabla^2 L(X) = \sum_{i_0=1}^{n}\sum_{j_0=1}^{d} \nabla c(X)_{i_0,j_0} \cdot \nabla c(X)_{i_0,j_0}^\top + c(X)_{i_0,j_0} \cdot \nabla^2 c(X)_{i_0,j_0}$$

Proof. This is directly given by the single-entry representation in Lemma E.1. □

F BOUNDS FOR BASIC FUNCTIONS

In this section, we prove the upper bound for each function, with following assumption about the domain of parameters. In Section F.1 we bound the basic terms. In Section F.2 we bound the gradient of $f(X)_{i_0}$. In Section F.3 we bound the gradient of $c(X)_{i_0,j_0}$

Assumption F.1 (Bounded parameters, formal version of Assumption 4.1)**.** *Let W, V, X, B be defined as in Section A.2,*

- *Let R be some fixed constant satisfies $R > 1$*
- *We have $\|W\| \leq R$, $\|V\| \leq R$, $\|X\| \leq R$ where $\|\cdot\|$ is the matrix spectral norm*
- *We have $b_{i,j} \leq R^2$*

F.1 BOUNDS FOR BASIC FUNCTIONS

Lemma F.2. *Under Assumption F.1, for all $i_0 \in [n], j_0 \in [d]$, we have following bounds:*

- *Part 1*
$$\|f(X)_{i_0}\|_2 \leq 1$$
- *Part 2*
$$\|h(X)_{i_0}\|_2 \leq R^2$$
- *Part 3*
$$|c(X)_{i_0,j_0}| \leq 2R^2$$
- *Part 4*
$$\|x^\top W_{*,j_0}\|_2 \leq R^2$$
- *Part 5*
$$|w(X)_{i_0,j_0}| \leq R^2$$
- *Part 6*
$$|z(X)_{i_0,j_0}| \leq R^2$$
- *Part 7*
$$|s(X)_{i_0,j_0}| \leq R^2$$

Proof. **Proof of Part 1**

The proof is similar to Deng et al. (2023d), and hence is omitted here.

Proof of Part 2

$$\begin{aligned}
\|h(X)_{j_0}\|_2 &= \|X^\top V_{*,j_0}\|_2 \\
&\leq \|V\| \cdot \|X\| \\
&\leq R^2
\end{aligned}$$

where the first step is by Definition A.7, the 2nd step is by basic algebra, the 3rd follows by Assumption F.1.

Proof of Part 3

$$\begin{aligned}
|c(X)_{i_0,j_0}| &= |\langle f(X)_{i_0}, h(X)_{j_0}\rangle - b_{i_0,j_0}| \\
&\leq |\langle f(X)_{i_0}, h(X)_{j_0}\rangle| + |b_{i_0,j_0}|
\end{aligned}$$

$$\leq \|f(X)_{i_0}\|_2 \cdot \|h(X)_{j_0}\|_2 + |b_{i_0,j_0}|$$
$$\leq 2R^2$$

where the first step is by Definition A.8, the 2nd step uses triangle inequality, the 3rd step uses Cauchy-Schwartz inequality, the 4th step is by Assumption F.1 and **Part 2**.

Proof of Part 4

$$\|x^\top W_{*,j_0}\|_2 \leq \|x\| \cdot \|W\|$$
$$\leq R^2$$

where the first step is by basic algebra, the second is by Assumption F.1.

Proof of Part 5

$$\begin{aligned}|w(X)_{i_0,j_0}| &= |\langle W_{j_0,*}, X_{*,i_0}|\\ &\leq \|W_{j_0,*}\|_2 \cdot \|X_{*,i_0}\|_2\\ &\leq R^2\end{aligned}$$

where the first step is by the definition of $w(X)_{i_0,j_0}$, the 2nd step is Cauchy-Schwartz inequality, the 3rd step is by Assumption F.1.

Proof of Part 6

$$\begin{aligned}|z(X)_{i_0,j_0}| &= |\langle f(X)_{i_0}, X^\top W_{*,j_0}\rangle|\\ &\leq \|f(X)_{i_0}\|_2 \cdot \|X\| \cdot \|W_{*,j_0}\|\\ &\leq R^2\end{aligned}$$

where the first step is by the definition of $z(X)_{i_0,j_0}$, the 2nd step is Cauchy-Schwartz inequality, the 3rd step is by Assumption F.1.

Proof of Part 7

$$\begin{aligned}|s(X)_{i_0,j_0}| &= |\langle f(X)_{i_0}, h(X)_{j_0}\rangle|\\ &\leq \|f(X)_{i_0}\|_2 \cdot \|h(X)_{j_0}\|_2\\ &\leq R^2\end{aligned}$$

where the first step is by the definition of $s(X)_{i_0,j_0}$, the 2nd step is Cauchy-Schwartz inequality, the 3rd step is by **Part 1** and **Part 2**. □

F.2 Bounds for gradient of $f(X)_{i_0}$

Lemma F.3. *Under following conditions*

- *Let $f(X)_{i_0}$ be defined as Definition A.6*
- *Assumption F.1 holds*
- *We use $\nabla f(X)_{i_0}$ to define a matrix that its $(j_0, i_1 \cdot j_1)$-th entry is*

$$\frac{\mathrm{d}f(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}}$$

  i.e., its $(i_1 \cdot j_1)$-th column is

$$\frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}$$

Then we have:

- *Part 1: for all $i_0, i_1 \in [n], j_1 \in [d]$,*

$$\|\frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}\|_2 \leq 4R^2$$

- *Part 2:*

$$\|\nabla f(X)_{i_0}\|_F \leq 4\sqrt{nd}R^2$$

Proof. **Proof of Part 1**

$$\begin{aligned}|\frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}| = & |-f(X)_{i_0}\cdot(f(X)_{i_0,i_0}\cdot\langle W_{j_1,*},X_{*,i_0}\rangle+\langle f(X)_{i_0},X^\top W_{*,j_1}\rangle) \\ & +f(X)_{i_0}\circ(e_{i_0}\cdot\langle W_{j_1,*},X_{*,i_0}\rangle+X^\top W_{*,j_1})| \\ \leq & \|f(X)_{i_0}\|_2^2\cdot|\langle W_{j_1,*},X_{*,i_0}\rangle|+\|f(X)_{i_0}\|_2^2\cdot\|X^\top W_{*,j_1}\| \\ & +\|f(X)_{i_0}\|_2\cdot|\langle W_{j_1,*},X_{*,i_0}\rangle|+\|f(X)_{i_0}\|_2\cdot\|X^\top W_{*,j_1})\|_2 \\ \leq & 4R^2\end{aligned}$$

where the 1st step is by Lemma A.14, the 2nd step is by Fact A.1, the 3rd step is by Lemma F.2.

Proof of Part 2

$$\begin{aligned}\|\nabla f(X)_{i_0}\|_F = & (\sum_{i_1=1}^n\sum_{j_1=1}^d\|\frac{\mathrm{d}f(X)_{i_0}}{\mathrm{d}x_{i_1,j_1}}\|_2^2)^{\frac{1}{2}} \\ \leq & (\sum_{i_1=1}^n\sum_{j_1=1}^d 16R^4)^{\frac{1}{2}} \\ = & 4\sqrt{nd}R^2\end{aligned}$$

where the first step is by the definition of $\nabla f(X)_{i_0}$, the 2nd step is by **Part 1**. □

F.3 BOUNDS FOR GRADIENT OF $c(X)_{i_0,j_0}$

Lemma F.4. *Under following conditions*

- *Let $c(X)_{i_0,j_0}$ be defined as Definition A.8*
- *Assumption F.1 holds*
- *We use $\nabla c(X)_{i_0,j_0}$ to denote the Hessian of $c(X)_{i_0,j_0}$ w.r.t. $\mathrm{vec}(X)$*

Then we have:

- *Part 1: for all $i_0, i_1 \in [n], j_1 \in [d]$,*

$$|\frac{c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}}|_2 \leq 5R^4$$

- *Part 2:*

$$\|\nabla c(X)_{i_0,j_0}\|_2 \leq 5\sqrt{nd}R^4$$

Proof. **Proof of part 1**

$$\begin{aligned}|\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}}| = & |C_1(X)+C_2(X)+C_3(X)+C_4(X)+C_5(X)| \\ \leq & |C_1(X)|+|C_2(X)|+|C_3(X)|+|C_4(X)|+|C_5(X)| \\ \leq & \|f(X)_{i_0}\|_2^2\cdot\|h(X)_{j_0}\|_2\cdot|w(X)_{i_0,j_0}|+\|f(X)_{i_0}\|_2\cdot\|h(X)_{j_0}\|_2\cdot|z(X)_{i_0,j_1}| \\ & +\|f(X)_{i_0}\|_2\cdot\|h(X)_{j_0}\|_2\cdot|w(X)_{i_0,j_0}| \\ & +\|f(X)_{i_0}\|_2\cdot\|X\|\cdot\|W_{*,j_1}\|_2\cdot\|h(X)_{j_0}\|_2+\|f(X)_{i_0}\|_2\cdot\|V\| \\ \leq & R^4+R^4+R^4+R^4+R^2 \\ \leq & 5R^4\end{aligned}$$

where the first step is by Lemma A.16, the 2nd step is by triangle inequality, the 3rd step is by Fact A.1, the 4th step is by Lemma F.2, the 5th step holds by $R > 1$.

Proof of Part 2

$$\begin{aligned}\|\nabla c(X)_{i_0,j_0}\|_2 &= (\sum_{i_1=1}^{n}\sum_{j_1=1}^{d}\|\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}}\|_2^2)^{\frac{1}{2}} \\ &\leq (\sum_{i_1=1}^{n}\sum_{j_1=1}^{d} 25R^8)^{\frac{1}{2}} \\ &= 5\sqrt{nd}R^4\end{aligned}$$

where the first step is by the definition of $\nabla f(X)_{i_0}$, the 2nd step is by **Part 1**.

□

F.4 Bounds for Hessian of $c(X)_{i_0,j_0}$

Lemma F.5. *Under following conditions*

- *Let $c(X)_{i_0,j_0}$ be defined as Definition A.8*
- *Assumption F.1 (Bounded parameter) holds*
- *Let $B_i(X)$ be defined as in Definition D.6*

we have

- *Part 1: For all $i_0 = i_1 = i_2 \in [n]$, we have*
$$\|H_1(X)^{(i_0,i_0)}\| \leq 23R^6 + R^5 + 12R^3$$
- *Part 2: For all $i_0 = i_1 \neq i_2 \in [n]$, we have*
$$\|H_2(X)^{(i_0,i_2)}\| \leq 11R^6 + 6R^3$$
- *Part 3: For all $i_0 = i_2 \neq i_1 \in [n]$, we have*
$$\|H_3(X)^{(i_1,i_0)}\| \leq 11R^6 + 6R^3$$
- *Part 4: For all $i_0 \neq i_1 = i_2 \in [n]$, we have*
$$\|H_4(X)^{(i_1,i_1)}\| \leq 5R^6 + 4R^3$$
- *Part 5: For all $i_0 \neq i_1, i_0 \neq i_2, i_1 \neq i_2 \in [n]$, we have*
$$\|H_5(X)^{(i_1,i_2)}\| \leq 4R^6 + 2R^3$$

Proof. The proof is similar to Lemma F.4 and hence omit. □

G Lipschitz of Hessian

In Section G.1 we provide tools and facts. In Sections G.2, G.3, G.4, G.7, G.6, G.7 and G.8 we provide proof of lipschitz property of several important terms. And finally in Section G.9 we provide the proof for Lipschitz property of gradient of $L(X)$. In Section G.10 we provide proof for Lipschitz property of Hessian of $L(X)$.

G.1 FACTS AND TOOLS

In this section, we introduce 2 tools for effectively calculate the Lipschitz for Hessian.

Fact G.1 (Mean value theorem for vector function, Fact 34 in Deng et al. (2023d)). *Under following conditions,*

- *Let $x, y \in C \subset \mathbb{R}^n$ where C is an open convex domain*
- *Let $g(x) : C \to \mathbb{R}^n$ be a differentiable vector function on C*
- *Let $\|g'(a)\|_F \leq M$ for all $a \in C$, where $g'(a)$ denotes a matrix which its (i, j)-th term is $\frac{\mathrm{d}g(a)_j}{\mathrm{d}a_i}$*

then we have

$$\|g(y) - g(x)\|_2 \leq M\|y - x\|_2$$

Fact G.2 (Lipschitz for product of functions). *Under following conditions*

- *Let $\{f_i(x)\}_{i=1}^n$ be a sequence of function with same domain and range*
- *For each $i \in [n]$ we have*
  - *$f_i(x)$ is bounded: $\forall x, \|f_i(x)\| \leq M_i$ with $M_i \geq 1$*
  - *$f_i(x)$ is Lipschitz continuous: $\forall x, y, \|f_i(x) - f_i(y)\| \leq L_i\|x - y\|$*

Then we have

$$\|\prod_{i=1}^n f_i(x) - \prod_{i=1}^n f_i(y)\| \leq 2^{n-1} \cdot \max_{i \in [n]}\{L_i\} \cdot (\prod_{i=1}^n M_i) \cdot \|x - y\|$$

Proof. We prove it by mathematical induction. The case that $i = 1$ obviously.

Now assume the case holds for $i = k$. Consider $i = k + 1$, we have.

$$\begin{aligned}
&\|\prod_{i=1}^{k+1} f_i(x) - \prod_{i=1}^{k+1} f_i(y)\| \\
\leq &\|\prod_{i=1}^{k+1} f_i(x) - f_{k+1}(x) \cdot \prod_{i=1}^{k} f_i(y)\| + \|f_{k+1}(x) \cdot \prod_{i=1}^{k} f_i(y) - \prod_{i=1}^{k+1} f_i(y)\| \\
\leq &\|f_{k+1}(x)\| \cdot \|\prod_{i=1}^{k} f_i(x) - \prod_{i=1}^{k} f_i(y)\| + \|f_{k+1}(x) - f_{k+1}(y)\| \cdot \|\prod_{i=1}^{k} f_i(y) - \prod_{i=1}^{k} f_i(y)\| \\
\leq &M_{k+1} \cdot \|\prod_{i=1}^{k} f_i(x) - \prod_{i=1}^{k} f_i(y)\| + (\prod_{i=1}^{k} M_i) \cdot \|f_{k+1}(x) - f_{k+1}(y)\| \\
\leq &2^{k-1}(\prod_{i=1}^{k+1} M_i) \cdot \max_{i \in [k]}\{L_i\}\|x - y\| + (\prod_{i=1}^{k} M_i) \cdot \|f_{k+1}(x) - f_{k+1}(y)\| \\
\leq &2^{k-1}(\prod_{i=1}^{k+1} M_i) \cdot \max_{i \in [k]}\{L_i\}\|x - y\| + (\prod_{i=1}^{k} M_i) \cdot L_{k+1}\|x - y\| \\
\leq &2^{k-1}(\prod_{i=1}^{k+1} M_i) \cdot \max_{i \in [k]}\{L_i\}\|x - y\| + (\prod_{i=1}^{k+1} M_i) \cdot L_{k+1}\|x - y\| \\
\leq &2^{k}(\prod_{i=1}^{k+1} M_i) \cdot \max_{i \in [k+1]}\{L_i\}\|x - y\|
\end{aligned}$$

where the first step is by triangle inequality, the 2nd step is by property of norm, the 3rd step is by upper bound of functions, the 4th step is by induction hypothesis, the 5th step is by Lipschitz of $f_{k+1}(x)$, the 6th step is by $M_{k+1} \geq 1$, the 7th step is a rearrangement.

Since the claim holds for $i = k+1$, we prove the desired result. $\square$

G.2 LIPSCHITZ FOR $f(X)_{i_0}$

Definition G.3 (Notation of norm). *For writing efficiency, we use* $\|X - Y\|$ *to denote* $\|\mathrm{vec}(X) - \mathrm{vec}(Y)\|_2$, *which is equivalent to* $\|X - Y\|_F$.

Lemma G.4. *Under following conditions*

- *Assumption F.1 holds*
- *Let* $f(X)_{i_0}$ *be defined as Definition A.6*

For $X, Y \in \mathbb{R}^{d \times n}$, *we have*

$$\|f(X)_{i_0} - f(Y)_{i_0}\|_2 \leq 4\sqrt{nd}R^2 \cdot \|X - Y\|$$

Proof.

$$\begin{aligned}\|f(X)_{i_0} - f(Y)_{i_0}\|_2 &\leq \|\nabla f(X)_{i_0}\|_F \cdot \|X - Y\| \\ &\leq 4\sqrt{nd}R^2 \cdot \|X - Y\|\end{aligned}$$

where the first step is given by Mean Value Theorem (Lemma G.1) and the 2nd step is due to upper bound for gradient of $f(X)_{i_0}$ (Lemma F.3). $\square$

G.3 LIPSCHITZ FOR $c(X)_{i_0,j_0}$

Lemma G.5. *Under following conditions*

- *Assumption F.1 holds*
- *Let* $c(X)_{i_0,j_0}$ *be defined as Definition A.8*

For $X, Y \in \mathbb{R}^{d \times n}$, *we have*

$$|c(X)_{i_0,j_0} - c(Y)_{i_0,j_0}| \leq 5\sqrt{nd}R^4 \cdot \|X - Y\|$$

Proof.

$$\begin{aligned}|c(X)_{i_0,j_0} - c(Y)_{i_0,j_0}| &\leq \|\nabla c(X)_{i_0,j_0}\|_2 \cdot \|X - Y\| \\ &\leq 5\sqrt{nd}R^4 \cdot \|X - Y\|\end{aligned}$$

where the first step is given by Mean Value Theorem (Lemma G.1) and the 2nd step is due to upper bound for gradient of $c(X)_{i_0,j_0}$ (Lemma F.4). $\square$

G.4 LIPSCHITZ FOR $h(X)_{j_0}$

Lemma G.6. *Under following conditions*

- *Assumption F.1 holds*
- *Let* $h(X)_{j_0}$ *be defined as Definition A.7*

For $X, Y \in \mathbb{R}^{d \times n}$, *we have*

$$\|h(X)_{j_0} - h(Y)_{j_0}\|_2 \leq R\|X - Y\|$$

Proof.

$$\begin{aligned}\|h(X)_{j_0} - h(Y)_{j_0}\| &= \|V_{*,j_0}\|_2 \cdot \|X - Y\| \\ &\leq R \cdot \|X - Y\|\end{aligned}$$

where the first step is from the definition of $h(X)_{j_0}$ (see Definition A.7), the 2nd step is by Assumption F.1. □

G.5 LIPSCHITZ FOR $w(X)_{i_0,j_0}$

Lemma G.7. *Under following conditions*

- *Assumption F.1 holds*

For $X, Y \in \mathbb{R}^{d\times n}$, we have

$$|w(X)_{i_0,j_0} - w(Y)_{i_0,j_0}| \leq R\|X - Y\|$$

Proof.

$$\begin{aligned}|w(X)_{i_0,j_0} - w(Y)_{i_0,j_0}| &= |\langle W_{j_0,*}, X_{*,i_0} - Y_{*,i_0}\rangle| \\ &\leq \|W_{j_0,*}\|_2 \cdot \|X - Y\| \\ &\leq R \cdot \|X - Y\|\end{aligned}$$

where the first step is from the definition of $w(X)_{i_0,j_0}$, the 2nd step is by Fact A.1, the 3rd step holds since Assumption F.1. □

G.6 LIPSCHITZ FOR $z(X)_{i_0,j_0}$

Lemma G.8. *Under following conditions*

- *Assumption F.1 holds*

For $X, Y \in \mathbb{R}^{d\times n}$, we have

$$|z(X)_{i_0,j_0} - z(Y)_{i_0,j_0}| \leq 5\sqrt{nd}R^4 \cdot \|X - Y\|$$

Proof.

$$\begin{aligned}|z(X)_{i_0,j_0} - z(Y)_{i_0,j_0}| &= |\langle f(X)_{i_0}, X^\top W_{*,j_0}\rangle - \langle f(Y)_{i_0}, Y^\top W_{*,j_0}\rangle| \\ &\leq |\langle f(X)_{i_0}, X^\top W_{*,j_0}\rangle - \langle f(X)_{i_0}, Y^\top W_{*,j_0}\rangle| \\ &\quad + |\langle f(X)_{i_0}, Y^\top W_{*,j_0}\rangle - \langle f(Y)_{i_0}, Y^\top W_{*,j_0}\rangle| \\ &\leq \|f(X)_{i_0}\|_2 \cdot \|X - Y\| \cdot \|W_{*,j_0}\|_2 + \|f(X)_{i_0} - f(Y)_{i_0}\| \cdot \|Y\| \cdot \|W_{*,j_0}\| \\ &\leq R \cdot \|X - Y\| + R^2\|f(X)_{i_0} - f(Y)_{i_0}\| \\ &\leq 5\sqrt{nd}R^4 \cdot \|X - Y\|\end{aligned}$$

where the first step is from the definition of $w(X)_{i_0,j_0}$, the 2nd step is by Fact A.1, the 3rd step holds since Assumption F.1, the 4th step uses Lemma G.4. □

G.7 LIPSCHITZ FOR FIRST ORDER DERIVATIVE OF $c(X)_{i_0,j_0}$

Lemma G.9. *Under following conditions*

- *Assumption F.1 holds*
- *Let $c(X)_{i_0,j_0}$ be defined as Definition A.8*

For $X, Y \in \mathbb{R}^{d\times n}$, we have

$$|\frac{c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}} - \frac{c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_1,j_1}}| \leq O(\sqrt{nd}R^6) \cdot \|X - Y\|$$

Proof. Recall $C_i(X)$ defined in Lemma A.16. The Lipschitz constant of $\frac{c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}}$ is bounded the summation of that of $C_i(X)$. We only present the proof for Lipschitz for $C_1(X)$ here.

Notice that

$$C_1(X) := -s(X)_{i_0,j_0} \cdot f(X)_{i_0,i_0} \cdot w(X)_{i_0,j_1}$$

By upper bound and lipschitz constant for basic functions, we have

- $|s(X)_{i_0,j_0}| \leq R^2$
- $|f(X)_{i_0,i_0}| \leq 1$
- $|w(X)_{i_0,j_1}| \leq R^2$
- $\max_{f \in \{s(X)_{i_0,j_0}, f(X)_{i_0,i_0}, w(X)_{i_0,j_1}\}} \{\mathrm{Lipschitz}(f)\} = 4\sqrt{nd}R^2$
- $n = 3$

By Fact G.2.

$$\begin{aligned} |C_1(X) - C_1(Y)| &\leq 2^{n-1} \cdot \max_{i \in [n]} \{L_i\} \cdot (\prod_{i=1}^{n} M_i) \cdot \|X - Y\| \\ &= 4 \cdot 4\sqrt{nd}R^2 \cdot R^4 \cdot \|X - Y\| \\ &= 16\sqrt{nd}R^6 \cdot \|X - Y\| \end{aligned}$$

□

G.8 Lipschitz for second order derivative of $c(X)_{i_0,j_0}$

Lemma G.10. *Under following conditions*

- *Assumption F.1 holds*
- *Let $c(X)_{i_0,j_0}$ be defined as Definition A.8*

For $X, Y \in \mathbb{R}^{d \times n}$, we have

$$|\frac{c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1} x_{i_2,j_2}} - \frac{c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_1,j_1} y_{i_2,j_2}}| \leq O(\sqrt{nd}R^8) \cdot \|X - Y\|$$

Proof. The proof is similar to Lemma G.9 and hence omit. Notice that the upper bound for $\frac{c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1} x_{i_2,j_2}}$ is given by Lemma F.5. □

G.9 Lipschitz for gradient of $L(X)$

Lemma G.11. *Under following conditions*

- *Assumption F.1 holds*
- *Let $c(X)_{i_0,j_0}$ be defined as Definition A.8*

For $X, Y \in \mathbb{R}^{d \times n}$, we have

$$\|\nabla^2 L(X) - \nabla^2 L(Y)\| \leq O(n^{1.5} d^{1.5} R^{10}) \cdot \|X - Y\|$$

Proof. We have calculated the gradient of $L(X)$ in Lemma A.17:

$$\frac{\mathrm{d}L(X)}{\mathrm{d}x_{i_1,j_1}} = \sum_{i_0=1}^{n} \sum_{j_0=1}^{d} c(X)_{i_0,j_0} \cdot \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}}$$

We can use the proof in Lemma G.9 to generate a Lipschitz bound for he gradient of $L(X)$. Notice that the Lipschitz of $c(X)_{i_0,j_0}$ is given in Lemma G.5 and the Lipschitz of $\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}}$ is given in Lemma G.9. □

G.10 LIPSCHITZ FOR HESSIAN OF $L(X)$

Lemma G.12. *Under following conditions*

- *Assumption F.1 holds*
- *Let $c(X)_{i_0,j_0}$ be defined as Definition A.8*

For $X, Y \in \mathbb{R}^{d\times n}$, we have

$$\|\nabla^2 L(X) - \nabla^2 L(Y)\| \le O(n^{3.5}d^{3.5}R^{10}) \cdot \|X - Y\|$$

Proof. Recall that

$$\begin{aligned}
\frac{\mathrm{d}L(X)}{\mathrm{d}x_{i_1,j_1}x_{i_2,j_2}} &= \sum_{i_0=1}^{n}\sum_{j_0=1}^{d} \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}} \cdot \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_2,j_2}} + c(X)_{i_0,j_0} \cdot \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}x_{i_2,j_2}} \\
&= \sum_{i_0=1}^{n}\sum_{j_0=1}^{d} U_1(X) + U_2(X)
\end{aligned}$$

For the first item $U_1(X)$, we have

$$\begin{aligned}
|U_1(X) - U_1(Y)| &= |\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}} \cdot \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_2}} - \frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}} \cdot \frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_1,j_2}}| \\
&\le |\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}}| \cdot |\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_2}} - \frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_2,j_2}}| \\
&\quad + |\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}} \cdot - \frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_1,j_1}}| \cdot |\frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_2,j_2}}| \\
&\le 10R^4 \cdot |\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}} \cdot - \frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_1,j_1}}| \\
&\le O(\sqrt{nd}R^{10}) \cdot \|X - Y\|
\end{aligned}$$

where the 2nd step is by triangle inequality, the 3rd step is by Lemma F.4, the 4th step uses Lemma G.9.

For the 2nd item $U_2(X)$, we have

$$\begin{aligned}
|U_2(X) - U_2(Y)| &= |c(X)_{i_0,j_0} \cdot \frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}x_{i_2,j_2}} - c(Y)_{i_0,j_0} \cdot \frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_1,j_1}y_{i_2,j_2}}| \\
&\le |c(X)_{i_0,j_0}| \cdot |\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}x_{i_2,j_2}} - \frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_1,j_1}y_{i_2,j_2}}| \\
&\quad + |c(X)_{i_0,j_0} - c(Y)_{i_0,j_0}| \cdot |\frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_1,j_1}y_{i_2,j_2}}| \\
&\le 2R^2 \cdot |\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}x_{i_2,j_2}} - \frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_1,j_1}y_{i_2,j_2}}| \\
&\quad + |c(X)_{i_0,j_0} - c(Y)_{i_0,j_0}| \cdot |\frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_1,j_1}y_{i_2,j_2}}| \\
&\le 2R^2 \cdot |\frac{\mathrm{d}c(X)_{i_0,j_0}}{\mathrm{d}x_{i_1,j_1}x_{i_2,j_2}} - \frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_1,j_1}y_{i_2,j_2}}| + 5\sqrt{nd}R^4 \cdot \|X - Y\| \cdot |\frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_1,j_1}y_{i_2,j_2}}| \\
&\le O(\sqrt{nd}R^{10}) \cdot \|X - Y\| + 5\sqrt{nd}R^4 \cdot \|X - Y\| \cdot |\frac{\mathrm{d}c(Y)_{i_0,j_0}}{\mathrm{d}y_{i_1,j_1}y_{i_2,j_2}}|
\end{aligned}$$

$$\leq O(\sqrt{nd}R^{10}) \cdot \|X - Y\|$$

where the 2nd step is by triangle inequality, the 3rd step uses Lemma F.2, the 4th step uses Lemma G.5, the 5th step uses Lemma G.10, the last step uses Lemma F.5.

Combining the above 2 items, we have

$$|\frac{\mathrm{d}L(X)}{\mathrm{d}x_{i_1,j_1}x_{i_2,j_2}} - \frac{\mathrm{d}L(Y)}{\mathrm{d}y_{i_1,j_1}y_{i_2,j_2}}| \leq O(n^{1.5}d^{1.5}R^{10}) \cdot \|X - Y\|$$

Then, we have

$$\begin{aligned}
\|\nabla^2 L(X) - \nabla^2 L(Y)\| &\leq \|\nabla^2 L(X) - \nabla^2 L(Y)\|_F \\
&\leq n^2 d^2 \cdot O(n^{1.5}d^{1.5}R^{10}\|X - Y\| \\
&= O(n^{3.5}d^{3.5}R^{10}) \cdot \|X - Y\|
\end{aligned}$$

where the 1st step is by matrix calculus, the 2nd is by the lipschitz for each entry of $\nabla^2 L(X)$. □

H STRONGLY CONVEXITY

In this section, we provide proof for PSD bounds for the Hessian of Loss function.

H.1 PSD BOUNDS FOR HESSIAN OF $c(X)_{i_0,j_0}$

Lemma H.1 (PSD bounds for $\nabla^2 c(X)_{i_0,j_0}$)**.** *Under following conditions,*

- *Let c_{i_0,j_0} be defined as in Definition A.8*
- *Let Assumption F.1 be satisfied*

For all $i_0 \in [n], j_0 \in [d]$, we have

$$-36R^6 \cdot \mathbf{I}_{nd} \preceq \nabla^2 c(X)_{i_0,j_0} \preceq 36R^6 \cdot \mathbf{I}_{nd}$$

Proof. We prove this statement by the definition of PSD. Let $p \in \mathbb{R}^{n\times d}$ be a vector. Let $i \in [n]$, we use $p_i \in \mathbb{R}^d$ to denote the vector formed by the $(i-1)\cdot n + 1$-th term to the $i \cdot n$-th term of vector p.

Then, we have

$$\begin{aligned}
|p^\top \nabla^2 c(X)_{i_0,j_0} p| = |p_{i_0}^\top H_1(X)^{i_0,i_0} p_{i_0} &+ \sum_{i\in[n]\backslash\{i_0\}} p_{i_0}^\top H_2(X)^{(i_0,i)} p_i \\
&+ \sum_{i\in[n]\backslash\{i_0\}} p_i^\top H_3(X)^{(i,i_0)} p_{i_0} + \sum_{i\in[n]\backslash\{i_0\}} p_i^\top H_4(X)^{(i,i)} p_i \\
&+ \sum_{i_1\in[n]\backslash\{i_0\}} \sum_{i_2\in[n]\backslash\{i_0\}} p_{i_1}^\top H_5(X)^{(i_1,i_2)} p_{i_2}| \\
\leq \max_{i\in[5]} \|H_i(X)\| \cdot \sum_{i_1\in[n]} \sum_{i_2\in[n]} p_{i_1}^\top p_{i_2} \\
\leq \max_{i\in[5]} \|H_i(X)\| \cdot p^\top p \\
\leq 36R^6 \cdot p^\top p
\end{aligned}$$

where the 1st step is by the formulation of $\nabla^2 c(X)_{i_0,j_0}$ (see Definition D.3), the 2nd and 3rd steps are from simple algebra, the 4th step uses Lemma F.5. □

H.2 PSD BOUNDS FOR HESSIAN OF LOSS

Lemma H.2 (PSD bound for $\nabla^2 L(X)$)**.** *Under following conditions,*

- *Let $L(X)$ be defined as in Definition A.9*
- *Let Assumption F.1 be satisfied*

we have

$$\nabla^2 L(X) \succeq -O(ndR^8) \cdot \mathbf{I}_{nd}$$

Proof. Recall in Lemma E.2, we have

$$\nabla^2 L(X) = \sum_{i_0=1}^{n} \sum_{j_0=1}^{d} \nabla c(X)_{i_0,j_0} \cdot \nabla c(X)_{i_0,j_0}^\top + c(X)_{i_0,j_0} \cdot \nabla^2 c(X)_{i_0,j_0} \quad (2)$$

Notice that the first term is PSD, so we omit it.

By Lemma F.2, we have

$$|c(X)_{i_0,j_0}| \le 2R^2$$

Therefore, we have

$$\nabla^2 c(X)_{i_0,j_0} \succeq -72R^8 \cdot \mathbf{I}_{nd}$$
$$i.e., \nabla^2 L(X) \succeq -72ndR^8 \cdot \mathbf{I}_{nd}$$

where the first line is by Lemma H.1 and the 2nd line is given by Eq. (2).

□

I Convergence Analysis

In this section, we give the convergence analysis of the gradient-based (see Section I.1 and Hessian-based method (see Section I.2) to conduct inverse attack. We utilize the Lipschitz and strongly-convexity properties proved in previous sections.

I.1 Gradient Method

We first state a canonical result for the convergence gradient-descent method under Lipschitz smoothness and strongly-convexity.

Theorem I.1 (Gradient descent). *Let the following conditions hold*

- *Let $f(x)$ be a convex and twice-differentiable function on $\mathbb{R}^n$*
- *Let $\nabla f(x)$ have Lipschitz constant L:*

$$\|\nabla f(x) - \nabla f(y)\|_2 \le L\|x - y\|_2 \quad \forall x, y \in \mathbb{R}^n$$

- *Let $f(x)$ be strongly convex with factor m:*

$$\nabla^2 f(x) \succeq m\mathbf{I}_n$$

- *$f(x)$ reaches its minimum (denoted as f^*) at some point x^**

Then, the gradient-descent algorithm with fixed step size $t < \frac{2}{m+L}$ satisfies

$$\|x_k - x^*\|_2 < (1 - \frac{m}{L})^{k/2} \cdot \|x_0 - x^*\|_2^2$$

where x_k is the update in k-th iteration.

In particular, it takes $O(\frac{L}{m} \cdot \log(|x_0 - x^*|_2/\epsilon))$ to find a ϵ-optimal solution.

Now, we use the above theorem to show the convergence of our regression problem.

Theorem I.2 (Formal version of Theorem 4.3)**.** *We assume our model satisfies the following conditions*

- *Bounded parameters: there exists $R > 1$ such that*
  - $\|W\|_F \leq R$, $\|V\|_F \leq R$
  - $\|X\|_F \leq R$
  - $\forall i \in [n], j \in [d], |b_{i,j}| \leq R$ *where $b_{i,j}$ denotes the i, j-th entry of B*
- *Regularization: we consider the following problem:*

$$\min_{X \in \mathbb{R}^{n \times d}} \|D(X)^{-1} \exp(X^\top W X) X^\top V - B\|_F^2 + \gamma \cdot \|\operatorname{vec}(X)\|_2^2$$

Then, for any accuracy parameter $\epsilon \in (0, 0.1)$, a gradient-descent algorithm can be employed to recover the initial data. The algorithm uses

$$T = O(\operatorname{poly}(n, d, R) \cdot \log(|X_0 - X^*|_F/\epsilon))$$

iterations, it outputs a matrix $\widetilde{X} \in \mathbb{R}^{d \times n}$ satisfying

$$\|\widetilde{X} - X^*\|_F \leq \epsilon$$

The execution time for each iteration is $\operatorname{poly}(n, d)$.

Proof. Choosing $\gamma \geq O(ndR^8)$, by Lemma H.2, we have our regression problem being strongly convex with factor $O(ndR^8)$. Notice that, we proved in Lemma G.11 that the gradient of our loss function is $O(n^{1.5}d^{1.5}R^{10})$-Lipschitz continuous. Applying Theorem I.1 with $L = O(n^{1.5}d^{1.5}R^{10})$ and $m = O(ndR^8)$, we have the result in this theorem.

The execution time for each iteration is the matrix-multiplication time. □

I.2 Hessian Method

Theorem I.3 (Formal version of Theorem 4.4, Main Result)**.** *We assume our model satisfies the following conditions*

- *Bounded parameters: there exists $R > 1$ such that*
  - $\|W\|_F \leq R$, $\|V\|_F \leq R$
  - $\|X\|_F \leq R$
  - $\forall i \in [n], j \in [d], |b_{i,j}| \leq R$ *where $b_{i,j}$ denotes the i, j-th entry of B*
- *Regularization: we consider the following problem:*

$$\min_{X \in \mathbb{R}^{n \times d}} \|D(X)^{-1} \exp(X^\top W X) X^\top V - B\|_F^2 + \gamma \cdot \|\operatorname{vec}(X)\|_2^2$$

- *Good initial point: We choose an initial point X_0 such that*

$$M \cdot \|X_0 - X^*\|_F \leq O(ndR^8),$$

  where $M = O(n^3 d^3 R^{10})$.

Then, for any accuracy parameter $\epsilon \in (0, 0.1)$ and any failure probability $\delta \in (0, 0.1)$, an algorithm based on the Newton method can be employed to recover the initial data. The result of this algorithm guarantee within

$$T = O(\log(|X_0 - X^*|_F/\epsilon))$$

iterations, it outputs a matrix $\widetilde{X} \in \mathbb{R}^{d \times n}$ satisfying

$$\|\widetilde{X} - X^*\|_F \leq \epsilon$$

with a probability of at least $1 - \delta$. The execution time for each iteration is $\operatorname{poly}(n, d, \log(1/\delta))$.

Proof. Choosing $\gamma \geq O(ndR^8)$, by Lemma H.2, we have the PD property of Hessian.

By Lemma G.12, we have the Lipschitz property of Hessian.

Since M is bounded (in the condition of Theorem), then by iterative shrinking lemma (see Lemma 6.9 in Li et al. (2023c) as an example), we prove the convergence. □

J SUPPLEMENTARY EXPERIMENTAL DETAILS

Here, we give the experimental details for our experiment as follows.

- Learning rate for fine-tuning: $\eta = 0.0001$ (for best effort).
- Learning rate for attack: $\eta = 0.001$ (default).
- Adam hyper-parameter $\beta_1 = 0.9$ (default).
- Adam hyper-parameter $\beta_2 = 0.999$ (default).
- Adam hyper-parameter $\epsilon = 1 \times 10^{-8}$ (default).
- Fine-tuning steps: 8000.
- Platform: PyTorch Paszke et al. (2019) and Huggingface Wolf et al. (2019).
- GPU device information: 1 RTX 4090 GPUs.
- Number of fine-tuning epochs 30.
- Batch size: 32 (for best effort).
- Quantization: fp16.