A Unified Scheme of ResNet and Softmax

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Abstract

Large language models (LLMs) have brought significant changes to human society. Softmax regression and residual neural networks (ResNet) are two important techniques in deep learning: they not only serve as significant theoretical components supporting the functionality of LLMs but also are related to many other machine learning and theoretical computer science fields, including but not limited to image classification, object detection, semantic segmentation, and tensors.

Previous research works studied these two concepts separately. In this paper, we provide a theoretical analysis of the regression problem:

$$\|\langle \exp(Ax) + Ax, \mathbf{1}_n \rangle^{-1} (\exp(Ax) + Ax) - b\|_2^2$$

where A is a matrix in $\mathbb{R}^{n \times d}$, b is a vector in \mathbb{R}^n , and $\mathbf{1}_n$ is the n-dimensional vector whose entries are all 1. This regression problem is a unified scheme that combines softmax regression and ResNet, which has never been done before. We derive the gradient, Hessian, and Lipschitz properties of the loss function. The Hessian is shown to be positive semidefinite, and its structure is characterized as the sum of a low-rank matrix and a diagonal matrix. This enables an efficient approximate Newton method.

As a result, this unified scheme helps to connect two previously thought unrelated fields and provides novel insight into loss landscape and optimization for emerging over-parameterized neural networks, which is meaningful for future research in deep learning models.

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1 Introduction

Softmax regression and residual neural networks (ResNet) are two emerging techniques in deep learning that have driven advances in computer vision and natural language processing tasks. In previous research, these two methods were studied separately.

Definition 1.1 (Softmax regression, [DLS23]). Given a matrix $A \in \mathbb{R}^{n \times d}$ and a vector $b \in \mathbb{R}^n$, the goal of the softmax regression is to compute the following problem:

$$\min_{x \in \mathbb{R}^d} \|\langle \exp(Ax), \mathbf{1}_n \rangle^{-1} \exp(Ax) - b\|_2^2,$$

where $\mathbf{1}_n$ denotes the n-dimensional vector whose entries are all 1.

Because of the explosive development of large language models (LLMs), there is an increasing amount of work focusing on the theoretical aspect of LLMs, aiming to improve the ability of LLMs from different aspects, including sentiment analysis [UAS+20], natural language translation [HWL21], creative writing [Ope22, Ope23], and language modeling [MMS+19]. One of the most important components of an LLM is its ability to identify and focus on the relevant information from the input text. Theoretical works [GSY23a, LSZ19, DLS23, BSZ23, GSY23b, GMS23, AS23, ZHDK23] analyze the attention computation to support this ability.

Definition 1.2 (Attention computation). Let Q, K, and V be $n \times d$ matrices whose entries are all real numbers.

Let $A = \exp(QK^{\top})$ and $D = \operatorname{diag}(A\mathbf{1}_n)$ be n-dimensional square matrices, where $\operatorname{diag}(A\mathbf{1}_n)$ is a diagonal matrix whose entries on the i-th row and i-th column is the same as the i-th entry of the vector $A\mathbf{1}_n$.

The static attention computation is defined as

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

In attention computation, the matrix Q is denoted as the query tokens, which are derived from the previous hidden state of decoders. K and V represent the key tokens and values. When computing A, the softmax function is applied to get the attention weight, namely $A_{i,j}$. Inspired by the role of the exponential functions in attention computation, prior research [GMS23, LSZ19] has built a theoretical framework of hyperbolic function regression, which includes the functions $f(x) = \exp(Ax), \cosh(Ax), and \sinh(Ax)$.

Definition 1.3 (Hyperbolic regression, [LSZ19]). Given a matrix $A \in \mathbb{R}^{n \times d}$ and a vector $b \in \mathbb{R}^n$, the goal of the hyperbolic regression problem is to compute the following regression problem:

$$\min_{x \in \mathbb{R}^d} ||f(x) - b||_2.$$

The approach developed by [DLS23] for analyzing the hyperbolic regression is to consider the normalization factor, namely $\langle f(x), \mathbf{1}_n \rangle^{-1} = \langle \exp(Ax), \mathbf{1}_n \rangle^{-1}$. By focusing on the exp, [DLS23] transform the hyperbolic regression problem (see Definition 1.3) to the softmax regression problem (see Definition 1.1). Later on, [LSX+23] studies the in-context learning based on a softmax regression of attention mechanism in the Transformer, which is an essential component within LLMs since it allows the model to focus on particular input elements. Moreover, [GSX23] utilize a tensor-trick from [SZZ21, Zha22, DJS+19, SWYZ21, SWZ19, DSSW18] simplifying the multiple softmax regression into a single softmax regression.

ResNet is a certain type of deep learning model: the weight layers can learn the residual functions [HZRS16]. It is characterized by skip connections, which may perform identity mappings by adding the layer's output to the initial input. This mechanism is similar to the Highway Network in [SGS15] that the gates are opened through highly positive bias weights. This innovation facilitates the training of deep learning models with a substantial number of layers, allowing them to achieve better accuracy as they become deeper. These identity skip connections, commonly known as "residual connections", are also employed in various other systems, including Transformer [VSP+17], BERT [DCLT18], and ChatGPT [Ope22]. Moreover, ResNets have achieved state-of-the-art performance across many computer vision tasks, including image classification [MC19, SPBA21], object detection [OYZ+19, LKNR19, LLGZ19, HLK19], and semantic segmentation [FEF+17, XYZ19, WCY+18, DZL+21]. Mathematically, it is defined as

$$y = F(x) + x,$$

where $x, F(x) \in \mathbb{R}^d$: x represents the input to the residual block, and F(x) represents the output of the residual path (the transformation applied to x).

In this paper, we combine the softmax regression (see Definition 1.1) with ResNet and give a theoretical analysis of this problem. We formally define it as follows:

Definition 1.4 (Soft-Residual Regression). Given a matrix $A \in \mathbb{R}^{n \times d}$ and a vector $b \in \mathbb{R}^n$, the goal is to compute the following regression problem:

$$\|\langle \exp(Ax) + Ax, \mathbf{1}_n \rangle^{-1} (\exp(Ax) + Ax) - b\|_2^2$$

We are motivated by the fact that the softmax regression and ResNets have mostly been studied separately in prior works. We would like to provide a theoretical analysis for combining them together. The unified perspective and analysis of the loss landscape could provide insights into optimization and generalization for emerging overparametrized models. We firmly believe that this lays the groundwork for further research at the intersection of softmax classification and residual architectures.

Roadmap In Section 2, we introduce the basic notations we use and present basic mathematical facts that may support the mathematical properties developed in this paper. In Section 3, we compute the gradient of the functions we defined earlier. In Section 4, we compute the Hessian of these functions based on their gradient. In Section 5, we formally define the key functions that appear in the Hessian and rewrite the Hessian functions in a more formal way. In Section 6, we show that the Hessian is positive semidefinite (PSD). In Section 7, we show that the Hessian is Lipschitz. In Section 8, we summarize the mathematical properties we developed in the previous sections and explain how they may support the main result of this paper. In Section 9, we conclude this paper, present the meaningfulness of our work, and discuss future research directions.

2 Preliminary

In this section, we first introduce the basic notations we use. Then, in section 2.1, we introduce the definition of the functions we analyze in the later sections. In Section 2.2, we present the basic mathematical properties of the derivative, vectors, norms, and matrices.

Notations Now, we define the notations used in this paper.

First, we define the notations related to sets. Let \mathbb{Z}_+ be the set containing all the positive integers, namely $\{1,2,3,\ldots\}$. Let n,d be arbitrary elements in \mathbb{Z}_+ . We define $[n] := \{1,2,\ldots,n\}$. We define $\mathbb{R}, \mathbb{R}^n, \mathbb{R}^{n \times d}$ to be the set containing all real numbers, the set containing all n-dimensional vectors whose entries are all real numbers, and the set containing all $n \times d$ matrices whose entries are all real numbers, respectively.

Then, we define the notations related to vectors. Let x, y be arbitrary elements in \mathbb{R}^n . We use x_i to denote the i-th entry of x, for all $i \in [n]$. $||x||_2 \in \mathbb{R}$ denotes the ℓ_2 norm of the vector x, which is defined as $||x||_2 := (\sum_{i=1}^n x_i^2)^{1/2}$. $\langle x, y \rangle \in \mathbb{R}$ represents the inner product of x and y, which is defined as $\langle x, y \rangle := \sum_{i=1}^n x_i y_i$. We use \circ to denote a binary operation between x and y, called the Hadamard product. $x \circ y \in \mathbb{R}^n$ is defined as $(x \circ y)_i := x_i \cdot y_i$, for all $i \in [n]$. $\mathbf{1}_n \in \mathbb{R}^n$ denotes a vector, where $(\mathbf{1}_n)_i := 1$ for all $i \in [n]$, and $\mathbf{0}_n \in \mathbb{R}^n$ denotes a vector, where $(\mathbf{0}_n)_i := 0$ for all $i \in [n]$.

After that, we introduce the notations related to matrices. Let A be an arbitrary element in $\mathbb{R}^{n\times d}$. We use $A_{i,j}$ to denote the entry of A which is at the i-th row and j-th column, for all $i\in [n]$ and $j\in [d]$. We define $A_{*,i}\in\mathbb{R}^n$ as $(A_{*,i})_j:=A_{j,i}$, for all $j\in [n]$ and $i\in [d]$. We use $\|A\|$ to denote the spectral norm of A, i.e., $\|A\|:=\max_{x\in\mathbb{R}^d}\|Ax\|_2/\|x\|_2$. This also implies that for any $x\in\mathbb{R}^d$, $\|Ax\|_2\leq \|A\|\cdot\|x\|_2$. For any $x\in\mathbb{R}^d$, we define $\mathrm{diag}(x)\in\mathbb{R}^{d\times d}$ as $(\mathrm{diag}(x))_{i,j}:=x_i$ for all i=j and $(\mathrm{diag}(x))_{i,j}:=0$ for all $i\neq j$, where $i,j\in [d]$. We use $A^\top\in\mathbb{R}^{d\times n}$ to denote the transpose of A, namely $(A^\top)_{i,j}:=A_{j,i}$, for all $i\in [d]$ and $j\in [n]$. We use I_n to denote the n-dimensional identity matrix. Let B and C be arbitrary symmetric matrices. We say $B\preceq C$ if, for all vector x, we have $x^\top Bx \leq x^\top Cx$. We say B is positive semidefinite (or B is a PSD matrix), denoted as $B\succeq 0$, if, for all vectors x, we have $x^\top Bx\geq 0$.

Finally, we define the notations related to functions. We define $\phi : \mathbb{R} \to \mathbb{R}$ as $\phi(z) := \max\{z, 0\}$. For a differentiable function f, we use $\frac{\mathrm{d}f}{\mathrm{d}x}$ to denote the derivative of f.

2.1 Basic Definitions

In this section, we define the basic functions which are analyzed in the later sections.

Definition 2.1 (Basic functions). Let $A \in \mathbb{R}^{n \times d}$ be an arbitrary matrix. Let $x \in \mathbb{R}^d$ be an arbitrary vector. Let $b \in \mathbb{R}^n$ be a given vector. Let $i \in [d]$ be an arbitrary positive integer. We define the functions $u_1, u_2, u, f, c, z, v_i : \mathbb{R}^d \to \mathbb{R}^n$ and $\alpha, L, \beta_i : \mathbb{R}^d \to \mathbb{R}$ as

$$\begin{array}{ll} u_1(x) := Ax & u_2(x) := \exp(Ax) \\ u(x) := u_1(x) + u_2(x) & \alpha(x) := \langle u(x), \mathbf{1}_n \rangle \\ f(x) := \alpha(x)^{-1} u(x) & c(x) := f(x) - b \\ L(x) := 0.5 \|c(x)\|_2^2 & z(x) := u_2(x) + \mathbf{1}_n \\ v_i(x) := (u_2(x) + \mathbf{1}_n) \circ A_{*,i} & \beta_i(x) := \langle v_i(x), \mathbf{1}_n. \end{array}$$

2.2 Basic Facts

In this section, we present the basic mathematical properties which are used to support our analysis in later sections.

Fact 2.2. Let f be a differentiable function. Then, we have

• Part 1.
$$\frac{d}{dx} \exp(x) = \exp(x)$$

• Part 2. For any $j \neq i$, $\frac{d}{dx_i} f(x_j) = 0$

Fact 2.3. For all vectors $u, v, w \in \mathbb{R}^n$, we have

- $\langle u, v \rangle = \langle u \circ v, \mathbf{1}_n \rangle = u^{\mathsf{T}} \mathrm{diag}(v) \mathbf{1}_n$
- $\langle u \circ v, w \rangle = \langle u \circ v \circ w, \mathbf{1}_n \rangle = u^{\top} \operatorname{diag}(v) w$
- $\langle u \circ v \circ w \circ z, \mathbf{1}_n \rangle = u^{\top} \operatorname{diag}(v \circ w) z$
- $u \circ v = v \circ u = \operatorname{diag}(u) \cdot v = \operatorname{diag}(v) \cdot u$
- $u^{\top}(v \circ w) = v^{\top}(u \circ w) = w^{\top}(u \circ v) = u^{\top}\operatorname{diag}(v)w = v^{\top}\operatorname{diag}(u)w = w^{\top}\operatorname{diag}(u)v$
- $\operatorname{diag}(u) \cdot \operatorname{diag}(v) \cdot \mathbf{1}_n = \operatorname{diag}(u)v$
- $\operatorname{diag}(u \circ v) = \operatorname{diag}(u)\operatorname{diag}(v)$
- $\operatorname{diag}(u) + \operatorname{diag}(v) = \operatorname{diag}(u+v)$
- $\langle u, v \rangle = \langle v, u \rangle$
- $\bullet \ \langle u, v \rangle = u^\top v = v^\top u$
- $\bullet \ u + vw^{\top}a = u + vu^{\top}w = (I_n + vw^{\top})u$
- $\bullet \ u + v^{\top}wu = (1 + v^{\top}w)u$

Fact 2.4. Let $f: \mathbb{R}^d \to \mathbb{R}^n$. Let $q: \mathbb{R}^d \to \mathbb{R}$. Let $g: \mathbb{R}^d \to \mathbb{R}^n$. Therefore, we have for any arbitrary $x \in \mathbb{R}^d$, $q(x) \in \mathbb{R}$, $f(x) \in \mathbb{R}^n$, and $g(x) \in \mathbb{R}^n$. Let $a \in \mathbb{R}$ be an arbitrary constant. Then, we have

- $\frac{\mathrm{d}q(x)^a}{\mathrm{d}x} = a \cdot q(x)^{a-1} \cdot \frac{\mathrm{d}q(x)}{\mathrm{d}x}$
- $\frac{\mathrm{d}\|f(x)\|_2^2}{\mathrm{d}t} = 2\langle f(x), \frac{\mathrm{d}f(x)}{\mathrm{d}t} \rangle$
- $\frac{\mathrm{d}\langle f(x), g(x)\rangle}{\mathrm{d}t} = \langle \frac{\mathrm{d}f(x)}{\mathrm{d}t}, g(x)\rangle + \langle f(x), \frac{\mathrm{d}g(x)}{\mathrm{d}t}\rangle$
- $\frac{\mathrm{d}(g(x)\circ f(x))}{\mathrm{d}t} = \frac{\mathrm{d}g(x)}{\mathrm{d}t} \circ f(x) + g(x) \circ \frac{\mathrm{d}f(x)}{\mathrm{d}t}$ (product rule for Hadamard product)

Fact 2.5 (Basic Vector Norm Bounds). For vectors $u, v, w \in \mathbb{R}^n$, we have

- Part 1. $\langle u, v \rangle \le ||u||_2 \cdot ||v||_2$ (Cauchy-Schwarz inequality)
- Part 2. $\|\operatorname{diag}(u)\| \le \|u\|_{\infty}$
- Part 3. $||u \circ v||_2 \le ||u||_{\infty} \cdot ||v||_2$
- Part 4. $||u||_{\infty} \le ||u||_2 \le \sqrt{n} ||u||_{\infty}$
- Part 5. $||u||_2 \le ||u||_1 \le \sqrt{n}||u||_2$
- Part 6. $\|\exp(u)\|_{\infty} \le \exp(\|u\|_{\infty}) \le \exp(\|u\|_2)$
- Part 7. Let α be a scalar, then $\|\alpha \cdot u\|_2 = |\alpha| \cdot \|u\|_2$
- Part 8. $||u+v||_2 \le ||u||_2 + ||v||_2$

- $Part \ 9. \ \|uv^{\top}\| \le \|u\|_2 \|v\|_2$
- Part 10. if $||u||_2, ||v||_2 \le R$, then $||\exp(u) \exp(v)||_2 \le \exp(R)||u v||_2$

Fact 2.6 (Matrices Norm Basics). For any matrices $U, V \in \mathbb{R}^{n \times n}$, given a scalar $\alpha \in \mathbb{R}$ and a vector $v \in \mathbb{R}^n$, we have

- Part 1. $||U^{\top}|| = ||U||$
- Part 2. $||U|| \ge ||V|| ||U V||$
- $Part 3. \|U + V\| \le \|U\| + \|V\|$
- $Part 4. \|U \cdot V\| \le \|U\| \cdot \|V\|$
- Part 5. If $U \leq \alpha \cdot V$, then $||U|| \leq \alpha \cdot ||V||$
- Part 6. $\|\alpha \cdot U\| \le |\alpha| \|U\|$
- Part 7. $||Uv||_2 \le ||U|| \cdot ||v||_2$
- Part 8. $||UU^{\top}|| \le ||U||^2$

Fact 2.7 (Basic algebraic properties). Let x be an arbitrary element in \mathbb{R} . Then, we have

- Part 1. $\exp(x^2) \ge 1$.
- Part 2. $\exp(x^2) \ge x$.

Proof. Proof of Part 1.

Consider

$$\frac{\mathrm{d}\exp(x^2)}{\mathrm{d}x} = 2x\exp(x^2) = 0.$$

This implies that

$$x = 0$$

since

$$\exp(x^2) \neq 0, \forall x \in \mathbb{R}.$$

Furthermore, since

$$\frac{\mathrm{d}\exp(x^2)}{\mathrm{d}x} < 0$$
, when $x < 0$

and

$$\frac{\mathrm{d}\exp(x^2)}{\mathrm{d}x} > 0, \text{ when } x > 0,$$

we have that

$$(0, \exp(0))$$

is the local minimum of $\exp(x^2)$.

Since x = 0 is the only critical point of $\exp(x^2)$ and $\exp(x^2)$ is differentiable over all $x \in \mathbb{R}$, so we have

$$\exp(x^2) \ge \exp(0^2) = 1,$$

which completes the proof of the first part.

Proof of Part 2.

This strategy of proofing this part is the same as the first part by considering the derivative of $\exp(x^2) - x$ and showing that the local minimum of $\exp(x^2) - x$ is greater than 0, so we omit the proof here.

Fact 2.8. For any vectors $u, v \in \mathbb{R}^n$, we have

- Part 1. $uu^{\top} \leq ||u||_2^2 \cdot I_n$
- Part 2. diag $(u) \leq ||u||_2 \cdot I_n$
- Part 3. diag $(u \circ u) \leq ||u||_2^2 \cdot I_n$
- $Part 4. uv^{\top} + vu^{\top} \leq uu^{\top} + vv^{\top}$
- $Part 5. uv^{\top} + vu^{\top} \succeq -(uu^{\top} + vv^{\top})$
- Part 6. $(v \circ u)(v \circ u)^{\top} \leq ||v||_{\infty}^{2} u u^{\top}$
- Part 7. diag $(u \circ v) \leq ||u||_2 ||v||_2 \cdot I_n$

3 Gradient

In this section, we compute the first-order derivatives of the functions defined earlier.

Lemma 3.1. Let $x \in \mathbb{R}^d$ be an arbitrary vector. Let $u_1(x), u_2(x), u(x), f(x), c(x), z(x), v_i(x) \in \mathbb{R}^n$ be defined as in Definition 2.1. Let $\alpha(x), L(x), \beta_i(x) \in \mathbb{R}$ be defined as in Definition 2.1. Then for each $i \in [d]$, we have

- Part 1. $\frac{du_1(x)}{dx_i} = A_{*,i}$
- Part 2. $\frac{du_2(x)}{dx_i} = u_2(x) \circ A_{*,i}$
- Part 3. $\frac{\mathrm{d}u(x)}{\mathrm{d}x_i} = v_i(x)$
- Part 4. $\frac{d\alpha(x)}{dx_i} = \beta_i(x)$
- Part 5. $\frac{d\alpha(x)^{-1}}{dx_i} = \alpha(x)^{-2} \cdot \beta_i(x)$
- Part 6. $\frac{\mathrm{d}f(x)}{\mathrm{d}x_i} = \alpha(x)^{-1}(I_n f(x) \cdot \mathbf{1}_n^\top) \cdot v_i(x)$
- Part 7. $\frac{\mathrm{d}c(x)}{\mathrm{d}x_i} = \alpha(x)^{-1}(I_n f(x) \cdot \mathbf{1}_n^\top) \cdot v_i(x)$
- Part 8. $\frac{\mathrm{d}L(x)}{\mathrm{d}x_i} = \alpha(x)^{-1}c(x)^{\top} \cdot (I_n f(x) \cdot \mathbf{1}_n^{\top}) \cdot v_i(x)$

- Part 9. $\frac{\mathrm{d}\beta_i(x)}{\mathrm{d}x_i} = \langle u_2(x), A_{*,i} \circ A_{*,i} \rangle$
- Part 10. For $j \in [d] \setminus \{i\}$, $\frac{d\beta_i(x)}{dx_j} = \langle u_2(x), A_{*,i} \circ A_{*,j} \rangle$
- Part 11. $\frac{dv_i(x)}{dx_i} = u_2(x) \circ A_{*,i} \circ A_{*,i}$
- Part 12. For $j \in [d] \setminus \{i\}$, $\frac{\mathrm{d}v_i(x)}{\mathrm{d}x_j} = u_2(x) \circ A_{*,j} \circ A_{*,i}$

Proof. Proof of Part 1. For each $i \in [d]$, we have

$$\frac{\mathrm{d}Ax}{\mathrm{d}x_i} = \frac{A\mathrm{d}x}{\mathrm{d}x_i}$$
$$= A_{*,i}$$

where the first step follows from simple algebra and the last step follows from the fact that only the *i*-th entry of $\frac{dx}{dx_i}$ is 1 and other entries of it are 0. Note that by definition 2.1,

$$u_1(x) = Ax$$
.

Therefore, we have

$$\frac{\mathrm{d}u_1(x)}{\mathrm{d}x_i} = A_{*,i}.$$

Proof of Part 2. For each $i \in [d]$, we have

$$\frac{\mathrm{d}(u_2(x))_i}{\mathrm{d}x_i} = u_2(x)_i \cdot \frac{\mathrm{d}(Ax)_i}{\mathrm{d}x_i}$$
$$= u_2(x)_i \cdot A_{*,i}$$

where the first step follows from simple algebra, and the last step follows from the result in Part 1. Thus, we have

$$\frac{\mathrm{d}u_2(x)}{\mathrm{d}x_i} = u_2(x) \circ A_{*,i}$$

Proof of Part 3.

We have

$$\frac{du(x)}{dx_i} = \frac{d(u_1(x) + u_2(x))}{dx_i}$$

$$= \frac{d(u_1(x))}{dx_i} + \frac{d(u_2(x))}{dx_i}$$

$$= A_{*,i} + u_2(x) \circ A_{*,i}$$

$$= (u_2(x) + \mathbf{1}_n) \circ A_{*,i}$$

$$= v_i(x),$$

where the first step follows from the definition of u(x) (see Definition 2.1), the second step follows from the basic derivative rule, the third step follows from results from Part 1 and Part 2, the fourth step follows from the basic properties of Hadamard product, and the last step follows from the definition of $v_i(x)$ (see Definition 2.1).

Proof of Part 4.

$$\frac{d\alpha(x)}{dx_i} = \frac{d(\langle u(x), \mathbf{1}_n \rangle)}{dx_i}$$

$$= \langle \frac{du(x)}{dx_i}, \mathbf{1}_n \rangle$$

$$= \langle v_i(x), \mathbf{1}_n \rangle$$

$$= \beta_i(x)$$

where the first step follows from the definition of $\alpha(x)$ (see Definition 2.1), the second step follows from Fact 2.4, the third step follows from Part 3, and the fourth step follows from the definition of $\beta_i(x)$ (see Definition 2.1).

Proof of Part 5.

$$\frac{d\alpha(x)^{-1}}{dx_i} = -1 \cdot \alpha(x)^{-2} \cdot \frac{d\alpha(x)}{dx_i}$$
$$= -\alpha(x)^{-2} \cdot \beta_i(x)$$

where the first step follows from the Fact 2.4, where the second step follows from the results of Part 4.

Proof of Part 6.

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x_i} = \frac{\mathrm{d}\alpha(x)^{-1}}{\mathrm{d}x_i} u(x) + \alpha(x)^{-1} \cdot \frac{\mathrm{d}u(x)}{\mathrm{d}x_i}
= -\alpha(x)^{-2} \cdot \beta_i(x) \cdot u(x) + \alpha(x)^{-1} \cdot v_i(x)
= -\alpha(x)^{-1} f(x) \cdot \beta_i(x) + \alpha(x)^{-1} \cdot v_i(x)
= \alpha(x)^{-1} \cdot (v_i(x) - f(x) \cdot \beta_i(x))
= \alpha(x)^{-1} \cdot (v_i(x) - f(x) \cdot \langle v_i(x), \mathbf{1}_n \rangle)
= \alpha(x)^{-1} \cdot (v_i(x) - f(x) \cdot \mathbf{1}_n^\top v_i(x))
= \alpha(x)^{-1} \cdot (I_n - f(x) \cdot \mathbf{1}_n^\top) \cdot v_i(x)$$

where the first step follows from the product rule and the definition of f(x) (see Definition 2.1), the second step follows from results of Part 3, 5, the third step follows from the definition of f(x) (see Definition 2.1), the fourth step follows from simple algebra, the fifth step follows from the definition of β_i (see Definition 2.1), the sixth step follows from Fact 2.3, and the last step follows from simple algebra.

Proof of Part 7.

$$\frac{\mathrm{d}c(x)}{\mathrm{d}x_i} = \frac{\mathrm{d}(f(x) - b)}{\mathrm{d}x_i}$$
$$= \frac{\mathrm{d}f(x)}{\mathrm{d}x_i}$$

where the first step follows from the definition of c(x) (see Definition 2.1), the second step follows from derivative rules.

Proof of Part 8.

$$\frac{\mathrm{d}L(x)}{\mathrm{d}x_i} = \frac{\mathrm{d}0.5 \|c(x)\|_2^2}{\mathrm{d}x_i}$$

$$= c(x)^\top \cdot \frac{\mathrm{d}c(x)}{\mathrm{d}x_i}$$

$$= \alpha(x)^{-1} \cdot c(x)^\top \cdot (I_n - f(x) \cdot \mathbf{1}_n^\top) \cdot v_i(x)$$

where the first step follows from the definition of L(x) (see Definition 2.1), the second step follows from Fact 2.4, and the last step follows from the results from Part 6 and 7.

Proof of Part 9.

$$\frac{\mathrm{d}\beta_{i}(x)}{\mathrm{d}x_{i}} = \frac{\mathrm{d}(\langle v_{i}(x), \mathbf{1}_{n} \rangle)}{\mathrm{d}x_{i}}$$

$$= \frac{\mathrm{d}(\langle (u_{2}(x) + \mathbf{1}_{n}) \circ A_{*,i}, \mathbf{1}_{n} \rangle)}{\mathrm{d}x_{i}}$$

$$= \frac{\mathrm{d}\langle u_{2}(x) + \mathbf{1}_{n}, A_{*,i} \rangle}{\mathrm{d}x_{i}}$$

$$= \langle \frac{\mathrm{d}(u_{2}(x) + \mathbf{1}_{n})}{\mathrm{d}x_{i}}, A_{*,i} \rangle$$

$$= \langle u_{2}(x) \circ A_{*,i}, A_{*,i} \rangle$$

$$= \langle u_{2}(x), A_{*,i} \circ A_{*,i} \rangle$$

where the first step follows from the definition of $\beta_i(x)$ (see Definition 2.1), the second step follows from the definition of $v_i(x)$ (see Definition 2.1), the third step follows from Fact 2.3, the fourth step follows from Fact 2.4, the fifth step follows from Part 2, and the last step follows from Fact 2.3.

Proof of Part 10.

$$\frac{\mathrm{d}\beta_{i}(x)}{\mathrm{d}x_{j}} = \frac{\mathrm{d}(\langle v_{i}(x), \mathbf{1}_{n} \rangle)}{\mathrm{d}x_{j}}$$

$$= \frac{\mathrm{d}(\langle (u_{2}(x) + \mathbf{1}_{n}) \circ A_{*,i}, \mathbf{1}_{n} \rangle)}{\mathrm{d}x_{j}}$$

$$= \frac{\mathrm{d}\langle u_{2}(x) + \mathbf{1}_{n}, A_{*,i} \rangle}{\mathrm{d}x_{j}}$$

$$= \langle \frac{\mathrm{d}(u_{2}(x) + \mathbf{1}_{n})}{\mathrm{d}x_{j}}, A_{*,i} \rangle$$

$$= \langle u_{2}(x) \circ A_{*,j}, A_{*,i} \rangle$$

$$= \langle u_{2}(x), A_{*,i} \circ A_{*,i} \rangle$$

where the first step follows from the definition of $\beta_i(x)$ (see Definition 2.1), the second step follows from the definition of $v_i(x)$ (see Definition 2.1), the third step follows from Fact 2.3, the fourth step follows from Fact 2.4, the fifth step follows from Part 2, and the last step follows from Fact 2.3.

Proof of Part 11.

$$\frac{\mathrm{d}v_i(x)}{\mathrm{d}x_i} = \frac{\mathrm{d}(u_2(x) + \mathbf{1}_n) \circ A_{*,i}}{\mathrm{d}x_i}$$

$$= \frac{\mathrm{d}(u_2(x) + \mathbf{1}_n)}{\mathrm{d}x_i} \circ A_{*,i}$$
$$= u_2(x) \circ A_{*,i} \circ A_{*,i}$$

where the first step follows from the definition of $v_i(x)$ (see Definition 2.1), the second step follows from Fact 2.4 as $\frac{dA_{*,i}}{dx_i} = 0$, and the last step follows from the results of Part 2.

Proof of Part 12.

$$\frac{\mathrm{d}v_i(x)}{\mathrm{d}x_j} = \frac{\mathrm{d}(u_2(x) + \mathbf{1}_n) \circ A_{*,i}}{\mathrm{d}x_j}$$
$$= \frac{\mathrm{d}(u_2(x) + \mathbf{1}_n)}{\mathrm{d}x_j} \circ A_{*,i}$$
$$= u_2(x) \circ A_{*,i} \circ A_{*,i}$$

where the first step follows from the definition of $v_i(x)$ (see Definition 2.1), the second step follows from Fact 2.4 as $\frac{dA_{*,i}}{dx_j} = 0$, and the last step follows from the results of Part 2.

4 Hessian

In Section 4.1, we introduce the basic definition of the matrices containing $B_1(x), B_2(x), B_3(x) \in \mathbb{R}^{n \times n}$, used for simplifying the expression of Hessian. In Section 4.2, we compute the second-order derivatives of the functions defined earlier. In Section 4.3, we present a helpful lemma. In Section 4.4, we decompose the matrices $B_1(x), B_2(x), B_3(x) \in \mathbb{R}^{n \times n}$ into low-rank matrices and diagonal matrices.

4.1 Basic Definition

In this section, we give the definition of the matrices containing $B_1(x), B_2(x), B_3(x) \in \mathbb{R}^{n \times n}$.

Definition 4.1. Let $x \in \mathbb{R}^d$ be an arbitrary vector. Let $u_1(x), u_2(x), u(x), f(x), c(x), z(x), v_i(x) \in \mathbb{R}^n$ and $\alpha(x), L(x), \beta_i(x) \in \mathbb{R}$ be defined as in Definition 2.1. Let $K(x) = (I_n - f(x) \cdot \mathbf{1}_n^\top) \in \mathbb{R}^{n \times n}$. Let $\widetilde{c}(x) = K(x)^\top c(x) \in \mathbb{R}^n$. We define

• $B_1(x) \in \mathbb{R}^{n \times n}$ as

$$A_{*,i}^{\top}B_1(x)A_{*,j}$$
:= $A_{*,i}^{\top}\underbrace{\alpha(x)^{-2}\underbrace{v_i(x)}^{\top}\underbrace{K(x)}^{\top}\underbrace{K(x)}^{\top}\underbrace{V_i(x)}_{n\times n}A_{*,j}$

• $B_2(x) \in \mathbb{R}^{n \times n}$ as

$$A_{*,i}^{\top} B_{2}(x) A_{*,j}$$

$$:= -A_{*,i}^{\top} \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \cdot \underbrace{\widetilde{c}(x)^{\top}}_{1 \times n} \cdot \underbrace{(v_{j}(x) \cdot \beta_{i}(x)}_{n \times 1} \cdot \underbrace{\beta_{i}(x)}_{\text{scalar}} + \underbrace{v_{i}(x) \cdot \beta_{j}(x)}_{n \times 1}) A_{*,j}$$

• $B_3(x) \in \mathbb{R}^{n \times n}$ as

$$A_{*,i}^{\top}B_3(x)A_{*,j} := \underbrace{\alpha(x)^{-1}}_{\text{scalar}} \cdot \underbrace{A_{*,i}^{\top}}_{1 \times n} \operatorname{diag}(\underbrace{\widetilde{c}(x)}_{n \times 1} \circ \underbrace{u_2(x)}_{n \times 1}) \underbrace{A_{*,j}}_{n \times 1}$$

4.2 Computation of Hessian

In this section, we present the computation of Hessian.

Lemma 4.2. Let $x \in \mathbb{R}^d$ be an arbitrary vector. Let $u_1(x), u_2(x), u(x), f(x), c(x), z(x), v_i(x) \in \mathbb{R}^n$ and $\alpha(x), L(x), \beta_i(x) \in \mathbb{R}$ be defined as in Definition 2.1. Let $K(x) \in \mathbb{R}^{n \times n}$ and $\widetilde{c}(x) \in \mathbb{R}^n$ be defined as in Definition 4.1.

Then for each $i, j \in [d]$, and $j \neq i$, we have

• Part 1.

$$\frac{\mathrm{d}^2 u_1(x)}{\mathrm{d}^2 x_i} = \mathbf{0}_n$$

• Part 2.

$$\frac{\mathrm{d}^2 u_1(x)}{\mathrm{d} x_i \mathrm{d} x_j} = \mathbf{0}_n$$

• Part 3.

$$\frac{\mathrm{d}^2 u_2(x)}{\mathrm{d}^2 x_i} = A_{*,i} \circ u_2(x) \circ A_{*,i}$$

• Part 4.

$$\frac{\mathrm{d}^2 u_2(x)}{\mathrm{d} x_i \mathrm{d} x_j} = A_{*,i} \circ u_2(x) \circ A_{*,j}$$

• Part 5.

$$\frac{\mathrm{d}^2 u(x)}{\mathrm{d}^2 x_i} = A_{*,i} \circ u_2(x) \circ A_{*,i}$$

• Part 6.

$$\frac{\mathrm{d}^2 u(x)}{\mathrm{d} x_i \mathrm{d} x_j} = A_{*,i} \circ u_2(x) \circ A_{*,j}$$

• Part 7.

$$\frac{\mathrm{d}^2 \alpha(x)}{\mathrm{d}^2 x_i} = \langle u_2(x), A_{*,i} \circ A_{*,i} \rangle$$

• Part 8.

$$\frac{\mathrm{d}^2 \alpha(x)}{\mathrm{d} x_i \mathrm{d} x_j} = \langle u_2(x), A_{*,j} \circ A_{*,i} \rangle$$

• Part 9.

$$\frac{\mathrm{d}^2 \alpha(x)^{-1}}{\mathrm{d}^2 x_i} = \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \underbrace{(\langle u_2(x), A_{*,i} \circ A_{*,i} \rangle}_{\text{scalar}} - 2\underbrace{\beta_i(x)^2}_{\text{scalar}}$$

• Part 10.

$$\frac{\mathrm{d}^2 \alpha(x)^{-1}}{\mathrm{d}x_i \mathrm{d}x_j} = \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \underbrace{(\langle u_2(x), A_{*,i} \circ A_{*,j} \rangle}_{\text{scalar}} - 2\underbrace{\beta_i(x)\beta_j(x)}_{\text{scalar}}$$

• Part 11.

$$\frac{\mathrm{d}^2 f(x)}{\mathrm{d}^2 x_i} = -2 \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \cdot \underbrace{\beta_i(x)}_{\text{scalar}} \cdot \underbrace{(I_n - f(x) \cdot \mathbf{1}_n^\top)}_{n \times n} \cdot \underbrace{v_i(x)}_{n \times 1} + \underbrace{\alpha(x)^{-1}}_{\text{scalar}} \cdot \underbrace{(I_n - f(x) \cdot \mathbf{1}_n^\top)}_{n \times n} \cdot \underbrace{(u_2(x) \circ A_{*,i} \circ A_{*,i})}_{n \times 1}$$

• Part 12.

$$\frac{\mathrm{d}^{2} f(x)}{\mathrm{d} x_{i} \mathrm{d} x_{j}} = \underbrace{-\underbrace{\alpha(x)^{-2}}_{\mathrm{scalar}} \cdot \underbrace{(I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top})}_{n \times n} \cdot \underbrace{(v_{j}(x) \cdot \underline{\beta_{i}(x)}}_{n \times 1} + \underbrace{v_{i}(x)}_{n \times 1} \cdot \underbrace{\underline{\beta_{j}(x)}}_{\mathrm{scalar}})}_{\mathrm{scalar}} + \underbrace{\alpha(x)^{-1}}_{n \times n} \underbrace{(I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top})}_{n \times n} \cdot \underbrace{(u_{2}(x) \circ A_{*,j} \circ A_{*,i})}_{n \times 1}$$

• Part 13.

$$\frac{\mathrm{d}^2 L(x)}{\mathrm{d}^2 x_i} = \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \cdot \underbrace{A_{*,i}^{\top}}_{1 \times n} \underbrace{B_1(x)}_{n \times n} \underbrace{A_{*,i}}_{n \times 1} - \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \cdot \underbrace{A_{*,i}^{\top}}_{1 \times n} \underbrace{B_2(x)}_{n \times n} \underbrace{A_{*,i}}_{n \times 1} + \underbrace{\alpha(x)^{-1}}_{\text{scalar}} \cdot \underbrace{A_{*,i}^{\top}}_{1 \times n} \underbrace{B_3(x)}_{n \times n} \underbrace{A_{*,i}}_{n \times 1}$$

• Part 14.

$$\frac{\mathrm{d}^2 L(x)}{\mathrm{d} x_i \mathrm{d} x_j} = \underbrace{\alpha(x)^{-2}}_{\mathrm{scalar}} \cdot \underbrace{A_{*,i}^\top}_{1 \times n} \underbrace{B_1(x)}_{n \times n} \underbrace{A_{*,j}}_{n \times 1} - \underbrace{\alpha(x)^{-2}}_{\mathrm{scalar}} \cdot \underbrace{A_{*,i}^\top}_{1 \times n} \underbrace{B_2(x)}_{n \times n} \underbrace{A_{*,j}}_{n \times 1} + \underbrace{\alpha(x)^{-1}}_{\mathrm{scalar}} \cdot \underbrace{A_{*,i}^\top}_{1 \times n} \underbrace{B_3(x)}_{n \times n} \underbrace{A_{*,j}}_{n \times 1}$$

Proof. Proof of Part 1

$$\frac{\mathrm{d}^2 u_1(x)}{\mathrm{d}^2 x_i} = \frac{\mathrm{d}}{\mathrm{d} x_i} (\frac{\mathrm{d} u_1(x)}{\mathrm{d} x_i})$$
$$= \frac{\mathrm{d} A_{*,i} \circ \mathbf{1}_n}{\mathrm{d} x_i}$$
$$= \mathbf{0}_n$$

where the first step follows from the expansion of the Hessian, the second step follows from Part 1 of Lemma 3.1, and the last step follows from derivative rules.

$$\frac{\mathrm{d}^2 u_1(x)}{\mathrm{d} x_i \mathrm{d} x_j} = \frac{\mathrm{d}}{\mathrm{d} x_j} \left(\frac{\mathrm{d} u_1(x)}{\mathrm{d} x_i}\right)$$

$$= \frac{\mathrm{d} A_{*,i} \circ \mathbf{1}_n}{\mathrm{d} x_j}$$
$$= \mathbf{0}_n$$

where the first step follows from the expansion of the Hessian, the second step follows from Part 1 of Lemma 3.1, and the last step follows from derivative rules.

Proof of Part 3

$$\frac{\mathrm{d}^2 u_2(x)}{\mathrm{d}^2 x_i} = \frac{\mathrm{d}}{\mathrm{d} x_i} \left(\frac{\mathrm{d} u_2(x)}{\mathrm{d} x_i} \right)$$

$$= \frac{\mathrm{d} (u_2(x) \circ A_{*,i})}{\mathrm{d} x_i}$$

$$= A_{*,i} \circ \frac{\mathrm{d} u_2(x)}{\mathrm{d} x_i}$$

$$= A_{*,i} \circ u_2(x) \circ A_{*,i}$$

where the first step follows from the expansion of Hessian, the second step follows from Part 2 of Lemma 3.1, the third step follows from extract constant $A_{*,i}$ out of derivative, and the last step follows from Part 2 of Lemma 3.1.

Proof of Part 4

$$\frac{\mathrm{d}^2 u_2(x)}{\mathrm{d}x_i x_j} = \frac{\mathrm{d}}{\mathrm{d}x_j} \left(\frac{\mathrm{d}u_2(x)}{\mathrm{d}x_i}\right)$$

$$= \frac{\mathrm{d}(u_2(x) \circ A_{*,i})}{\mathrm{d}x_j}$$

$$= A_{*,i} \circ \frac{\mathrm{d}u_2(x)}{\mathrm{d}x_j}$$

$$= A_{*,i} \circ u_2(x) \circ A_{*,i}$$

where the first step follows from the expansion of Hessian, the second step follows from Part 2 of Lemma 3.1, the third step follows from extract constant $A_{*,i}$ out of derivative, and the last step follows from Part 2 of Lemma 3.1.

Proof of Part 5

$$\frac{\mathrm{d}^2 u(x)}{\mathrm{d}^2 x_i} = \frac{\mathrm{d}}{\mathrm{d}x_i} \left(\frac{\mathrm{d}u_1(x) + u_2(x)}{\mathrm{d}x_i} \right)$$

$$= \frac{\mathrm{d}}{\mathrm{d}x_i} \frac{\mathrm{d}u_1(x)}{\mathrm{d}x_i} + \frac{\mathrm{d}}{\mathrm{d}x_i} \frac{\mathrm{d}u_2(x)}{\mathrm{d}x_i}$$

$$= \frac{\mathrm{d}(u_2(x) \circ A_{*,i})}{\mathrm{d}x_i}$$

$$= A_{*,i} \circ \frac{\mathrm{d}u_2(x)}{\mathrm{d}x_i}$$

$$= A_{*,i} \circ u_2(x) \circ A_{*,i}$$

where the first step follows from the expansion of Hessian and Definition 2.1, the second step follows from the expansion of derivative, the third step follows from Part 1 and 2 of Lemma 3.1, the fourth step follows from extract constant $A_{*,i}$ out of derivative, and the last step follows from Part 2 of Leamm 3.1.

Proof of Part 6

$$\frac{\mathrm{d}^2 u(x)}{\mathrm{d}x_i x_j} = \frac{\mathrm{d}}{\mathrm{d}x_j} \left(\frac{\mathrm{d}u_1(x) + u_2(x)}{\mathrm{d}x_i} \right)$$

$$= \frac{\mathrm{d}}{\mathrm{d}x_j} \frac{\mathrm{d}u_1(x)}{\mathrm{d}x_i} + \frac{\mathrm{d}}{\mathrm{d}x_j} \frac{\mathrm{d}u_2(x)}{\mathrm{d}x_i}$$

$$= \frac{\mathrm{d}(u_2(x) \circ A_{*,i})}{\mathrm{d}x_j}$$

$$= A_{*,i} \circ \frac{\mathrm{d}u_2(x)}{\mathrm{d}x_j}$$

$$= A_{*,i} \circ u_2(x) \circ A_{*,j}$$

where the first step follows from the expansion of Hessian and Definition 2.1, the second step follows from the expansion of derivative, the third step follows from Part 1 and 2 of Lemma 3.1, the fourth step follows from extract constant $A_{*,i}$ out of derivative, and the last step follows from Part 2 of Lemma 3.1.

Proof of Part 7

$$\frac{\mathrm{d}^2 \alpha(x)}{\mathrm{d}^2 x_i} = \frac{\mathrm{d}}{\mathrm{d} x_i} (\frac{\mathrm{d} \alpha(x)}{\mathrm{d} x_i})$$
$$= \frac{\mathrm{d} \beta_i(x)}{\mathrm{d} x_i}$$
$$= \langle u_2(x), A_{*,i} \circ A_{*,i} \rangle$$

where the first step follows from the expansion of Hessian, the second step follows from Part 4 of Lemma 3.1, and the last step follows from Part 9 of Lemma 3.1.

Proof of Part 8

$$\frac{\mathrm{d}^2 \alpha(x)}{\mathrm{d}x_i x_j} = \frac{\mathrm{d}}{\mathrm{d}x_j} \left(\frac{\mathrm{d}\alpha(x)}{\mathrm{d}x_i}\right)$$
$$= \frac{\mathrm{d}\beta_i(x)}{\mathrm{d}x_j}$$
$$= \langle u_2(x), A_{*,j} \circ A_{*,i} \rangle$$

where the first step follows from the expansion of Hessian, the second step follows from Part 4 of Lemma 3.1, and the last step follows from Part 10 of Lemma 3.1.

$$\frac{\mathrm{d}^{2}\alpha(x)^{-1}}{\mathrm{d}^{2}x_{i}} = \frac{\mathrm{d}}{\mathrm{d}x_{i}} \left(\frac{\mathrm{d}\alpha(x)^{-1}}{\mathrm{d}x_{i}} \right)
= \frac{\mathrm{d}(\alpha(x)^{-2} \cdot \beta_{i}(x))}{\mathrm{d}x_{i}}
= \frac{\mathrm{d}\alpha(x)^{-2}}{\mathrm{d}x_{i}} \cdot \beta_{i}(x) + \alpha(x)^{-2} \cdot \frac{\mathrm{d}\beta_{i}(x)}{\mathrm{d}x_{i}}
= -2\alpha(x)^{-3} \cdot \frac{\mathrm{d}\alpha(x)}{\mathrm{d}x_{i}} \cdot \beta_{i}(x) + \alpha(x)^{-2} \cdot \langle u_{2}(x), A_{*,i} \circ A_{*,i} \rangle
= -2\alpha(x)^{-3} \cdot \beta_{i}(x)^{2} + \alpha(x)^{-2} \cdot \langle u_{2}(x), A_{*,i} \circ A_{*,i} \rangle
= \alpha(x)^{-2} (\langle u_{2}(x), A_{*,i} \circ A_{*,i} \rangle - 2\alpha(x)^{-1} \cdot \beta_{i}(x)^{2})$$

where the first step follows from the expansion of Hessian, the second step follows from Part 5 of Lemma 3.1, the third step follows from the chain rule of derivative, the fourth step follows from the chain rule of derivative and Part 9 of Lemma 3.1, the fifth step follows from Part 2, 4 of Lemma 3.1, and the last step follows from simple algebra.

Proof of Part 10

$$\frac{\mathrm{d}^{2}\alpha(x)^{-1}}{\mathrm{d}^{2}x_{i}} = \frac{\mathrm{d}}{\mathrm{d}x_{i}} \left(\frac{\mathrm{d}\alpha(x)^{-1}}{\mathrm{d}x_{i}}\right)$$

$$= \frac{\mathrm{d}(\alpha(x)^{-2} \cdot \beta_{i}(x))}{\mathrm{d}x_{j}}$$

$$= \frac{\mathrm{d}\alpha(x)^{-2}}{\mathrm{d}x_{j}} \cdot \beta_{i}(x) + \alpha(x)^{-2} \cdot \frac{\mathrm{d}\beta_{i}(x)}{\mathrm{d}x_{j}}$$

$$= -2\alpha(x)^{-3} \cdot \frac{\mathrm{d}\alpha(x)}{\mathrm{d}x_{j}} \cdot \beta_{i}(x) + \alpha(x)^{-2} \cdot \langle u_{2}(x), A_{*,j} \circ A_{*,i} \rangle$$

$$= -2\alpha(x)^{-3} \cdot \beta_{i}(x) \cdot \beta_{j}(x) + \alpha(x)^{-2} \cdot \langle u_{2}(x), A_{*,j} \circ A_{*,i} \rangle$$

$$= \alpha(x)^{-2} (\langle u_{2}(x), A_{*,j} \circ A_{*,i} \rangle - 2\alpha(x)^{-1} \cdot \beta_{i}(x) \cdot \beta_{j}(x))$$

where the first step follows from the expansion of Hessian, the second step follows from Part 5 of Lemma 3.1, the third step follows from the chain rule of derivative, the fourth step follows from the chain rule of derivative and Part 10 of Lemma 3.1, the fifth step follows from Part 2, 4 of Lemma 3.1, and the last step follows from simple algebra.

Proof of Part 11

$$\frac{\mathrm{d}^{2}f(x)}{\mathrm{d}^{2}x_{i}} = \frac{\mathrm{d}}{\mathrm{d}x_{i}} \left(\frac{\mathrm{d}f(x)}{\mathrm{d}x_{i}} \right) \\
= \frac{\mathrm{d}(\alpha(x)^{-1} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x))}{\mathrm{d}x_{i}} \\
= \frac{\mathrm{d}\alpha(x)^{-1}}{\mathrm{d}x_{i}} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x) + \alpha(x)^{-1} \cdot \frac{\mathrm{d}(I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x))}{\mathrm{d}x_{i}} \\
= -\alpha(x)^{-2} \cdot \beta_{i}(x) \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x) \\
+ \alpha(x)^{-1} \cdot \left(\frac{\mathrm{d}(I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top})}{\mathrm{d}x_{i}} \cdot v_{i}(x) + (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot \frac{\mathrm{d}v_{i}(x)}{\mathrm{d}x_{i}} \right) \\
= -\alpha(x)^{-2} \cdot \beta_{i}(x) \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x) \\
+ -\alpha(x)^{-2} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x) + \alpha(x)^{-1} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot (u_{2}(x) \circ A_{*,i} \circ A_{*,i}) \\
= -2\alpha(x)^{-2} \cdot \beta_{i}(x) \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x) + \alpha(x)^{-1} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot (u_{2}(x) \circ A_{*,i} \circ A_{*,i})$$

where the first step follows from the expansion of Hessian, the second step follows from Part 6 of Lemma 3.1, the third step follows from the chain rule of derivative, the fourth step follows from the chain rule of derivative and Part 4 of Lemma 3.1, the fifth step follows from Part 4,6,11 of Lemma 3.1, and the last step follows from simple algebra.

$$\frac{\mathrm{d}^2 f(x)}{\mathrm{d}x_i x_j} = \frac{\mathrm{d}}{\mathrm{d}x_j} \left(\frac{\mathrm{d}f(x)}{\mathrm{d}x_i} \right)$$
$$= \frac{\mathrm{d}(\alpha(x)^{-1} \cdot (I_n - f(x) \cdot \mathbf{1}_n^\top) \cdot v_i(x))}{\mathrm{d}x_j}$$

$$= \frac{\mathrm{d}\alpha(x)^{-1}}{\mathrm{d}x_{i}} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x) + \alpha(x)^{-1} \cdot \frac{\mathrm{d}(I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x)}{\mathrm{d}x_{j}}$$

$$= -\alpha(x)^{-2} \cdot \beta_{j}(x) \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x)$$

$$+ \alpha(x)^{-1} \cdot \left(\frac{\mathrm{d}(I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top})}{\mathrm{d}x_{j}} \cdot v_{i}(x) + (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot \frac{\mathrm{d}v_{i}(x)}{\mathrm{d}x_{j}}\right)$$

$$= -\alpha(x)^{-2} \cdot \beta_{j}(x) \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x)$$

$$+ -\alpha(x)^{-2} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{j}(x) \cdot \beta_{i}(x) + \alpha(x)^{-1} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot (u_{2}(x) \circ A_{*,j} \circ A_{*,i})$$

$$= -\alpha(x)^{-2} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot (v_{j}(x) \cdot \beta_{i}(x) + v_{i}(x) \cdot \beta_{j}(x))$$

$$+ \alpha(x)^{-1} (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot (u_{2}(x) \circ A_{*,j} \circ A_{*,i})$$

where the first step follows from the expansion of Hessian, the second step follows from Part 6 of Lemma 3.1, the third step follows from the chain rule of derivative, the fourth step follows from the chain rule of derivative and Part 4 of Lemma 3.1, the fifth step follows from Part 4,6,12 of Lemma 3.1, and the last step follows from simple algebra.

Proof of Part 13

$$\frac{\mathrm{d}^{2}L(x)}{\mathrm{d}^{2}x_{i}} = \frac{\mathrm{d}}{\mathrm{d}x_{i}} \left(\frac{\mathrm{d}L(x)}{\mathrm{d}x_{i}}\right)
= \frac{\mathrm{d}}{\mathrm{d}x_{i}} \left\langle c(x), \frac{\mathrm{d}c(x)}{\mathrm{d}x_{i}} \right\rangle
= \frac{\mathrm{d}}{\mathrm{d}x_{i}} \left\langle c(x), \frac{\mathrm{d}f(x)}{\mathrm{d}x_{i}} \right\rangle
= \left\langle \frac{\mathrm{d}c(x)}{\mathrm{d}x_{i}}, \frac{\mathrm{d}f(x)}{\mathrm{d}x_{i}} \right\rangle + c(x)^{\top} \cdot \frac{\mathrm{d}^{2}f(x)}{\mathrm{d}^{2}x_{i}}
= \left(\alpha(x)^{-1} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x)\right)^{\top} \cdot \alpha(x)^{-1} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x)
+ c(x)^{\top} \cdot -2\alpha(x)^{-2} \cdot \beta_{i}(x) \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x)
+ \alpha(x)^{-1} \cdot c(x)^{\top} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot (u_{2}(x) \circ A_{*,i} \circ A_{*,i})
= \alpha(x)^{-2} v_{i}(x)^{\top} K(x)^{\top} K(x) v_{i}(x)
+ -2\alpha(x)^{-2} \cdot \tilde{c}(x)^{\top} \cdot v_{i}(x) \cdot \beta_{i}(x)
+ \alpha(x)^{-1} \cdot A_{*,i}^{\top} \mathrm{diag}(\tilde{c}(x) \circ u_{2}(x)) A_{*,i}
= A_{*,i}^{\top} B_{1}(x) A_{*,i} + A_{*,i}^{\top} B_{2}(x) A_{*,i} + A_{*,i}^{\top} B_{3}(x) A_{*,i}$$

where the first step follows from the expansion of Hessian, the second step follows from Part 8 of Lemma 3.1, the third step follows from Part 6 of Lemma 3.1, the fourth step follows from the chain rules of derivative, the fifth step follows from Part 7 of Lemma 3.1 and Lemma 4.2, the sixth step follows from Definition of \tilde{c} , K, and the last step follow from Definitions of B_1 , B_2 , B_3

$$\frac{\mathrm{d}^2 L(x)}{\mathrm{d}x_i x_j} = \frac{\mathrm{d}}{\mathrm{d}x_j} \left(\frac{\mathrm{d}L(x)}{\mathrm{d}x_i} \right)$$

$$= \frac{\mathrm{d}}{\mathrm{d}x_j} \langle c(x), \frac{\mathrm{d}c(x)}{\mathrm{d}x_i} \rangle$$

$$= \frac{\mathrm{d}}{\mathrm{d}x_j} \langle c(x), \frac{\mathrm{d}f(x)}{\mathrm{d}x_i} \rangle$$

$$= \frac{\mathrm{d}c(x)^{\top}}{\mathrm{d}x_{j}} \cdot \frac{\mathrm{d}f(x)}{\mathrm{d}x_{i}} + c(x)^{\top} \cdot \frac{\mathrm{d}^{2}f(x)}{\mathrm{d}x_{i}x_{j}}$$

$$= (\alpha(x)^{-1} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{j}(x))^{\top} \cdot \alpha(x)^{-1} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot v_{i}(x)$$

$$+ c(x)^{\top} \cdot (-\alpha(x)^{-2} \cdot (I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot (v_{j}(x) \cdot \beta_{i}(x) + v_{i}(x) \cdot \beta_{j}(x))$$

$$+ \alpha(x)^{-1}(I_{n} - f(x) \cdot \mathbf{1}_{n}^{\top}) \cdot (u_{2}(x) \circ A_{*,j} \circ A_{*,i}))$$

$$= \alpha(x)^{-2}v_{i}(x)^{\top}K(x)^{\top}K(x)v_{j}(x)$$

$$+ -\alpha(x)^{-2} \cdot \tilde{c}(x)^{\top} \cdot (v_{j}(x) \cdot \beta_{i}(x) + v_{i}(x) \cdot \beta_{j}(x))$$

$$+ \alpha(x)^{-1} \cdot A_{*,i}^{\top}\mathrm{diag}(\tilde{c}(x) \circ u_{2}(x))A_{*,j}$$

$$= A_{*,i}^{\top}B_{1}(x)A_{*,j} + A_{*,i}^{\top}B_{2}(x)A_{*,j} + A_{*,i}^{\top}B_{3}(x)A_{*,j}$$

where the first step follows from the expansion of Hessian, the second step follows from Part 8 of Lemma 3.1, the third step follows from Part 6 of Lemma 3.1, the fourth step follows from the chain rules of derivative, the fifth step follows from Part 7 of Lemma 3.1 and Lemma 4.2, the sixth step follows from Definition of \tilde{c} , K, and the last step follow from Definitions of B_1 , B_2 , B_3

4.3 Helpful Lemma

In this section, we present a helpful lemma that is used for further analysis of Hessian.

Lemma 4.3. Let $x \in \mathbb{R}^d$ be an arbitrary vector. Let $u_1(x), u_2(x), u(x), f(x), c(x), z(x), v_i(x) \in \mathbb{R}^n$ and $\alpha(x), L(x), \beta_i(x) \in \mathbb{R}$ be defined as in Definition 2.1. Let $K(x) \in \mathbb{R}^{n \times n}$ and $\widetilde{c}(x) \in \mathbb{R}^n$ be defined as in Definition 4.1.

Then, for each $i, j \in [d]$,

• Part 1.

$$A_{*,i}^{\top} \alpha(x)^{-2} \cdot v_i(x)^{\top} K(x)^{\top} K(x) v_j(x) A_{*,j}$$

$$= \underbrace{A_{*,i}^{\top}}_{1 \times n} \cdot \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \cdot \underbrace{\operatorname{diag}(z(x))}_{n \times n}$$

$$\cdot \underbrace{K(x)^{\top}}_{n \times n} \underbrace{K(x)}_{n \times n} \cdot \underbrace{\operatorname{diag}(z(x))}_{n \times 1} \cdot \underbrace{A_{*,j}}_{n \times 1}$$

• Part 2.

$$A_{*,i}^{\top} \alpha(x)^{-2} \cdot \widetilde{c}(x)^{\top} \cdot (v_{j}(x) \cdot \beta_{i}(x) + v_{i}(x) \cdot \beta_{j}(x)) A_{*,j}$$

$$= \underbrace{A_{*,i}^{\top}}_{1 \times n} \cdot \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \cdot \underbrace{z(x)}_{n \times 1} \cdot \underbrace{\widetilde{c}(x)^{\top}}_{1 \times n} \cdot \underbrace{\text{diag}(z(x))}_{n \times n} \cdot \underbrace{A_{*,j}}_{n \times 1}$$

$$+ \underbrace{A_{*,i}^{\top}}_{1 \times n} \cdot \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \cdot \underbrace{\text{diag}(z(x))}_{n \times n} \cdot \underbrace{\widetilde{c}(x)}_{n \times 1} \cdot \underbrace{z(x)^{\top}}_{1 \times n} \cdot \underbrace{A_{*,j}}_{n \times 1}$$

• Part 3.

$$=\underbrace{A_{*,i}^{\top} \cdot A_{*,i}^{\top} \operatorname{diag}(\widetilde{c}(x) \circ u_{2}(x)) A_{*,j}}_{1 \times n} \underbrace{A_{*,i}^{\top} \cdot \underbrace{\alpha(x)^{-1}}_{scalar} \cdot \underbrace{\operatorname{diag}(\widetilde{c}(x) \circ u_{2}(x))}_{n \times n} \underbrace{A_{*,j}}_{n \times 1}}_{n \times 1}$$

Proof. Proof of Part 1.

$$\alpha(x)^{-2} \cdot v_i(x)^\top K(x)^\top K(x) v_j(x)$$

$$= \alpha(x)^{-2} \cdot ((z(x) \circ A_{*,i})^\top \cdot K(x)^\top K(x) \cdot (z(x) \circ A_{*,j})$$

$$= \alpha(x)^{-2} \cdot (\operatorname{diag}(z(x)) \cdot A_{*,i})^\top \cdot K(x)^\top K(x) \cdot \operatorname{diag}(z(x)) \cdot A_{*,j}$$

$$= A_{*,i}^\top \cdot \alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot K(x)^\top K(x) \cdot \operatorname{diag}(z(x)) \cdot A_{*,j}$$

where the first step follows from the definition of $v_i(x)$ (see Definition 2.1), the second step follows from Fact 2.3, and the last step follows from simple algebra and the definition of z(x) (see Definition 2.1).

Proof of Part 2.

$$\alpha(x)^{-2} \cdot \widetilde{c}(x)^{\top} \cdot (v_{j}(x) \cdot \beta_{i}(x) + v_{i}(x) \cdot \beta_{j}(x))$$

$$= \alpha(x)^{-2} \cdot \widetilde{c}(x)^{\top} \cdot z(x) \circ A_{*,j} \cdot \langle z(x), A_{*,i} \rangle$$

$$+ \alpha(x)^{-2} \cdot \widetilde{c}(x)^{\top} \cdot z(x) \circ A_{*,i} \cdot \langle z(x), A_{*,j} \rangle$$

$$= \alpha(x)^{-2} \cdot \widetilde{c}(x)^{\top} \operatorname{diag}(z(x)) \cdot A_{*,j} \cdot z(x)^{\top} \cdot A_{*,i}$$

$$+ \alpha(x)^{-2} \cdot \widetilde{c}(x)^{\top} \operatorname{diag}(z(x)) \cdot A_{*,i} \cdot z(x)^{\top} \cdot A_{*,j}$$

$$= (A_{*,j}^{\top} \cdot \alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot \widetilde{c}(x) \cdot z(x)^{\top} \cdot A_{*,i})^{\top}$$

$$+ A_{*,i}^{\top} \cdot \alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot \widetilde{c}(x) \cdot (z(x))^{\top} \cdot A_{*,j}$$

$$= A_{*,i}^{\top} \cdot \alpha(x)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x)) \cdot A_{*,j}$$

$$+ A_{*,i}^{\top} \cdot \alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot \widetilde{c}(x) \cdot z(x)^{\top} \cdot A_{*,j}$$

where the first step follows from the definition of $\beta_i(x)$ and $v_i(x)$ (see Definition 2.1), the second step follows from Fact 2.3, the third step follows from Fact 2.3 and the last step follows from simple algebra and the definition of z(x) (see Definition 2.1).

Proof of Part 3.

$$\alpha(x)^{-1} \cdot A_{*,i}^{\top} \operatorname{diag}(\widetilde{c}(x) \circ u_2(x)) A_{*,i}$$
$$= A_{*,i}^{\top} \cdot \alpha(x)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x)) A_{*,i}$$

where the first step follows from the simple algebra.

4.4 Decomposing $B_1(x), B_2(x)$ and $B_3(x)$ into low rank plus diagonal

In this section, we decompose the matrices $B_1(x)$, $B_2(x)$ and $B_3(x)$ into low rank plus diagonal.

Lemma 4.4. Let $x \in \mathbb{R}^d$ be an arbitrary vector. Let $u_1(x), u_2(x), u(x), f(x), c(x), z(x), v_i(x) \in \mathbb{R}^n$ and $\alpha(x), L(x), \beta_i(x) \in \mathbb{R}$ be defined as in Definition 2.1. Let $K(x), B_1(x), B_2(x), B_3(x) \in \mathbb{R}^{n \times n}$ and $\widetilde{c}(x) \in \mathbb{R}^n$ be defined as in Definition 4.1 and $B(x) = B_1(x) + B_2(x) + B_3(x) \in \mathbb{R}^{n \times n}$.

Then, we show that

• Part 1. For $B_1(x) \in \mathbb{R}^{n \times n}$, we have

$$B_1(x) = \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \cdot \underbrace{\operatorname{diag}(z(x))}_{n \times n} \cdot \underbrace{K(x)^{\top}}_{n \times n} \underbrace{K(x)}_{n \times n} \cdot \operatorname{diag}(\underline{z(x)})$$

• Part 2. For $B_2(x) \in \mathbb{R}^{n \times n}$, we have

$$B_{2}(x) = -\underbrace{\alpha(x)^{-2}}_{\text{scalar}} \cdot \underbrace{\widetilde{c}(x)}_{n \times 1} \cdot \underbrace{z(x)^{\top}}_{1 \times n} \cdot \underbrace{\operatorname{diag}(z(x))}_{n \times n}$$
$$- \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \cdot \underbrace{\operatorname{diag}(z(x))}_{n \times n} \cdot \underbrace{z(x)}_{n \times 1} \cdot \underbrace{\widetilde{c}(x)^{\top}}_{1 \times n}$$

• Part 3. For $B_3(x) \in \mathbb{R}^{n \times n}$, we have

$$B_3(x) = \underbrace{\alpha(x)^{-1}}_{\text{scalar}} \cdot \operatorname{diag}(\underbrace{\widetilde{c}(x)}_{n \times 1} \circ \underbrace{u_2(x)}_{n \times 1})$$

• Part 4. For $B(x) \in \mathbb{R}^{n \times n}$, we have

$$B(x) = \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \underbrace{\operatorname{diag}(z(x))}_{n \times n} \cdot \underbrace{K(x)^{\top}}_{n \times n} \underbrace{K(x)}_{n \times n} \cdot \operatorname{diag}(\underline{z(x)})$$

$$- \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \cdot \underbrace{\widetilde{c}(x)}_{n \times 1} \cdot \underbrace{z(x)^{\top}}_{1 \times n} \cdot \underbrace{\operatorname{diag}(z(x))}_{n \times n}$$

$$- \underbrace{\alpha(x)^{-2}}_{\text{scalar}} \cdot \underbrace{\operatorname{diag}(z(x))}_{n \times n} \cdot \underbrace{z(x)}_{n \times 1} \cdot \underbrace{\widetilde{c}(x)^{\top}}_{1 \times n}$$

$$+ \underbrace{\alpha(x)^{-1}}_{\text{scalar}} \cdot \operatorname{diag}(\underbrace{\widetilde{c}(x)}_{n \times 1} \circ \underbrace{u_2(x)}_{n \times 1})$$

$$= \underbrace{\alpha(x)^{-1}}_{\text{scalar}} \cdot \underbrace{\operatorname{diag}(z(x))}_{n \times 1} \cdot \underbrace{u_2(x)}_{n \times 1}$$

Proof. Proof of Part 1

$$A_{*,i}^{\top}B_{1}(x)A_{*,j} = A_{*,i}^{\top}\underbrace{\alpha(x)^{-2}}_{\text{scalar}} \cdot \underbrace{v_{i}(x)^{\top}}_{1\times n} \underbrace{K(x)^{\top}}_{n\times n} \underbrace{K(x)}_{n\times n} \underbrace{v_{i}(x)}_{n\times 1} A_{*,j}$$
$$= A_{*,i}^{\top} \cdot \alpha(x)^{-2} \cdot \operatorname{diag}(z(x))^{\top}$$
$$\cdot K(x)^{\top}K(x) \cdot \operatorname{diag}(z(x)) \cdot A_{*,j}$$

where the first step follows from Definition 4.1, and the last step follows from Lemma 4.3. Thus, by extracting $A_{*,i}^{\top}$ and $A_{*,j}$, we get:

$$B_1(x) = \alpha(x)^{-2} \cdot \operatorname{diag}(z(x))^{\top} \cdot K(x)^{\top} K(x) \cdot \operatorname{diag}(z(x))$$

Proof of Part 2.

$$A_{*,i}^{\top} B_2(x) A_{*,j}$$

$$= -A_{*,i}^{\top} \alpha(x)^{-2} \cdot \widetilde{c}(x)^{\top} \cdot (v_j(x) \cdot \beta_i(x) + v_i(x) \cdot \beta_j(x)) A_{*,j}$$

$$= -(A_{*,i}^{\top} \cdot \alpha(x)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x)) \cdot A_{*,j}$$

$$+ A_{*,i}^{\top} \cdot \alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot \widetilde{c}(x) \cdot z(x)^{\top} \cdot A_{*,j})$$

where the first step follows from the Definition of $A_{*,i}^{\top}B_2(x)A_{*,j}$ (see Definition 4.1), and the last step follows from Lemma 4.3.

Thus, by extracting $A_{*,i}^{\top}$ and $A_{*,j}$, we get:

$$B_2(x) = -(\alpha(x)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))$$

$$+ \alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot \widetilde{c}(x) \cdot z(x)^{\top}$$

Proof of Part 3.

$$A_{*,i}^{\top} B_3(x) A_{*,i} = A_{*,i}^{\top} \cdot \alpha(x)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x)) A_{*,i}$$

where the first step follows from Lemma 4.3.

Thus, by extracting $A_{*,i}^{\top}$ and $A_{*,j}$, we get:

$$B_3(x) = \alpha(x)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x))$$

Proof of Part 4. Since $B(x) = B_1(x) + B_2(x) + B_3(x)$, by combining the first three part, we can get B(x).

5 Rewrite Hessian

In Section 5.1, we present the mathematical properties of the PSD matrices. In Section 5.2, we rewrite the hessian.

5.1 Basic Fact

In this section, we introduce a basic mathematical property.

Fact 5.1. Let f(x) be defined as Definition 2.1

- $0 \leq f(x)f(x)^{\top} \leq I_n$.
- $||f(x)||_1 = 1$

5.2 Re-write Hesisan

For convenient of analysis, we formally make a definition block for B(x).

Definition 5.2. Let $x \in \mathbb{R}^d$ be an arbitrary vector. Let $u_1(x), u_2(x), u(x), f(x), c(x), z(x), v_i(x) \in \mathbb{R}^n$ and $\alpha(x), L(x), \beta_i(x) \in \mathbb{R}$ be defined as in Definition 2.1. Let $K(x) \in \mathbb{R}^{n \times n}$ and $\widetilde{c}(x) \in \mathbb{R}^n$ be defined as in Definition 4.1.

Then, we define $B(x) \in \mathbb{R}^{n \times n}$ as follows:

$$B(x) := \alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot K(x)^{\top} K(x) \cdot \operatorname{diag}(z(x))$$
$$- \alpha(x)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x)) - \alpha(x)^{-2}$$
$$\cdot \operatorname{diag}(z(x)) \cdot \widetilde{c}(x) \cdot z(x)^{\top}$$
$$+ \alpha(x)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x)).$$

Furthermore, we defined $B_{\text{mat}}(x), B_{\text{rank}}(x), B_{\text{diag}}(x) \in \mathbb{R}^{n \times n}$ as follows:

$$B_{\text{mat}}(x) := \alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot K(x)^{\top} K(x) \cdot \operatorname{diag}(z(x))$$

$$B_{\text{rank}}(x) := \alpha(x)^{-2} \cdot (z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))$$

$$+ \operatorname{diag}(z(x)) \cdot \widetilde{c}(x) \cdot z(x)^{\top})$$

$$B_{\text{diag}}(x) := \alpha(x)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x)),$$

so that

$$B(x) = B_{\text{mat}}(x) - B_{\text{rank}}(x) + B_{\text{diag}}(x).$$

6 Hessian is PSD

In this section, we mainly prove Lemma 6.1.

6.1 PSD Lower Bound

Lemma 6.1. Let $x \in \mathbb{R}^d$ be an arbitrary vector. Let $u_1(x), u_2(x), u(x), f(x), c(x), z(x), v_i(x) \in \mathbb{R}^n$ and $\alpha(x), L(x), \beta_i(x) \in \mathbb{R}$ be defined as in Definition 2.1. Let $K(x), B(x), B_{\text{mat}}(x), B_{\text{rank}}(x), B_{\text{diag}}(x) \in \mathbb{R}^{n \times n}$ and $\widetilde{c}(x) \in \mathbb{R}^n$ be defined as in Definition 5.2. Let $1 < \beta < \alpha(x)$.

Then, we have

• Part 1.

$$0 \leq B_{\text{mat}}(x) \leq \beta^{-2} \cdot 16n^2 \exp(2R^2) \cdot I_n$$

• Part 2.

$$-10\beta^{-2}n\exp(R^2)\cdot I_n \leq B_{\text{rank}}(x) \leq 10\beta^{-2}n\exp(R^2)\cdot I_n$$

• Part 3.

$$-4\beta^{-1}n\exp(R^2)\cdot I_n \leq B_{\operatorname{diag}}(x) \leq 4\beta^{-1}n\exp(R^2)\cdot I_n$$

• Part 4.

$$6\beta^{-2}n\exp(R^2)\cdot I_n \le B(x) \le 10\beta^{-2}n^2\exp(2R^2)\cdot I_n$$

Proof. Proof of Part 1.

On the one hand,

$$B_{\text{mat}} = \alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot K(x)^{\top} K(x) \cdot \operatorname{diag}(z(x))$$

$$\leq \alpha(x)^{-2} \| \operatorname{diag}(z(x)) K(x)^{\top} \|^{2} \cdot I_{n}$$

$$\leq \alpha(x)^{-2} \| \operatorname{diag}(z(x)) \|^{2} \| K(x)^{\top} \|^{2} \cdot I_{n}$$

$$\leq \alpha(x)^{-2} \| z(x) \|_{2}^{2} \cdot 4n \cdot I_{n}$$

$$\leq \beta^{-2} \cdot 16n^{2} \exp(2R^{2}) \cdot I_{n}$$

where the first step follows from definition of $B_{\rm mat}$, the second step follows from Part 1 of Fact 2.8, the third step follows from Part 4 of Fact 2.6, the fourth step follows from Part 2,4 of Fact 2.5 and Part 7 of Lemma 7.2, and the final step follows from Part 8 of Lemma 7.2 and $\alpha(x) > \beta$.

On the other hand, since B_{mat} is a positive semi-definite matrix, then $B_{\text{mat}} \succeq 0$.

Proof of Part 2

On the one hand

$$B_{\text{rank}}(x) = \alpha(x)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))$$

$$+ \alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot \widetilde{c}(x) \cdot z(x)^{\top}$$

$$\leq \alpha(x)^{-2} \cdot (z(x)z(x)^{\top}$$

$$+ \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x)) \cdot (\widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x)))^{\top})$$

$$\leq \alpha(x)^{-2} (\|z(x)\|_{2}^{2} + \|\widetilde{c}(x)^{\top} \operatorname{diag}(z(x))\|_{2}^{2}) \cdot I_{n}$$

$$\leq \alpha(x)^{-2} (2\sqrt{n} \exp(R^{2}) + \|\widetilde{c}(x)\|_{2}^{2} \|z(x)\|_{2}^{2}) \cdot I_{n}$$

$$\leq \alpha(x)^{-2} (2\sqrt{n} \exp(R^{2}) + 8n \exp(R^{2})) \cdot I_{n}$$

$$\leq 10\beta^{-2} n \exp(R^{2}) \cdot I_{n}$$

where the first step follows from the definition of $B_{\rm rank}(x)$, the second step follows from Part 4 of Fact 2.8, the third step follows from Part 1 of Fact 2.8, the fourth step follows from Part 8 of Lemma 7.2 and Part 9 of Fact 2.5, the fifth step follows from Part 8, 10 of Lemma 7.2, and the last step follows from n > 1 and $\alpha(x) > \beta$.

On the other hand, the proof of the lower bound is similar to the previous one, we omit it here.

Proof of Part 3

On the one hand

$$B_{\text{diag}}(x) = \alpha(x)^{-1} \cdot \text{diag}(\widetilde{c}(x) \circ u_2(x))$$

$$\leq \alpha(x)^{-1} \|\widetilde{c}(x)\|_2 \|u_2(x)\|_2 \cdot I_n$$

$$\leq 4\beta^{-1} n \exp(R^2) \cdot I_n$$

where the first step follows from the definition of $B_{\text{diag}}(x)$, the second step follows from Part 7 of Fact 2.8, and the last step follows from 1, 10 of Lemma 7.2 and $\alpha(x) > \beta$.

On the other hand, the proof of the lower bound is similar to the previous one, we omit it here.

Proof of Part 4

On the one hand

$$B(x) = B_{\text{mat}}(x) - B_{\text{rank}}(x) + B_{\text{diag}}(x)$$

$$\leq \beta^{-2} \cdot 16n^2 \exp(2R^2) \cdot I_n - 10\beta^{-2}n \exp(R^2) \cdot I_n$$

$$+ 4\beta^{-1}n \exp(R^2) \cdot I_n$$

$$\leq 10\beta^{-2}n^2 \exp(2R^2) \cdot I_n$$

where the first step follows from Definition 5.2, the second step follows Part 1, 2, 3, and the last step follows from $\beta^{-1} > 1$, n > 1, and $\exp(2R^2) > \exp(R^2)$.

On the other hand, we have

$$B(x) = B_{\text{mat}}(x) - B_{\text{rank}}(x) + B_{\text{diag}}(x)$$

$$\succeq 10\beta^{-2}n \exp(R^2) \cdot I_n - 4\beta^{-1}n \exp(R^2) \cdot I_n)$$

$$\succeq 6\beta^{-2}n \exp(R^2) \cdot I_n$$

where the first step follows from Definition 5.2, the second step follows Part 1, 2, 3, and the last step follows from $\beta^{-1} > 1$.

7 Hessian is Lipschitz

In this section, we find the upper bound of $\|\nabla^2 L(x) - \nabla^2 L(y)\|$ and thus proved that $\nabla^2 L$ is Lipschitz. More specifically, in section 7.1, we give a summary of the main properties developed in this whole section. In Section 7.2, we present the upper bound of the norms of the functions we analyzed before. In Section 7.3, we present the Lipschitz properties of the functions we analyzed before. In Section 7.4, we summarize the four steps of the Lipschitz for matrix functions. In

Section 7.5, we analyze the first step of the Lipschitz for matrix function $\alpha(x)^{-2} \cdot \operatorname{diag}(z(x))^{\top} \cdot K(x)^{\top} K(x) \cdot \operatorname{diag}(z(x))$. In Section 7.6, we analyze the second step of the Lipschitz for matrix function $\alpha(x)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))$. In Section 7.7, we analyze the third step of the Lipschitz for matrix function $\alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot \widetilde{c}(x) \cdot z(x)^{\top}$. In Section 7.8, we analyze the fourth step of the Lipschitz for matrix function $\alpha(x)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x))$.

7.1 Main results

In this section, we present the main lemma which is the summary of the properties developed in this whole section.

Lemma 7.1. Let $H(x) = \frac{d^2L}{dx^2}$.

Then we have

$$||H(x) - H(y)|| \le 700\beta^{-4}n^3 \exp(6R^2)||x - y||_2$$

Proof.

$$||H(x) - H(y)|| = ||A|| ||\sum_{i=1}^{4} G_i(x) - G_i(y)|| ||A||$$

$$\leq R^2 \cdot ||\sum_{i=1}^{4} G_i(x) - G_i(y)||$$

$$\leq R^2 \cdot 700\beta^{-4} n^3 \exp(5R^2) ||x - y||_2$$

$$< 700\beta^{-4} n^3 \exp(6R^2) ||x - y||_2$$

where the first step follows from Definition of G_i and matrix spectral norm, the second step follows from $||A|| \leq R$, the second step follows from Lemma 7.4, and the last step follows from $R^2 \leq \exp(R^2)$

7.2 A core Tool: Upper Bound for Several Basic Functions

In this section, we find the upper bound for the norms of the functions we analyze.

Lemma 7.2. Let $R \geq 4$. Let $A \in \mathbb{R}^{n \times d}$ and $x \in \mathbb{R}^d$ satisfy $||A|| \leq R$ and $||x||_2 \leq R$. Let $b \in \mathbb{R}^n$ satisfy $||b||_1 \leq 1$. Let $u_1(x), u_2(x), u(x), f(x), c(x), z(x), v_i(x) \in \mathbb{R}^n$ and $\alpha(x), L(x), \beta_i(x) \in \mathbb{R}$ be defined as in Definition 2.1. Let $K(x), B(x), B_{\text{mat}}(x), B_{\text{rank}}(x), B_{\text{diag}}(x) \in \mathbb{R}^{n \times n}$ and $\widetilde{c}(x) \in \mathbb{R}^n$ be defined as in Definition 5.2. Let $\beta \in (0, 0.1)$, and $\langle \exp(Ax), \mathbf{1}_n \rangle$, $\langle \exp(Ay), \mathbf{1}_n \rangle$, $\langle \exp(Ax) + Ax, \mathbf{1}_n \rangle$, and $\langle \exp(Ay) + Ay, \mathbf{1}_n \rangle$ be greater than or equal to β , respectively. Let $R_f = 2\beta^{-1} \cdot (R \exp(R^2) + R) \cdot (n \cdot \exp(R^2) + \sqrt{n} \cdot R^2)$.

Then, we have

- Part 1. $\|\exp(Ax)\|_2 \le \sqrt{n}\exp(R^2)$
- Part 2. $\|\exp(Ax) + Ax\|_2 \le 2\sqrt{n}\exp(R^2)$
- Part 3. $|\alpha(x)| \ge \beta$
- Part 4. $|\alpha(x)^{-1}| \le \beta^{-1}$
- Part 5. $||f(x)||_2 \le 1$

- Part 6. $||c(x)||_2 \le 2$
- Part 7. $||K(x)|| \le 2\sqrt{n}$
- Part 8 $||z(x)||_2 \le \sqrt{n} \cdot \exp(R^2)$
- Part $9 |\alpha(x)^{-2}| \le \beta^{-2}$
- Part $10 \|\widetilde{c}(x)\|_2 \le 4\sqrt{n}$

Proof. Proof of Part 1

$$\|\exp(Ax)\|_{2} \leq \sqrt{n} \cdot \|\exp(Ax)\|_{\infty}$$

$$\leq \sqrt{n} \cdot \exp(\|(Ax)\|_{\infty})$$

$$\leq \sqrt{n} \cdot \exp(\|(Ax)\|_{2})$$

$$\leq \sqrt{n} \cdot \exp(R^{2})$$

where the first step follows from Part 4 of Fact 2.5, the second step follows from Part 6 of Fact 2.5, the third step follows from Part 6 of Fact 2.5, and the last step follows from $||A|| \le R$ and $||x||_2 \le R$.

Proof of Part 2

$$\| \exp(Ax) + Ax \|_2 \le \| \exp(Ax) \|_2 + \|Ax\|_2$$

 $\le \sqrt{n} \cdot \exp(R^2) + R^2$
 $\le 2\sqrt{n} \exp(R^2)$

where the first step follows from Part 8 of Fact 2.5, the second step follows from Part 1 and $||A|| \le R$, $||x||_2 \le R$, and the last step follows from n > 1, $\exp(R^2) \ge R^2$.

Proof of Part 3

$$|\alpha(x)| = |\langle u(x), \mathbf{1}_n \rangle|$$

$$\geq |\langle \exp(Ax) + Ax, \mathbf{1}_n \rangle|$$

$$> \beta$$

where the first step follows from the definition of $\alpha(x)$ (see Definition 2.1), the second step follows the definition of u(x) (see Definition 2.1), and the last step follows from the assumption $\langle \exp(Ax) + Ax, \mathbf{1}_n \rangle \geq \beta$.

Proof of Part 4

We have

$$|\alpha(x)^{-1}| \le |\beta^{-1}|$$

 $\le \beta^{-1}$

where the first step follows from Part 3 of Lemma 7.2, the second step follows from $\beta^{-1} > 0$.

Proof of Part 5

$$||f(x)||_2 \le ||f(x)||_1$$
= 1

where the first step follows from $||f(x)||_2 \le ||f(x)||_1 \le 1$.

Proof of Part 6

$$||c(x)|| = ||f(x) - b||_2$$

 $\leq ||f(x)||_2 + ||b||_2$
 ≤ 2

where the first step follows from the definition of c(x) (see Definition 2.1), the second step follows from Part 8 of Fact 2.5, and the last step follows from Part 5 of Lemma 7.2 and $||b||_2 \le ||b||_1 \le 1$.

Proof of Part 7

$$||K(x)|| = ||(I_n - f(x) \cdot \mathbf{1}_n^\top)||$$

$$\leq ||I_n|| + ||f(x) \cdot \mathbf{1}_n^\top||$$

$$\leq 1 + ||f(x)||_2 \cdot ||\mathbf{1}_n^\top||_2$$

$$\leq 1 + 1 \cdot \sqrt{n}$$

$$\leq 2\sqrt{n}$$

where the first step follows from the Definition of K(x), the second step follows from the Part 3 of Fact 2.6, the third step follows from $||I_n|| = 1$ and Part 9 of Fact 2.5, and the fourth step follows from Part 5 of Lemma 7.2, and the last step follows from the simple algebra.

Proof of Part 8

$$||z(x)||_2 = ||u_2(x) + \mathbf{1}_n||$$

$$\leq ||u_2(x)||_2 + ||\mathbf{1}_n||_2$$

$$\leq \sqrt{n} \cdot (\exp(R^2) + 1)$$

$$\leq 2\sqrt{n} \exp(R^2)$$

where the first step follows from the the definition of z(x) (see Definition 2.1), the second step follows from Part 8 of Fact 2.5, the third step follows from Part 1 of Lemma 7.2, and the last step follows from Fact 2.7.

Proof of Part 9

$$|\alpha(x)^{-2}| = |\alpha(x)^{-1}|^2$$

$$\leq \beta^{-2}$$

where the first step follows from simple algebra, and the last step follows from Part 4 of Lemma 7.2 **Proof of Part 10**

$$\|\widetilde{c}(x)\|_2 = \|K(x)^{\top} c(x)\|_2$$

 $\leq \|K(x)\| \|c(x)\|_2$
 $\leq 4\sqrt{n}$

where the first step follows from Definition of $\widetilde{c}(x)$, the second step follows from Part 7 of Fact 2.6, and the last step follows from Part 6 and 7 of Lemma 7.2.

7.3 A core Tool: Lipschitz Property for Several Basic Functions

In this section, we present the Lipschitz property for the functions we analyze.

Lemma 7.3 (Basic Functions Lipschitz Property). Let $R \geq 4$. Let $A \in \mathbb{R}^{n \times d}$ and $x \in \mathbb{R}^d$ satisfy $||A|| \leq R$ and $||x||_2 \leq R$. Let $b \in \mathbb{R}^n$ satisfy $||b||_1 \leq 1$. Let $u_1(x), u_2(x), u(x), f(x), c(x), z(x), v_i(x) \in \mathbb{R}^n$ and $\alpha(x), L(x), \beta_i(x) \in \mathbb{R}$ be defined as in Definition 2.1. Let $K(x), B(x), B_{\max}(x), B_{\max}(x), B_{\dim}(x), B_{\dim}(x) \in \mathbb{R}^{n \times n}$ and $\widetilde{c}(x) \in \mathbb{R}^n$ be defined as in Definition 5.2. Let $\beta \in (0, 0.1)$, and $\langle \exp(Ax), \mathbf{1}_n \rangle$, $\langle \exp(Ay), \mathbf{1}_n \rangle$, $\langle \exp(Ay) + Ax, \mathbf{1}_n \rangle$, and $\langle \exp(Ay) + Ay, \mathbf{1}_n \rangle$ be greater than or equal to β , respectively. Let $R_f = 6\beta^{-2} \cdot n \cdot \exp(3R^2)$.

Then, we have

- Part 1. $||Ax Ay||_2 \le R \cdot ||x y||_2$
- Part 2. $\|\exp(Ax) \exp(Ay)\|_2 \le R\exp(R^2) \cdot \|x y\|_2$
- Part 3. $|\alpha(x) \alpha(y)| \le 2\sqrt{n}R \exp(R^2)||x y||_2$
- Part 4. $|\alpha(x)^{-1} \alpha(y)^{-1}| \le \beta^{-2} \cdot |\alpha(x) \alpha(y)|$
- Part 5. $||f(x) f(y)||_2 \le R_f \cdot ||x y||_2$
- Part 6. $||c(x) c(y)||_2 \le R_f \cdot ||x y||_2$
- Part 7. $||z(x) z(y)||_2 \le R \exp(R^2) ||x y||_2$
- Part 8. $||K(x) K(y)|| \le \sqrt{n} \cdot R_f \cdot ||x y||_2$
- $Part \ 9$. $\|\operatorname{diag}(z(x)) \operatorname{diag}(z(y))\| \le R \exp(R^2) \|x y\|_2$
- Part 10. $|\alpha(x)^{-2} \alpha(y)^{-2}| \le 2\beta^{-3}|\alpha(x) \alpha(y)|$
- Part 11. $\|\widetilde{c}(x) \widetilde{c}(y)\|_2 \le 4\sqrt{n} \cdot R_f \cdot \|x y\|_2$
- Part 12. $\|\operatorname{diag}(\widetilde{c}(x) \circ u_2(x)) \operatorname{diag}(\widetilde{c}(y) \circ u_2(y))\| \le 48n^2 \cdot 6\beta^{-2} \exp(4R^2) \|x y\|_2$

Proof. Proof of Part 1

$$||Ax - Ay||_2 \le ||A||_2 ||x - y||_2$$

 $\le R \cdot ||x - y||_2$

where the first step follows from Part 7 of Fact 2.6, and the last step follows from $||A|| \le R$ and $||x||_2 \le R$.

Proof of Part 2

$$\|\exp(Ax) - \exp(Ay)\|_2 \le \exp(R^2) \|Ax - Ay\|_2$$

 $\le \exp(R^2) \|A\| \|x - y\|_2$
 $\le R \exp(R^2) \|x - y\|_2$

where the first step follows from Part 10 of Fact 2.5, the second step follows from Part 4 of Fact 2.6, the third step follows from $||A|| \le R$.

$$|\alpha(x) - \alpha(y)|$$

$$= |\langle (\exp(Ax) + Ax) - (\exp(Ay) + Ay), \mathbf{1}_n \rangle|$$

$$\leq \|(\exp(Ax) + Ax) - (\exp(Ay) + Ay)\|_2 \cdot \sqrt{n}$$

$$\leq (\|\exp(Ax) - \exp(Ay)\|_2 + \|Ax - Ay\|_2) \cdot \sqrt{n}$$

$$\leq \sqrt{n}(R\exp(R^2) + R) \cdot \|x - y\|_2$$

$$\leq 2\sqrt{n}R\exp(R^2) \cdot \|x - y\|_2$$

where the first step follows from the definition of $\alpha(x)$ (see Definition 2.1), the second step follows from Part 1 of Fact 2.5 (Cauchy-Schwarz inequality), the third step follows from Part 8 of Fact 2.5, the fourth step follows from Part 1 and 2 of Lemma 7.3, and the last step follows from Part 1 of Fact 2.7.

Proof of Part 4

$$|\alpha(x)^{-1} - \alpha(y)^{-1}| = \alpha(x)^{-1} \cdot \alpha(y)^{-1} |\alpha(x) - \alpha(y)|$$

 $\leq \beta^{-2} \cdot |\alpha(x) - \alpha(y)|$

where the first step follows from the simple algebra, and the last step follows from $\alpha(x)$, $\alpha(y) \ge \beta$. **Proof of Part 5**

$$||f(x) - f(y)||_{2}$$

$$= ||\alpha(x)^{-1} \cdot (\exp(x) + Ax) - \alpha(y)^{-1} \cdot (\exp(y) + Ay)||_{2}$$

$$\leq ||\alpha(x)^{-1} \cdot (\exp(x) + Ax) - \alpha(x)^{-1} \cdot (\exp(y) + Ay)||_{2}$$

$$+ ||\alpha(x)^{-1} \cdot (\exp(y) + Ay) - \alpha(y)^{-1} \cdot (\exp(y) + Ay)||_{2}$$

$$\leq \alpha(x)^{-1} \cdot ||(\exp(x) + Ax) - (\exp(y) + Ay)||_{2}$$

$$+ |\alpha(x)^{-1} - \alpha(y)^{-1}|||\exp(Ay) + Ay||$$

where the first step follows from the definition of f(x) and $\alpha(x)$ (see Definition 2.1), the second step follows from triangle inequality (Part 3 of Fact 2.5), and the last step follows from Part 7 of Fact 2.5.

For the first term in the above, we have

$$\alpha(x)^{-1} \cdot \|(\exp(x) + Ax) - (\exp(y) + Ay)\|_{2}$$

$$\leq \beta^{-1} \cdot \|(\exp(x) + Ax) - (\exp(y) + Ay)\|_{2}$$

$$\leq \beta^{-1} \cdot (\|\exp(x) - \exp(y)\|_{2} + \|Ax - Ay\|_{2})$$

$$\leq \beta^{-1} \cdot (R\exp(R^{2})\|x - y\|_{2} + R \cdot \|x - y\|_{2})$$

$$= \beta^{-1} \cdot (R\exp(R^{2}) + R) \cdot \|x - y\|_{2}$$

$$\leq 2\beta^{-1} \cdot R\exp(R^{2}) \cdot \|x - y\|_{2}$$

$$\leq 2\beta^{-1} \cdot R\exp(R^{2}) \cdot \|x - y\|_{2}$$
(1)

where the first step follows from $\alpha(x) \geq \beta$, the second step follows from Part 8 of Fact 2.5, the third step follows from Part 1 and Part 2 of Lemma 7.3, the fourth step follows from simple algebra, and the last step follows from Part 1 of Fact 2.7.

For the second term in the above, we have

$$|\alpha(x)^{-1} - \alpha(y)^{-1}| \| \exp(Ay) + Ay \|_{2}$$

$$\leq \beta^{-2} \cdot |\alpha(x) - \alpha(y)| \cdot \| \exp(Ay) + Ay \|_{2}$$

$$\leq \beta^{-2} \cdot |\alpha(x) - \alpha(y)| \cdot 2\sqrt{n} \exp(R^{2})$$

$$\leq \beta^{-2} \cdot 2R \exp(R^{2}) \cdot \|x - y\|_{2} \cdot \sqrt{n} \cdot 2\sqrt{n} \exp(R^{2})$$

$$= 4\beta^{-2} \cdot R \cdot n \exp(2R^{2}) \cdot \|x - y\|_{2}$$
(2)

where the first step follows from the result of Part 4 of Lemma 7.3, the second step follows from the result of Part 2 of Lemma 7.2, the third step follows from the result of Part 1,2, and 3 of Lemma 7.3, and the last step follows from simple algebra.

Combining Eq. (1) and Eq. (2) together, we have

$$||f(x) - f(y)||_2 \le 2\beta^{-1} \cdot R \exp(R^2) \cdot ||x - y||_2 + 4\beta^{-2} \cdot n \cdot R \exp(2R^2) \cdot ||x - y||_2 \le 6\beta^{-2} \cdot n \cdot \exp(3R^2) \cdot ||x - y||_2$$

where the first step follows the combination of Eq. (1) and Eq. (2), and the last step follows from $\beta^{-1} \ge 1$ and $n \ge 1, R \ge 4, \exp(R^2) \ge R$.

Proof of Part 6

$$||c(x) - c(y)||_2 = ||f(x) - f(y)||_2$$

 $\leq R_f \cdot ||x - y||_2$

where the first step follows from the definition of c(x) (see Definition 2.1), and the last step follows from Part 5 of Lemma 7.3.

Proof of Part 7

$$||z(x) - z(y)||_2 = ||u_2(x) + \mathbf{1}_n - u_2(y) - \mathbf{1}_n||$$

= $||u_2(x) - u_2(y)||_2$
 $\leq R \exp(R^2) ||x - y||_2$

where the first step follows from the definition of z(x) (see Definition 2.1), the second step follows from simple algebra, and the last step follows from the definition of $u_2(x)$ (see Definition 2.1) and Part 2 of Lemma 7.3.

Proof of Part 8

$$||K(x) - K(y)|| = ||(I_n - f(x) \cdot \mathbf{1}_n^\top) - (I_n - f(y) \cdot \mathbf{1}_n^\top)||$$

$$= || - (f(x) - f(y)) \cdot \mathbf{1}_n^\top||$$

$$\leq ||f(x) - f(y)||_2 \cdot ||\mathbf{1}_n^\top||_2$$

$$\leq \sqrt{n} \cdot R_f \cdot ||x - y||_2$$

where the first step follows from K(x), the second step follows from the simple algebra, the third step follows from Part 9 of Fact 2.5, and the last step follows from Part 5 of Lemma 7.3.

Proof of Part 9

$$\|\operatorname{diag}(z(x)) - \operatorname{diag}(z(y))\| = \|\operatorname{diag}(z(x) - z(y))\|$$

$$\leq \|z(x) - z(y)\|_{\infty}$$

$$\leq \|z(x) - z(y)\|_{2}$$

$$\leq R \exp(R^{2}) \|x - y\|_{2}$$

where the first step follows from the simple algebra, the second step follows from Part 2 of Fact 2.5, the third step follows from Part 4 of Fact 2.5, and the last step follows from Part 7 of Lemma 7.3.

$$|\alpha(x)^{-2} - \alpha(y)^{-2}| = |(\alpha(x)^{-1} - \alpha(y)^{-1})(\alpha(x)^{-1} + \alpha(y)^{-1})|$$

$$\leq |\alpha(x)^{-1} - \alpha(y)^{-1}| |\alpha(x)^{-1} + \alpha(y)^{-1}|$$

$$\leq \beta^{-2} \cdot |\alpha(x) - \alpha(y)| \cdot |2\beta^{-1}|$$

$$\leq 2\beta^{-3} |\alpha(x) - \alpha(y)|$$

$$\leq 4\beta^{-3} \sqrt{n} R \exp(R^2) \cdot ||x - y||_2$$

where the first step follows from the simple algebra, the second step follows from the simple algebra, the third step follows from Part 4 of Lemma 7.2, and Part 4 of Lemma 7.3, the fourth step follows from the simple algebra, and the last step follows from Part 3 of Lemma 7.3.

Proof of Part 11

$$\|\widetilde{c}(x) - \widetilde{c}(y)\|_{2}$$

$$= \|K(x)^{\top} c(x) - K(y)^{\top} c(y)\|$$

$$\leq \|K(x)^{\top} c(x) - K(y)^{\top} c(x)\| + \|K(y)^{\top} c(x) - K(y)^{\top} c(y)\|$$

$$\leq \|K(x)^{\top} - K(y)^{\top}\| \cdot \|c(x)\|_{2} + \|K(y)^{\top}\| \cdot \|c(x) - c(y)\|_{2}$$

$$\leq \sqrt{n} R_{f} \cdot \|x - y\|_{2} \cdot 2 + 2\sqrt{n} \cdot R_{f} \cdot \|x - y\|_{2}$$

$$\leq 4\sqrt{n} \cdot R_{f} \cdot \|x - y\|_{2}$$

where the first step follows from Definition of $\tilde{c}(x)$, the second step follows from the triangle inequality, the third step follows from Part 7 of Fact 2.6, the fourth step follows from Part 6, 8 of Lemma 7.3 and 6, 7 of Lemma 7.2, and the last step follows from the simple algebra.

Proof of Part 12

$$\|\operatorname{diag}(\widetilde{c}(x) \circ u_{2}(x)) - \operatorname{diag}(\widetilde{c}(y) \circ u_{2}(y))\|$$

$$\leq \|\operatorname{diag}(\widetilde{c}(x))\operatorname{diag}(u_{2}(x)) - \operatorname{diag}(\widetilde{c}(y))\operatorname{diag}(u_{2}(y))\|$$

$$\leq \|\operatorname{diag}(\widetilde{c}(x))\operatorname{diag}(u_{2}(x)) - \operatorname{diag}(\widetilde{c}(x))\operatorname{diag}(u_{2}(y))\|$$

$$+ \|\operatorname{diag}(\widetilde{c}(y))\operatorname{diag}(u_{2}(x)) - \operatorname{diag}(\widetilde{c}(y))\operatorname{diag}(u_{2}(y))\|$$

$$\leq \|\operatorname{diag}(\widetilde{c}(x)) - \operatorname{diag}(\widetilde{c}(y))\|\|\operatorname{diag}(u_{2}(x))\|$$

$$+ \|\operatorname{diag}(\widetilde{c}(y))\|\|\operatorname{diag}(u_{2}(x)) - \operatorname{diag}(u_{2}(y))\|$$

$$\leq \|\widetilde{c}(x) - \widetilde{c}(y)\|_{2} \cdot \|u_{2}(x)\|_{2} + \|\widetilde{c}(y)\|_{2} \cdot \|u_{2}(x) - u_{2}(y)\|_{2}$$

$$\leq 4\sqrt{n} \cdot R_{f}\|x - y\|_{2}\sqrt{n}\exp(R^{2}) + 4\sqrt{n}R\exp(R^{2})\|x - y\|_{2}$$

$$\leq (24n^{2} \cdot \beta^{-2}\exp(4R^{2}) + 4\sqrt{n}\exp(2R^{2}))\|x - y\|_{2}$$

$$\leq 48n^{2} \cdot \beta^{-2}\exp(4R^{2})\|x - y\|_{2}$$

where the first step follows from Fact 2.3, the second step follows from triangle inequality, the third step follows from Part 4 of Fact 2.6, the fourth step follows from 2 and 4 of Fact 2.5, the fifth step follows from Part 2,11 of Lemma r7.3 and Part 1,10 of Lemma 7.2, the sixth step follows from definition of R_f , and the last step follows from R > 4, R > 1, R > 1, R > 1 and R > 1, R > 1

7.4 Summary of Four Steps

In this section, we summarize the four steps which are discussed in the next four sections, respectively.

Lemma 7.4. If the following conditions hold

•
$$G_1(x) = \alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot K(x)^{\top} K(x) \cdot \operatorname{diag}(z(x))$$

•
$$G_2(x) = -\alpha(x)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))$$

•
$$G_3(x) = -\alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot \widetilde{c}(x) \cdot z(x)^{\top}$$

•
$$G_4(x) = \alpha(x)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x))$$

Then, we have

$$\sum_{i=1}^{4} \|G_i(x) - G_i(y)\| \le 700\beta^{-4} n^3 \exp(5R^2)$$

Proof.

$$\sum_{i=1}^{4} \|G_i(x) - G_i(y)\| \le 200\beta^{-4} n^3 \exp(5R^2) \cdot \|x - y\|_2$$

$$+ 200\beta^{-4} n^2 \exp(5R^2) \cdot \|x - y\|_2$$

$$+ 200\beta^{-4} n^2 \exp(5R^2) \cdot \|x - y\|_2$$

$$+ 100\beta^{-3} n^2 \cdot \exp(4R^2) \|x - y\|_2$$

$$\le 700\beta^{-4} n^3 \exp(5R^2) \|x - y\|_2$$

where the first step follows from Lemma 7.5, 7.6, 7.7, 7.8, the last step follows from $\beta^{-1} > 1, n > 1, R > 4$.

7.5 Calculation: Step 1 Lipschitz for Matrix Function $\alpha(x)^{-2} \cdot \operatorname{diag}(z(x))^{\top} \cdot K(x)^{\top} K(x) \cdot \operatorname{diag}(z(x))$

In this section, we analyze the first step, namely the Lipschitz for the matrix function $\alpha(x)^{-2}$ · $\operatorname{diag}(z(x))^{\top} \cdot K(x)^{\top} K(x) \cdot \operatorname{diag}(z(x))$.

Lemma 7.5. Let $G_1(x) = \alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot K(x)^{\top} K(x) \cdot \operatorname{diag}(z(x))$. Then we have

$$||G_1(x) - G_1(y)|| \le 200\beta^{-4}n^3 \exp(5R^2) \cdot ||x - y||_2$$

Proof. We define

$$G_{1,1} := \alpha(x)^{-2} \operatorname{diag}(z(x)) K(x)^{\top} K(x) \operatorname{diag}(z(x))$$

$$- \alpha(y)^{-2} \operatorname{diag}(z(x)) K(x)^{\top} K(x) \operatorname{diag}(z(x))$$

$$G_{1,2} := \alpha(y)^{-2} \operatorname{diag}(z(x)) K(x)^{\top} K(x) \operatorname{diag}(z(x))$$

$$- \alpha(y)^{-2} \operatorname{diag}(z(y)) K(x)^{\top} K(x) \operatorname{diag}(z(x))$$

$$G_{1,3} := \alpha(y)^{-2} \operatorname{diag}(z(y)) K(x)^{\top} K(x) \operatorname{diag}(z(x))$$

$$- \alpha(y)^{-2} \operatorname{diag}(z(y)) K(y)^{\top} K(x) \operatorname{diag}(z(x))$$

$$G_{1,4} := \alpha(y)^{-2} \operatorname{diag}(z(y)) K(y)^{\top} K(x) \operatorname{diag}(z(x))$$

$$- \alpha(y)^{-2} \operatorname{diag}(z(y)) K(y)^{\top} K(y) \operatorname{diag}(z(x))$$

$$G_{1,5} := \alpha(y)^{-2} \operatorname{diag}(z(y)) K(y)^{\top} K(y) \operatorname{diag}(z(x))$$

$$-\alpha(y)^{-2}\operatorname{diag}(z(y))K(y)^{\top}K(y)\operatorname{diag}(z(y))$$

we have

$$G_1 = G_{1.1} + G_{1.2} + G_{1.3} + G_{1.4} + G_{1.5}$$

Let's prove the $G_{1,1}$,

$$||G_{1,1}||$$

$$= ||\alpha(x)^{-2}\operatorname{diag}(z(x))K(x)^{\top}K(x)\operatorname{diag}(z(x))$$

$$- \alpha(y)^{-2}\operatorname{diag}(z(x))K(x)^{\top}K(x)\operatorname{diag}(z(x))||$$

$$\leq |\alpha(x)^{-2} - \alpha(y)^{-2}| \cdot ||\operatorname{diag}(z(x))K(x)^{\top}K(x)\operatorname{diag}(z(x))||$$

$$\leq |\alpha(x)^{-2} - \alpha(y)^{-2}|$$

$$\cdot ||\operatorname{diag}(z(x))|| \cdot ||K(x)^{\top}|||K(x)|| \cdot ||\operatorname{diag}(z(x))||$$

$$\leq |\alpha(x)^{-2} - \alpha(y)^{-2}| \cdot ||z(x)||_{\infty}^{2} \cdot ||K(x)||^{2}$$

$$\leq 2\beta^{-3}|\alpha(x) - \alpha(y)| \cdot ||z(x)||_{2}^{2} \cdot (2\sqrt{n})^{2}$$

$$\leq 2\beta^{-3} \cdot 4n \cdot (2\sqrt{n}\exp(R^{2}))^{2} \cdot 2\sqrt{n}R\exp(R^{2}) \cdot ||x - y||_{2}$$

$$\leq 64\beta^{-3}n^{1.5}R \cdot \exp(3R^{2})||x - y||_{2}$$

$$\leq 64\beta^{-3}n^{1.5} \cdot \exp(4R^{2})||x - y||_{2}$$

where the first step follows from Definition of $G_{1,1}$, the second step follows from Part 6 of Fact 2.6, the third step follows from Part 4 of Fact 2.6, the fourth step follows from Part 2 of Fact 2.5, the fifth step follows from Part 4 of Fact 2.5 and Part 10 of Lemma 7.3, the sixth step follows from Part 8 of Lemma 7.2, the seventh step follows from simple algebra, and the last step follows from $R \leq \exp(R^2)$.

Then let's prove the $G_{1,2}$

$$||G_{1,2}||$$

$$= ||\alpha(y)^{-2} \operatorname{diag}(z(x))K(x)^{\top}K(x) \operatorname{diag}(z(x))$$

$$- \alpha(y)^{-2} \operatorname{diag}(z(y))K(x)^{\top}K(x) \operatorname{diag}(z(x))||$$

$$\leq ||\operatorname{diag}(z(x)) - \operatorname{diag}(z(y))||$$

$$\cdot ||\alpha(y)^{-2}K(x)^{\top}K(x) \operatorname{diag}(z(x))||$$

$$\leq R \exp(R^{2})||x - y||_{2} \cdot |\alpha(y)^{-2}|||K(x)^{\top}||||K(x)|| \cdot ||\operatorname{diag}(z(x))||$$

$$\leq R \exp(R^{2})||x - y||_{2} \cdot \beta^{-2} \cdot ||z(x)||_{2} \cdot 4n$$

$$\leq 4\beta^{-2} \cdot n \cdot R \exp(R^{2}) \cdot 2\sqrt{n} \cdot \exp(R^{2})||x - y||_{2}$$

$$\leq 8\beta^{-2}n^{1.5} \exp(3R^{2})||x - y||_{2}$$

where the first step follows from the Definition of $G_{1,2}$, the second step follows from the Part 6 of Fact 2.6, the third step follows from Part 4 of Fact 2.6 and Part 10 of Lemma 7.3, the fourth step follows from the Part 10 of Lemma 7.2 and Part 2 of Lemma 2.5, the fifth step follows from Part 8 of Lemma 7.2, and the last step follows from $R \leq \exp(R^2)$

Let's prove the $G_{1,3}$

$$||G_{1,3}||$$

$$= \|\alpha(y)^{-2} \operatorname{diag}(z(y)) K(x)^{\top} K(x) \operatorname{diag}(z(x)) - \alpha(y)^{-2} \operatorname{diag}(z(y)) K(y)^{\top} K(x) \operatorname{diag}(z(x)) \| \leq \|K(x)^{\top} - K(y)^{\top} \| \cdot \|\alpha(y)^{-2} \operatorname{diag}(z(y)) K(x) \operatorname{diag}(z(x)) \| \leq \|K(x)^{\top} - K(y)^{\top} \| |\alpha(y)^{-2}| \cdot \| \operatorname{diag}(z(y)) \| \cdot \| K(x) \| \cdot \| \operatorname{diag}(z(x)) \| \leq \sqrt{n} \cdot R_f \cdot \|x - y\|_2 \cdot \beta^{-2} \cdot \|z(y)\|_2 \cdot \|z(x)\|_2 \cdot 2\sqrt{n} \leq 2n \cdot \beta^{-2} \cdot (2\sqrt{n} \cdot \exp(R^2))^2 \cdot \|x - y\|_2 \leq 8\beta^{-2} \cdot n^2 \cdot R_f \cdot \exp(2R^2) \cdot \|x - y\|_2 \leq 48\beta^{-4} \cdot n^3 \cdot \exp(5R^2) \cdot \|x - y\|_2$$

where the first step follows from the Definition of $G_{1,3}$, the second step follows from Part 4 of Fact 2.6, the third step follows from Part 4, 6 of Fact 2.6, the fourth step follows from Part 8 of Lemma 7.3 and Part 3 of Fact 2.5, the fifth step follows from Part 8 of Lemma 7.2, the sixth step follows from simple algebra, and the last step follows from $R_f = 6\beta^{-2} \cdot n \cdot \exp(3R^2)$.

Proof of $G_{1,4}$ is similar to $G_{1,3}$, and the proof of $G_{1,5}$ is similar to $G_{1,2}$, so we skip them. Then, by combining all results we get

$$||G_1(x) - G_1(y)|| = ||G_{1,1} + G_{1,2} + G_{1,3} + G_{1,4} + G_{1,5}||$$

$$\leq 64\beta^{-3}n^{1.5} \cdot \exp(4R^2)||x - y||_2$$

$$+ 16\beta^{-2}n^{1.5} \exp(3R^2)||x - y||_2$$

$$+ 48\beta^{-4} \cdot n^3 \cdot \exp(5R^2) \cdot ||x - y||_2$$

$$\leq 200\beta^{-4}n^3 \exp(5R^2) \cdot ||x - y||_2$$

where the first step follows from the Definitions of $G_{1,1}$, $G_{1,2}$, $G_{1,3}$, $G_{1,4}$, $G_{1,5}$, the second step follows from previous results, and the last step follows from simple algebra

7.6 Calculation: Step 2 Lipschitz for Matrix Function $\alpha(x)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))$

In this section, we analyze the second step, namely the Lipschitz for the matrix function $\alpha(x)^{-2}$ $\cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))$.

Lemma 7.6. Let
$$G_2(x) = \alpha(x)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))$$
.
Then we have

$$||G_2(x) - G_2(y)|| \le 200\beta^{-4}n^2 \exp(5R^2) \cdot ||x - y||_2$$

Proof. We define

$$G_{2,1} := -(\alpha(x)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))$$

$$-\alpha(y)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x)))$$

$$G_{2,2} := -(\alpha(y)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))$$

$$-\alpha(y)^{-2} \cdot z(y) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x)))$$

$$G_{2,3} := -(\alpha(y)^{-2} \cdot z(y) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))$$

$$-\alpha(y)^{-2} \cdot z(y) \cdot \widetilde{c}(y)^{\top} \cdot \operatorname{diag}(z(x)))$$

$$G_{2,4} := -(\alpha(y)^{-2} \cdot z(y) \cdot \widetilde{c}(y)^{\top} \cdot \operatorname{diag}(z(x))$$

$$-\alpha(y)^{-2} \cdot z(y) \cdot \widetilde{c}(y)^{\top} \cdot \operatorname{diag}(z(y)))$$

Then let's prove $G_{2,1}$ first

$$||G_{2,1}||$$

$$= || - (\alpha(x)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))$$

$$- \alpha(y)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x)))||$$

$$\leq |\alpha(x)^{-2} - \alpha(y)^{-2}| \cdot ||z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))||$$

$$\leq 4\beta^{-3} \sqrt{n} R \exp(R^{2}) \cdot ||x - y||_{2} \cdot ||z(x)||_{2} \cdot ||\widetilde{c}(x)^{\top}||_{2}$$

$$\cdot ||z(x)||_{2}$$

$$\leq 4\beta^{-3} \sqrt{n} R \exp(R^{2}) \cdot ||x - y||_{2} \cdot 4n \cdot \exp(2R^{2}) \cdot 4\sqrt{n}$$

$$\leq 64\beta^{-3} n^{2} \cdot \exp(4R^{2}) \cdot ||x - y||_{2}$$

where the first step follows from definition of $G_{2,1}$, the second step follows from Part 6 of Fact 2.6, the third step follows from Part 10 of Lemma 7.2 and Part 7 of Fact 2.6, the fourth step follows from Part 8, 10 of Lemma 7.2, and the last step follow from simple algebra.

let's prove $G_{2,2}$

$$||G_{2,2}||$$

$$= || - (\alpha(y)^{-2} \cdot z(x) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))$$

$$- \alpha(y)^{-2} \cdot z(y) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x)))||$$

$$\leq ||z(x) - z(y)||_{2} \cdot ||\alpha(y)^{-2} \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x))||_{2}$$

$$\leq R \exp(R^{2}) \cdot ||x - y||_{2} \cdot |\alpha(y)^{-2}| \cdot ||\widetilde{c}(x)^{\top}||_{2} \cdot ||z(x)||_{2}$$

$$\leq R \exp(R^{2}) \cdot ||x - y||_{2} \cdot \beta^{-2} \cdot 4\sqrt{n} \cdot 2\sqrt{n} \exp(R^{2})$$

$$\leq 8\beta^{-2} n \exp(3R^{2}) \cdot ||x - y||_{2}$$

where the first step follows from the definition of $G_{2,2}$, the second step follows from Part 9 of Fact 2.5, the third step follows from Part 2, 4, and 8 of Fact 2.5, the fourth step follows from Part 8,9, and 10 of Lemma 7.2, and the last step follows from $\exp(R^2) > R$.

Then, let's prove $G_{2,3}$

$$||G_{2,3}|| = || - (\alpha(y)^{-2} \cdot z(y) \cdot \widetilde{c}(x)^{\top} \cdot \operatorname{diag}(z(x)) - \alpha(y)^{-2} \cdot z(y) \cdot \widetilde{c}(y)^{\top} \cdot \operatorname{diag}(z(x)))||$$

$$\leq ||\widetilde{c}(x)^{\top} - \widetilde{c}(y)^{\top}||_{2} \cdot ||\alpha(y)^{-2} \cdot z(y) \cdot \operatorname{diag}(z(x))||_{2}$$

$$\leq 4\sqrt{n} \cdot R_{f} \cdot ||x - y||_{2} \cdot |\alpha(y)^{-2}| \cdot ||z(y)||_{2} \cdot ||z(x)||_{2}$$

$$\leq 4\sqrt{n} \cdot \beta^{-2} \cdot R_{f} \cdot 4n \exp(2R^{2}) \cdot ||x - y||_{2}$$

$$\leq 100\beta^{-4}n^{2} \exp(5R^{2})||x - y||_{2}$$

where the first step follows from the definition of $G_{2,3}$, the second step follows from Part 9 of Fact 2.5, the third step follows from Part 2, 4, and 8 of Fact 2.5, the fourth step follows from Part 8 of Lemma 7.2, and the last step follows from $R_f = 6\beta^{-2} \cdot n \cdot \exp(3R^2)$

Let's prove $G_{2,4}$

$$||G_{2,4}|| = || - (\alpha(y)^{-2} \cdot z(y) \cdot \widetilde{c}(y)^{\top} \cdot \operatorname{diag}(z(x)) - \alpha(y)^{-2} \cdot z(y) \cdot \widetilde{c}(y)^{\top} \cdot \operatorname{diag}(z(y)))||$$

$$\leq ||\alpha(y)^{-2} \cdot z(y) \cdot \widetilde{c}(y)^{\top}|| || \operatorname{diag}(z(x)) - \operatorname{diag}(z(y))||$$

$$\leq |\alpha(y)^{-2}| \cdot ||z(y)||_{2} \cdot ||\widetilde{c}(x)^{\top}||_{2} \cdot R \exp(R^{2}) \cdot ||x - y||_{2}$$

$$\leq \beta^{-2} \cdot 2\sqrt{n} \cdot \exp(R^{2}) \cdot 4\sqrt{n} \cdot R \exp(R^{2}) \cdot ||x - y||_{2}$$

$$\leq 8\beta^{-2} n \exp(3R^{2}) ||x - y||_{2}$$

where the first step follows from the definition of $G_{2,4}$, the second step follows from Part 4 of Fact 2.6, the third step follows from Part 8 of Fact 2.5, the fourth step follows from Part 8,9, and 10 of Lemma 7.2, and the last step follows from simple algebra.

Finally, by combining above results we can get

$$||G_2(x) - G_2(y)|| = ||G_{2,1} + G_{2,2} + G_{2,3} + G_{2,4}||$$

$$\leq 64\beta^{-3}n^2 \cdot \exp(4R^2) \cdot ||x - y||_2$$

$$+ 16\beta^{-2}n \exp(3R^2) \cdot ||x - y||_2$$

$$+ 100\beta^{-4}n^2 \exp(5R^2)||x - y||_2$$

$$\leq 200\beta^{-4}n^2 \exp(5R^2) \cdot ||x - y||_2$$

where the first step follows from the definitions of $G_{1,1}, G_{1,2}, G_{1,3}, G_{1,4}, G_{1,5}$, the second step follows from previous results, and the last step follows from simple algebra.

7.7 Calculation: Step 3 Lipschitz for Matrix Function $\alpha(x)^{-2} \cdot \mathrm{diag}(z(x)) \cdot \widetilde{c}(x) \cdot z(x)^{\top}$

In this section, we analyze the third step, namely the Lipschitz for the matrix function $\alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot \widetilde{c}(x) \cdot z(x)^{\top}$.

Lemma 7.7. Let
$$G_3 = \alpha(x)^{-2} \cdot \operatorname{diag}(z(x)) \cdot \widetilde{c}(x) \cdot z(x)^{\top}$$
.

Then we have

$$||G_3(x) - G_3(y)|| \le 200\beta^{-4}n^2 \exp(5R^2) \cdot ||x - y||_2$$

Proof. The proof of $||G_3(x) - G_3(y)||$ is similar to $||G_2(x) - G_2(y)||$, so we omit it here.

7.8 Calculation: Step 4 Lipschitz for Matrix Function $\alpha(x)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x))$

In this section, we analyze the fourth step, namely the Lipschitz for the matrix function $\alpha(x)^{-1}$ diag $(\tilde{c}(x) \circ u_2(x))$.

Lemma 7.8. Let
$$G_4 = \alpha(x)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x))$$
.
Then we have

$$||G_4(x) - G_4(y)|| \le 100\beta^{-3}n^2 \cdot \exp(4R^2)||x - y||_2$$

Proof. We define

$$G_{4,1} := \alpha(x)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x))$$
$$- \alpha(y)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x))$$
$$G_{4,2} := \alpha(y)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x))$$
$$- \alpha(y)^{-1} \cdot \operatorname{diag}(\widetilde{c}(y) \circ u_2(y))$$

Let's prove $G_{4,1}$ first,

$$||G_{4,1}||$$

$$= ||\alpha(x)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x)) - \alpha(y)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x))||$$

$$\leq ||\alpha(x)^{-1} - \alpha(y)^{-1}|| \cdot ||\operatorname{diag}(\widetilde{c}(x) \circ u_2(x))||$$

$$\leq ||\alpha(x)^{-1} - \alpha(y)^{-1}|| \cdot ||\operatorname{diag}(\widetilde{c}(x))|| \cdot ||\operatorname{diag}(u_2(x))||$$

$$\leq 4\beta^{-2} \cdot R \cdot n \exp(2R^2) \cdot ||x - y||_2 \cdot ||\widetilde{c}(x)||_2 \cdot ||u_2(x)||_2$$

$$\leq 4\beta^{-2} \cdot R \cdot n \exp(2R^2) \cdot ||x - y||_2 \cdot 4\sqrt{n} \cdot \sqrt{n} \exp(R^2)$$

$$\leq 16\beta^{-2}n^2 \exp(4R^2)||x - y||_2$$

where the first step follows from definition of $G_{4,1}$, the second step follows from Part 6 of Fact 2.6, the third step follows from Fact 2.3, the forth step follows from Part 4 of Lemma 7.3 and Part 4 of Fact 2.5, the fifth step follows from Part 2, 10 of Lemma 7.2, and the last step follows from $\exp(R^2) > R$.

Then let's prove $G_{4,2}$

$$||G_{4,2}||$$

$$= ||\alpha(y)^{-1} \cdot \operatorname{diag}(\widetilde{c}(x) \circ u_2(x)) - \alpha(y)^{-1} \cdot \operatorname{diag}(\widetilde{c}(y) \circ u_2(y))||$$

$$\leq ||\operatorname{diag}(\widetilde{c}(x) \circ u_2(x)) - \operatorname{diag}(\widetilde{c}(y) \circ u_2(y))|| ||\alpha(y)^{-1}||$$

$$\leq 48\beta^{-3}n^2 \cdot \exp(4R^2)||x - y||_2$$

where the first step follows from the definition of $G_{4,2}$, the second step follows from Part 6 of Fact 2.5, and the last step follows from Part 12 of Lemma 7.3.

By combining the above results, we can get

$$||G_4(x) - G_4(y)||$$

$$= ||G_{4,1} + G_{4,2}||$$

$$\leq (16\beta^{-2}n^2 \exp(4R^2) + 48\beta^{-3}n^2 \cdot \exp(4R^2))||x - y||_2$$

$$< 100\beta^{-3}n^2 \cdot \exp(4R^2)||x - y||_2$$

where the first step follows from the definitions of $G_{4,1}$, $G_{4,2}$, the second step follows from previous results, and last step follows from $\beta^{-1} > 1$.

8 Main Result

Now, we present our main theorem and algorithm.

Algorithm 1 Main algorithm of solving the Soft-Residual Regression problem in Definition 1.4.

```
1: procedure IterativeSoftResidualRegression(A \in \mathbb{R}^{n \times d}, b \in \mathbb{R}^n, w \in \mathbb{R}^n, \epsilon, \delta)
     Theorem 8.1
          Choose x_0 (suppose it satisfies Definition A.1)
 2:
          We use T \leftarrow \log(\|x_0 - x^*\|_2/\epsilon) to denote the number of iterations.
 3:
          for t = 0 \rightarrow T do
 4:
                D \leftarrow B_{\text{diag}}(x_t) + \text{diag}(w \circ w)
 5:
                D \leftarrow \text{SUBSAMPLE}(D, A, \epsilon_1 = \Theta(1), \delta_1 = \delta/T)
                                                                                                                                   ▶ Lemma A.5
 6:
                g \leftarrow A^{\top}(f(x_t)\langle c(x_t), f(x_t)\rangle + \operatorname{diag}(f(x_t))c(x_t))
 7:
 8:
                x_{t+1} \leftarrow x_t + \widetilde{H}^{-1}a
 9:
          end for
10:
          \widetilde{x} \leftarrow x_{T+1}
11:
12:
          return \tilde{x}
13: end procedure
```

Theorem 8.1 (Main theorem). Let A be an arbitrary matrix in $\mathbb{R}^{n \times d}$. Let b and w be arbitrary vectors in \mathbb{R}^n . Let $f(x) = \langle \exp(Ax) + Ax, \mathbf{1}_n \rangle^{-1} (\exp(Ax) + Ax) \in \mathbb{R}^n$ be defined as in Definition 2.1. Let x^* as the optimal solution of

$$\|\langle \exp(Ax) + Ax, \mathbf{1}_n \rangle^{-1} (\exp(Ax) + Ax) - b\|_2^2$$

for $g(x^*) = \nabla f(x^*) = \mathbf{0}_d$ and $||x^*||_2 \le R$, with R > 4. Suppose $||A|| \le R$, each entry of b is greater than or equal to 0, $||b||_1 \le 1$, $w_i^2 \ge 100 + l/\sigma_{\min}(A)^2$ for all $i \in [n]$, and $M = n^{1.5} \exp(30R^2)$.

Let x_0 denote an initial point for which it holds that $M||x_0 - x^*||_2 \le 0.1l$.

Then for all accuracy parameter $\epsilon \in (0,0.1)$ and failure probability $\delta \in (0,0.1)$, there exists a randomized algorithm (Algorithm 1) such that, with probability at least $1-\delta$, it runs $T = \log(\|x_0 - x^*\|_2/\epsilon)$ iterations and outputs a vector $\widetilde{x} \in \mathbb{R}^d$ such that

$$\|\widetilde{x} - x^*\|_2 \le \epsilon,$$

and the time cost per iteration is

$$O((\operatorname{nnz}(A) + d^{\omega}) \cdot \operatorname{poly}(\log(n/\delta)).$$

Here ω denotes the exponent of matrix multiplication. Currently $\omega \approx 2.373$ [Wil12, LG14, AW21].

9 Conclusion

In this paper, we propose a unified scheme of combining the softmax regression and ResNet by analyzing the regression problem

$$\|\langle \exp(Ax) + Ax, \mathbf{1}_n \rangle^{-1} (\exp(Ax) + Ax) - b\|_2,$$

where $A \in \mathbb{R}^{n \times d}$ and $b \in \mathbb{R}^n$. The softmax regression focuses on analyzing $\exp(Ax)$, and the ResNet focuses on analyzing F(x) + x. We combine these together and study $\exp(Ax) + Ax$.

Specifically, we formally define this regression problem. We show that the Hessian matrix is positive semidefinite with the loss function L(x). We analyze the Lipschitz properties and

approximate Newton's method. Our unified scheme builds a connection between two previously thought unrelated areas in machine learning, providing new insight into the loss landscape and optimization for the emerging over-parametrized neural networks.

In the future, researchers may implement an experiment with the proposed unified scheme on large datasets to test our theoretical analysis. Moreover, extending the current analysis to multilayer networks is another promising direction. We believe that our unified perspective between softmax regression and ResNet will inspire more discoveries at the intersection of theory and practice of deep learning.

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A Approximate Newton Method

In this section, we provide an approximate version of the newton method for convex optimization. In Section A.1, we state some assumptions of the traditional newton method and the exact update rule of the traditional algorithm. In Section A.2, we provide the approximate update rule of the approximate newton method, we also implement a tool for compute the approximation of $\nabla^2 L$ and use some lemmas from [LSZ19] to analyze the approximate newton method. In Section A.3, we prove a lower bound on β . In Section A.4, we prove an upper bound on M.

A.1 Definition and Update Rule

Here in this section, we focus on the local convergence of the Newton method. We consider the following target function

$$\min_{x \in \mathbb{R}^d} L(x)$$

with these assumptions:

Definition A.1 ((l, M)-good Loss function). For a function $L : \mathbb{R}^d \to \mathbb{R}$, we say L is (l, M)-good it satisfies the following conditions,

- l-local Minimum. We define l > 0 to be a positive scalar. If there exists a vector $x^* \in \mathbb{R}^d$ such that the following holds
 - $\nabla L(x^*) = \mathbf{0}_d.$ $\nabla^2 L(x^*) \succeq l \cdot I_d.$
- Hessian is M-Lipschitz. If there exists a positive scalar M > 0 such that

$$\|\nabla^2 L(y) - \nabla^2 L(x)\| \le M \cdot \|y - x\|_2$$

• Good Initialization Point. Let x_0 denote the initialization point. If $r_0 := ||x_0 - x_*||_2$ satisfies

$$r_0 M \leq 0.1 l$$

We define gradient and Hessian as follows

Definition A.2 (Gradient and Hessian). The gradient $g : \mathbb{R}^d \to \mathbb{R}^d$ of the loss function is defined as

$$g(x) := \nabla L(x)$$

The Hessian $H: \mathbb{R}^d \to \mathbb{R}^{d \times d}$ of the loss function is defined as,

$$H(x) := \nabla^2 L(x)$$

With the gradient function $g: \mathbb{R}^d \to \mathbb{R}^d$ and the Hessian matrix $H: \mathbb{R}^d \to \mathbb{R}^{d \times d}$, we define the exact process of the Newton method as follows:

Definition A.3 (Exact update of the Newton method).

$$x_{t+1} = x_t - H(x_t)^{-1} \cdot g(x_t)$$

A.2 Approximate of Hessian and Update Rule

In many real-world tasks, it is very hard and expensive to compute exact $\nabla^2 L(x_t)$ or $(\nabla^2 L(x_t))^{-1}$. Thus, it is natural to consider the approximated computation of the gradient and Hessian. The computation is defined as

Definition A.4 (Approximate Hessian). For any Hessian $H(x_t) \in \mathbb{R}^{d \times d}$, we define the approximated Hessian $\widetilde{H}(x_t) \in \mathbb{R}^{d \times d}$ to be a matrix such that the following holds,

$$(1 - \epsilon_0) \cdot H(x_t) \leq \widetilde{H}(x_t) \leq (1 + \epsilon_0) \cdot H(x_t).$$

In order to get the approximated Hessian $\widetilde{H}(x_t)$ efficiently, here we state a standard tool (see Lemma 4.5 in [DSW22]).

Lemma A.5 ([DSW22, SYYZ22]). Let $\epsilon_0 = 0.01$ be a constant precision parameter. Let $A \in \mathbb{R}^{n \times d}$ be a real matrix, then for any positive diagonal (PD) matrix $D \in \mathbb{R}^{n \times n}$, there exists an algorithm which runs in time

$$O((\operatorname{nnz}(A) + d^{\omega})\operatorname{poly}(\log(n/\delta)))$$

and it outputs an $O(d \log(n/\delta))$ sparse diagonal matrix $\widetilde{D} \in \mathbb{R}^{n \times n}$ for which

$$(1 - \epsilon_0)A^{\top}DA \prec A^{\top}\widetilde{D}A \prec (1 + \epsilon_0)A^{\top}DA.$$

Note that, ω denotes the exponent of matrix multiplication, currently $\omega \approx 2.373$ [Wil12, LG14, AW21].

Following the standard of Approximate Newton Hessian literature [Ans00, JKL⁺20, BPSW21, SZZ21, HJS⁺22, LSZ19], we consider the following.

Definition A.6 (Approximate update). We consider the following process

$$x_{t+1} = x_t - \widetilde{H}(x_t)^{-1} \cdot g(x_t).$$

We state a tool from prior work,

Lemma A.7 (Iterative shrinking Lemma, Lemma 6.9 on page 32 of [LSZ19]). If the following condition hold

- Loss Function L is (l, M)-good (see Definition A.1).
- Let $\epsilon_0 \in (0, 0.1)$ (see Definition A.4).
- Let $r_t := ||x_t x^*||_2$.
- Let $\overline{r}_t := M \cdot r_t$

Then we have

$$r_{t+1} \leq 2 \cdot (\epsilon_0 + \overline{r}_t/(l - \overline{r}_t)) \cdot r_t$$

Let T denote the total number of iterations of the algorithm, to apply Lemma A.7, we will need the following induction hypothesis lemma. This is very standard in the literature, see [LSZ19].

Lemma A.8 (Induction hypothesis, Lemma 6.10 on page 34 of [LSZ19]). For each $i \in [t]$, we define $r_i := ||x_i - x^*||_2$. If the following condition hold

- $\epsilon_0 = 0.01$ (see Definition A.4 for ϵ_0)
- $r_i \leq 0.4 \cdot r_{i-1}$, for all $i \in [t]$
- $M \cdot r_i \leq 0.1l$, for all $i \in [t]$ (see Definition A.1 for M)

Then we have

- $r_{t+1} \leq 0.4r_t$
- $M \cdot r_{t+1} \le 0.1l$

A.3 Lower bound on β

Lemma A.9. If the following conditions holds

- $||A|| \leq R$
- $||x||_2 \le R$
- Let β be lower bound on $\langle \exp(Ax), \mathbf{1}_n \rangle$

Then we have

$$\beta \ge \exp(-R^2)$$

Proof. We have

$$\langle \exp(Ax), \mathbf{1}_n \rangle \ge \max_{i \in [n]} \exp(-|(Ax)_i|)$$

 $\ge \exp(-\|Ax\|_{\infty})$
 $\ge \exp(-\|Ax\|_2)$
 $> \exp(-R^2)$

the 1st step follows from simple algebra, the 2nd step follows from definition of ℓ_{∞} norm, the 3rd step follows from Fact 2.5.

A.4 Upper bound on M

Lemma A.10. If the following conditions holds

- $||A|| \le R$.
- $||x||_2 \le R$.
- Let H denote the hessian of loss function L.
- $||H(x) H(y)|| \le \beta^{-2} n^{1.5} \exp(20R^2) \cdot ||x y||_2$ (Lemma 7.3)

Then, we have

$$M \le n^{1.5} \exp(30R^2).$$

Proof. It follows from Lemma A.9.