Attention Scheme Inspired Softmax Regression

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Abstract

Large language models (LLMs) have made transformed changes for human society. One of the key computation in LLMs is the softmax unit. This operation is important in LLMs because it allows the model to generate a distribution over possible next words or phrases, given a sequence of input words. This distribution is then used to select the most likely next word or phrase, based on the probabilities assigned by the model. The softmax unit plays a crucial role in training LLMs, as it allows the model to learn from the data by adjusting the weights and biases of the neural network.

In the area of convex optimization such as using central path method to solve linear programming. The softmax function has been used a crucial tool for controlling the progress and stability of potential function [Cohen, Lee and Song STOC 2019, Brand SODA 2020].

In this work, inspired the softmax unit, we define a softmax regression problem. Formally speaking, given a matrix $A \in \mathbb{R}^{n \times d}$ and a vector $b \in \mathbb{R}^n$, the goal is to use greedy type algorithm to solve

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

In certain sense, our provable convergence result provides theoretical support for why we can use greedy algorithm to train softmax function in practice.

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1 Introduction

In the past few years, Large Language Models (LLMs) have experienced an explosive development. There is a series of results of LLMs, like Transformer [VSP+17], GPT-1 [RNS+18], BERT [DCLT18], GPT-2 [RWC+19], GPT-3 [BMR+20], PaLM [CND+22], OPT [ZRG+22]. The success of a recent chatbot named ChatGPT [Cha22] by OpenAI has exemplified the use of LLMs in human-interaction tasks. Very recently, OpenAI released their new version of LLM, named GPT-4 [Ope23], which has been tested to perform much better even than previous ChatGPT [BCE+23]. These LLMs are trained on massive amounts of textual data to generate natural language text. They have already shown their power on various real-work tasks, including natural language translation [HWL21], sentiment analysis [UAS+20], language modeling [MMS+19], and even creative writing [Cha22, Ope23].

In the construction of the LLMs, attention computation is a key component which is used to enhance the model's ability to focus on relevant parts of the input text [VSP+17, RNS+18, DCLT18, RWC+19, BMR+20]. The attention matrix is defined as a squared matrix consisted of rows and columns related to the words or tokens, and the entries in the matrix represent the correlations between the words/tokens in the input text. The attention mechanism allows the model to selectively focus on specific parts of the input text when generating the output, rather than treating all input tokens equally. The attention mechanism is based on the idea that different parts of the input sequence contribute differently to the output sequence, and the model should learn to weigh these contributions accordingly. In LLMs, attention computation is typically implemented as a soft attention mechanism, where the weights are computed using a softmax function over the input sequence. The Attention computation can be described as follows (see [ZHDK23, AS23, BSZ23] as an example).

Definition 1.1 (Static Attention Computation). Given matrix $Q, K, V \in \mathbb{R}^{n \times d}$, we define

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

where $A := \exp(QK^{\top}) \in \mathbb{R}^{n \times n}$ is a square matrix and $D := \operatorname{diag}(A\mathbf{1}_n) \in \mathbb{R}^{n \times n}$ is a diagonal matrix.

In the above definition, We use matrix $Q \in \mathbb{R}^{n \times d}$ to denote the query tokens, which are typically derived from the previous hidden state of the decoder. And we use matrix $K \in \mathbb{R}^{n \times d}$ and $V \in \mathbb{R}^{n \times d}$ to denote the key tokens and values. By the way we compute A, each entry of A is computed as a dot product between the query vector q and the key vector k_i , and the softmax function is applied to obtain the attention weights $A_{i,j}$.

Motivated by the exp function in attention computation, previous work [LSZ23, GMS23] has formally defined hyperbolic function (for example $f(x) = \exp(Ax), \cosh(Ax), \sinh(Ax)$) regression problems.

Definition 1.2 (Hyperbolic Regression [LSZ23]). Given $A \in \mathbb{R}^{n \times d}$ and $b \in \mathbb{R}^n$, the softmax regression problem is aiming for minimize the following objective function

$$\min_{x \in \mathbb{R}^d} ||f(x) - b||_2^2.$$

Here f(x) can be either of $\exp(Ax)$, $\cosh(Ax)$ and $\sinh(Ax)$.

In this work, we move one more step forward and to consider the normalization factor, $\langle f(x), \mathbf{1}_n \rangle^{-1} = \langle \exp(Ax), \mathbf{1}_n \rangle^{-1}$. We will focus on the exp in the rest of the paper. Inspired by the softmax formulation in each row of the above attention computation, we formally define the softmax regression problem,

Definition 1.3 (Softmax Regression). Given $A \in \mathbb{R}^{n \times d}$ and $b \in \mathbb{R}^n$, the softmax regression problem is aiming for minimize the following objective function

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

It is natural in practice to consider regularization [LLR23], then we consider the regularized version of softmax regression.

Definition 1.4 (Regularized Softmax Regression). Given $A \in \mathbb{R}^{n \times d}$, $b \in \mathbb{R}^n$, and $w \in \mathbb{R}^n$, the goal of the regularized softmax regression is to solve the following minimization problem,

$$\min_{x \in \mathbb{P}^d} 0.5 \cdot \|\langle \exp(Ax), \mathbf{1}_n \rangle^{-1} \exp(Ax) - b\|_2^2 + 0.5 \cdot \|\operatorname{diag}(w)Ax\|_2^2.$$

1.1 Our Result

Here we state our main result. We remark that since $\langle \exp(Ax), \mathbf{1}_n \rangle^{-1} \exp(Ax)$ is always a probability distribution. Therefore, it is a natural to consider each entry in b is nonnegative and its ℓ_1 norm is at most 1.

Theorem 1.5 (Main Result, informal). Given matrix $A \in \mathbb{R}^{n \times d}$, $b \in \mathbb{R}^n$, and $w \in \mathbb{R}^n$.

- We define $f(x) := \langle \exp(Ax), \mathbf{1}_n \rangle^{-1} \exp(Ax)$.
- We use x^* to denote the optimal solution of

$$\min_{x \in \mathbb{R}^d} 0.5 ||f(Ax) - b||_2^2 + 0.5 ||\operatorname{diag}(w)Ax||_2^2$$

that

$$-g(x^*)=\mathbf{0}_d.$$

$$- \|x^*\|_2 \le R.$$

- Suppose that $R \ge 10$.
- Assume that $||A|| \leq R$. Here ||A|| denotes the spectral norm of matrix A.
- Suppose that $b \geq \mathbf{0}_n$ and $||b||_1 \leq 1$. Here $\mathbf{0}_n$ denotes a length-n vector where all the entries are zeros.
- Assume that $w_i^2 \ge 100 + l/\sigma_{\min}(A)^2$ for all $i \in [n]$. Here $\sigma_{\min}(A)$ denotes the smallest singular value of matrix A.
- Let $M = n^{1.5} \exp(30R^2)$.
- Let l > 0.
- Let x_0 denote an starting/initial point such that $M||x_0 x^*||_2 \le 0.1l$.
- Let $\epsilon \in (0, 0.1)$ be our accuracy parameter.
- Let $\delta \in (0, 0.1)$ be our failure probability.
- Let ω denote the exponent of matrix multiplication.

There is a randomized algorithm (Algorithm 1) that

- runs $\log(\|x_0 x^*\|_2/\epsilon)$ iterations
- spend

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

time per iteration,

• and finally outputs a vector $\widetilde{x} \in \mathbb{R}^d$ such that

$$\Pr[\|\widetilde{x} - x^*\|_2 \le \epsilon] \ge 1 - \delta.$$

We remark that, in previous work [LSZ23], they only assume $||b||_2 \leq R$. The reason is in their setting, they don't consider the normalization parameter. It doesn't make sense for them to assume that $||b||_1 \leq 1$ because they're not trying to learn the distribution.

Roadmap. We organize the following paper as follows. In Section 2, we introduce some other projects that's related to or that has inspired our work. In Section 3 we provide a sketch for the techniques used in our project. In Section 4 we define the notations used in our work and provide some useful tools for exact algebra, approximate algebra and differential computation. In Section 5 we provide detailed analysis of $L_{\rm exp}$, including its gradient and hessian. In Section 6 we proved that $L = L_{\rm exp} + L_{\rm reg}$ is a convex function. In Section 7 we proved that the hessian of $L_{\rm exp}$ is Lipschitz. In Section 8 we provide an approximate version of newton method for solving convex optimization problem which is more efficient under certain assumptions. In Section 9 we state our result of this paper and provide the algorithm for tackling the softmax regression problem.

2 Related Work

2.1 Attention Theory

Computation. Since the explosion of LLM, there have been a lot of theoretical works about the computation of attention [KKL20, CLP+21, ZHDK23, AS23, BSZ23, LSZ23, DMS23]. Locality sensitive hashing (LSH) techniques have been employed in research to approximate attention. [KKL20, CLP+21, ZHDK23]. Based on it, [ZHDK23] proposed KDEformer, an efficient approximation algorithm for the dot-product attention mechanism, with provable spectral norm bounds and superior performance on various pre-trained models. Recent research has investigated both static and dynamic approaches to attention computation [AS23, BSZ23]. Additionally, [LSZ23] delved into regularized hyperbolic regression problems involving exponential, cosh, and sinh functions. [DMS23] proposed randomized and deterministic algorithms to sparsify the attention matrix in large language models, achieving high accuracy with significantly reduced feature dimension.

Convergence and Optimization. There have been works trying to understanding attention computation on optimization and convergence perspective [ZKV⁺20, SZKS21, GMS23, LSZ23, LLR23]. In practical attention models, adaptive methods often performs better than SGD. To understand this, [ZKV⁺20] showed that heavy-tailed distribution of the noise is one of the reason of the bad performance of SGD compared to adaptive methods, and provided new upper and lower bounds for convergence of adaptive methods under heavy-tailed noise in attention models. This

answered the question of why adaptive methods performs better in attention models. [SZKS21] explained why models sometimes attend to salient words and how the attention mechanism evolves throughout training, using a model property they defined, named Knowledge to Translate Individual Words (KTIW), which is learned early on from word co-occurrence statistics and later used to attend to input words while predicting the output. Recently, [GMS23] studied the regression problem inspired by the neural network with exponential activation function, and showed the convergence of a two-layer NN with large width (over-parameterized), while [LSZ23] focused on solving regularized exp, cosh and sinh regression problems inspired by Attention computation. [LLR23] explored how transformers learn the co-occurrence structure of words by examining attention-based network size, depth, and complexity through experiments and mathematical analysis, showing that the embedding and self-attention layers encode topical structure with higher average inner product and pairwise attention between same-topic words.

Privacy and Security. With the fast development of LLMs, the potential negative impact of abusing LLM has also been considered. To overcome this, without influencing the quality of the generated text, $[KGW^+23]$ proposed a novel method to add watermark in LLM-generated text. The method needs no access to the parameters or API of the LLM. [VKB23] introduced a formal definition of near access-freeness (NAF) and develops generative model learning algorithms to ensure that the model outputs do not resemble copyrighted data by more than k-bits, with experiments on language (transformers) and image (diffusion) generative models demonstrating strong protection against sampling protected content.

2.2 Fast Linear Algebra

Applications of Exponential Functions There are many theory problem use exp, sinh, cosh function as potential functions to prove the convergence of iterative optimization algorithms. In the work of [CLS19, Bra20, JSWZ21], they use cosh function to define a potential function for measuring the central path. Such design can guarantee the central path method is robust and stable. Let $x \in \mathbb{R}^n$ denote the primal variables and let s denote the slack variables of the central path algorithm. The central path is defined as tuple (x, y, s, t) that satisfies

$$Ax = b, x > 0$$

$$A^{\top}y + s = c, s > 0$$

$$x_i s_i = t \text{ for all } i \in [n].$$

Let t denote the target at one step of central (also mathematically called the complementarity gap). The xs can viewed as reality. In the ideal case, they hope xs = t. However, this is unlikely to happen. They are using the potential function $\Phi(xs) = \sum_{i=1}^{n} \cosh(x_i s_i - t)$ to measure the difference between reality and target.

In [QSZ23], they use cosh function to build a potential for rank-1 matrix sensing problem. Given a matrix $A \in \mathbb{R}^{d \times n}$, there are n observations x_i, y_i and $b_i = x_i^\top A y_i$. The goal of matrix sensing is to recover A by using observations $\{(x_i, y_i, b_i)\}_{i \in [n]}$. They use the potential function $\Phi(x, y) = \sum_{i=1}^{n} \cosh(x_i^\top A y_i - b_i)$.

In standard linear ℓ_2 regression, given matrix $A \in \mathbb{R}^{n \times d}$ and vector $b \in \mathbb{R}^n$, the formulation is usually $L(x) = \|Ax - b\|_2^2 = (\sum_{i=1}^n (Ax)_i - b_i)^2$. In [LSZ23], they use cosh function to construct a ℓ_2 loss such that $L(x) = \sum_{i=1}^n (\cosh((Ax)_i) - b_i)^2$. Furthermore, [LSZ23] also studied exp and sinh functions.

Sketching for Convex Optimization. Sketching technique has been widely-used in optimization problems such as linear programming [CLS19, JSWZ21, DLY21, SY21, GS22], empirical risk minimization [LSZ19, QSZZ23], cutting plane method [JLSW20], computing John Ellipsoid [CCLY19, SYYZ22], integral minimization problem [JLSZ23], matrix completion [GSYZ23], training over-parameterized neural tangent kernel regression [BPSW21, SZZ21, Zha22, ALS⁺22], matrix sensing [DLS23].

3 Technique Overview

Here in this section, we provide an overview of our techniques.

Decomposition of Hessian for Softmax Regression. Recall the target function of our problem is in the form of

$$\min_{x \in \mathbb{R}^d} 0.5 \cdot ||f(Ax) - b||_2^2 + 0.5 \cdot ||WAx||_2^2,$$

We divide the loss function with respect to above target function to the following two terms $L(x) := L_{\exp}(x) + L_{\operatorname{reg}}(x)$, where

$$L_{\text{exp}}(x) := 0.5 \cdot \|\langle \exp(Ax), \mathbf{1}_n \rangle^{-1} \cdot \exp(Ax) - b\|_2^2$$

$$L_{\text{reg}}(x) := 0.5 \cdot \|WAx\|_2^2$$

Calculating the Hessian of $L_{\exp}(x)$ directly is too complicated. To simplify this, we define two terms of $\alpha(x) := \langle \exp(Ax), \mathbf{1}_n \rangle$, $f(x) := \langle \exp(Ax), \mathbf{1}_n \rangle^{-1} \cdot \exp(Ax)$. Then to get the final Hessian to the loss functions, we calculate the Hessian step by step. To be specific, we divide the Hessian calculation into the following items:

- Hessian of $\exp(Ax)$;
- Hessian of $\alpha(x)$ and $\alpha^{-1}(x)$;
- Hessian of f(x).

After that, we notice a structured decomposition of Hessian of L(x). We show that

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

where B(x) is only function with x and has no relation with respect to i and j. In order to apply existing sparsification tool to boost the Hessian calculation (which is one of our main motivations), we construct specific decomposition to the two terms B(x). We show that, B can be viewed as sums of several rank-1 matrices and diagonal matrices.

Hessian is Positive Definite. The key insight of this section lies in the analysis of volumetric barrier functions for solving semidefinite programming. [Ans00, HJS⁺22]. With the decomposition of the Hessian matrix for L_{exp} , the next step is to bound it. To be specific, by dividing B(x) in the way of low-rank parts and diagonal parts, we can lower and upper bound each segment of them. And by combining them, we can get the bound for B(x),

$$-4I_n \leq B(x) \leq 8I_n$$
.

Now combine the Hessian for L_{exp} and $L_{\text{reg}}(x)$ (Hessian for $L_{\text{reg}}(x)$ is trivial $A^{\top}W^2A$) we get

$$\frac{\mathrm{d}^2 L}{\mathrm{d}x^2} = A^{\top} (B(x) + W^2) A.$$

We show that, by assuming all w_i^2 's are lower bounded by $4 + l/\sigma_{\min}(A)^2$, the Hessian is positive definite $\frac{d^2L}{dx^2} \succeq l \cdot I_d$. Further more, we show if all w_i^2 's are lower bounded by $100 + l/\sigma_{\min}(A)^2$, then the matrix W^2 can approximate the sum of $B(x) + W^2$ with a constant guarantee, i.e.,

$$(1 - 1/10) \cdot (B(x) + W^2) \leq W^2 \leq (1 + 1/10) \cdot (B(x) + W^2).$$

This allows us to apply sparsification tool on W to approximate the Hessian.

Lipschitz property for Hessian. The key insight of this section lies in the analysis of previous analysis for recurrent neural networks [AZLS19a, AZLS19b]. By the above calculation of Hessian, we divide the Hessian matrix to different segments. Now with the decomposition (to be specific, we divide the Hessian into low-rank parts and diagonal parts), we show Lipschitz property for each term. We first show Lipschitz property for the basic terms:

- $\|\exp(Ax)\|_2 \le \sqrt{n} \cdot \exp(R^2)$
- $\|\exp(Ax) \exp(Ay)\|_2 \le 2\sqrt{n} \cdot R \exp(R^2) \cdot \|x y\|_2$;
- $|\alpha(x) \alpha(y)| \le \sqrt{n} \cdot \|\exp(Ax) \exp(Ay)\|_2$;
- $|\alpha(x)^{-1} \alpha(y)^{-1}| \le \beta^{-2} \cdot |\alpha(x) \alpha(y)|$; (Later we will also prove an upper bound for β^{-1} , see Lemma 8.9)
- $||f(x)-f(y)||_2 \le R_f \cdot ||x-y||_2$. (Here R_f is a function of β^{-1} , $\exp(R^2)$, see concrete definition in Lemma 7.2)

Then, following the decomposition of the Hessian matrix, we show the Lipschitz property for each of the divided terms (we use G_i for $i \in 1, ..., 8$ to denote the terms) and combine them together to get the property of

$$||G_1|| + \sum_{i=1}^{8} ||G_i|| \le 100R \cdot ||f(x) - f(y)||_2.$$

With this property and a fact that $\|\frac{\mathrm{d}^2L}{\mathrm{d}x^2}(x) - \frac{\mathrm{d}^2L}{\mathrm{d}x^2}(y)\| \le \|A\| \cdot (\|G_1\| + \sum_{i=1}^8 \|G_i\|) \cdot \|A\|$, by assuming any two points x,y satisfy $\|x\|_2, \|y\|_2 \le R$ and $\|A(x-y)\|_{\infty} < 0.01$, we can show that the Hessian matrix is Lipschitz, i.e.,

$$\left\| \frac{\mathrm{d}^2 L}{\mathrm{d}x^2}(x) - \frac{\mathrm{d}^2 L}{\mathrm{d}x^2}(y) \right\| \le \beta^{-2} n^{1.5} \exp(20R^2) \cdot \|x - y\|_2,$$

for some small constant $\beta \in (0, 0.1)$, which implies the Lipschitz property for the Hessian.

Approximated Newton Method with Sparsification Tool. Newton method is a widely-used and traditional tool used in optimization questions. In many optimization applications, computing $\nabla^2 L(x_t)$ or $(\nabla^2 L(x_t))^{-1}$ is quite expensive. Therefore, a natural motivation is to approximately formulate its Hessian or inverse of Hessian. In our setting, we want a faster implementation of Newton method. By above steps, we show our Hessian can be approximated by a matrix in the form of $A^{\top}DA$, where $D = W^2$ is a diagonal matrix. This inspires us to implement a standard tool [DSW22, SYYZ22] that can generate a sparse matrix \widetilde{D} such that

$$(1 - \epsilon) \cdot A^{\top} DA \leq A^{\top} \widetilde{D}A \leq (1 + \epsilon) \cdot A^{\top} DA$$

in near input-sparsity time of A. By this tool, we can reduce the time for Hessian calculation of each iteration to the time of $\widetilde{O}(\text{nnz}(A) + d^{\omega})$. Here nnz(A) denotes the number of non-zero entries in matrix A. Let ω denote the exponent of matrix multiplication. Currently, $\omega \approx 2.373$ [Wil12, LG14, AW21].

4 Preliminary

In this section, we provide the preliminaries used in our paper. In Section 4.1 we introduce the notations we use. In Section 4.2 we provide some basic facts for exact computation. In Section 4.3 we provide some tools for finding the bound of norms based on vectors. In Section 4.4 we provide some tools for finding the bound of norms related to matrices. In Section 4.5, we provide basic inequalities for psd matrices. In Section 4.6, we state several basic rules for calculus. In Section 4.7 we provide the regularization term L_{reg} and compute ∇L_{reg} and $\nabla^2 L_{\text{reg}}$.

4.1 Notations

We denote the ℓ_p norm of a vector x by $\|x\|_p$, i.e., $\|x\|_1 := \sum_{i=1}^n |x_i|$, $\|x\|_2 := (\sum_{i=1}^n x_i^2)^{1/2}$ and $\|x\|_{\infty} := \max_{i \in [n]} |x_i|$. For a vector $x \in \mathbb{R}^n$, $\exp(x) \in \mathbb{R}^n$ denotes a vector where $\exp(x)_i$ is $\exp(x_i)$ for all $i \in [n]$. For n > k, for any matrix $A \in \mathbb{R}^{n \times k}$, we denote the spectral norm of A by $\|A\|$, i.e., $\|A\| := \sup_{x \in \mathbb{R}^k} \|Ax\|_2 / \|x\|_2$. We use $\sigma_{\min}(A)$ to denote the minimum singular value of A. Given two vectors $x, y \in \mathbb{R}^n$, we use $\langle x, y \rangle$ to denote $\sum_{i=1}^n x_i y_i$. Given two vectors $x, y \in \mathbb{R}^n$, we use $x \circ y$ to denote a vector that its i-th entry is $x_i y_i$ for all $i \in [n]$. We use $e_i \in \mathbb{R}^n$ to denote a vector where i-th entry is 1 and all the other entries are 0. Let $x \in \mathbb{R}^n$ be a vector. We define $\operatorname{diag}(x) \in \mathbb{R}^{n \times n}$ as the diagonal matrix whose diagonal entries are given by $\operatorname{diag}(x)_{i,i} = x_i$ for $i = 1, \ldots, n$, and all off-diagonal entries are zero. For a symmetric matrix $A \in \mathbb{R}^{n \times n}$, we say $A \succ 0$ (positive definite (PD)), if for all $x \in \mathbb{R}^n \setminus \{\mathbf{0}_n\}$, we have $x^\top Ax > 0$. For a symmetric matrix $A \in \mathbb{R}^{n \times n}$, we say $A \succeq 0$ (positive semidefinite (PSD)), if for all $x \in \mathbb{R}^n$, we have $x^\top Ax \ge 0$. The Taylor Series for $\exp(x)$ is $\exp(x) = \sum_{i=0}^\infty \frac{x^i}{i!}$.

4.2 Basic Algebras

Fact 4.1. For vectors $u, v, w \in \mathbb{R}^n$. We have

- $\langle u, v \rangle = \langle u \circ v, \mathbf{1}_n \rangle$
- $\langle u \circ v, w \rangle = \langle u \circ v \circ w, \mathbf{1}_n \rangle$
- $\langle u, v \rangle = \langle v, u \rangle$
- $\bullet \langle u, v \rangle = u^{\top}v = v^{\top}u$

Fact 4.2. For any vectors $u, v, w \in \mathbb{R}^n$, we have

- $u \circ v = v \circ u = \operatorname{diag}(u) \cdot v = \operatorname{diag}(v) \cdot u$
- $u^{\top}(v \circ w) = u^{\top} \operatorname{diag}(v) w$
- $\bullet \ u^{\top}(v \circ w) = v^{\top}(u \circ w) = w^{\top}(u \circ v)$
- $u^{\top} \operatorname{diag}(v) w = v^{\top} \operatorname{diag}(u) w = u^{\top} \operatorname{diag}(w) v$
- $\operatorname{diag}(u) \cdot \operatorname{diag}(v) \cdot \mathbf{1}_n = \operatorname{diag}(u)v$
- $\operatorname{diag}(u \circ v) = \operatorname{diag}(u) \operatorname{diag}(v)$
- $\operatorname{diag}(u) + \operatorname{diag}(v) = \operatorname{diag}(u+v)$

4.3 Basic Vector Norm Bounds

Fact 4.3. For vectors $u, v \in \mathbb{R}^n$, we have

- $\langle u, v \rangle \le ||u||_2 \cdot ||v||_2$ (Cauchy-Schwarz inequality)
- $\|\operatorname{diag}(u)\| \le \|u\|_{\infty}$
- $||u \circ v||_2 \le ||u||_{\infty} \cdot ||v||_2$
- $||u||_{\infty} \le ||u||_2 \le \sqrt{n} \cdot ||u||_{\infty}$
- $||u||_2 \le ||u||_1 \le \sqrt{n} \cdot ||u||_2$
- $\|\exp(u)\|_{\infty} \le \exp(\|u\|_{\infty}) \le \exp(\|u\|_2)$
- Let α be a scalar, then $\|\alpha \cdot u\|_2 = |\alpha| \cdot \|u\|_2$
- $||u+v||_2 \le ||u||_2 + ||v||_2$.
- For any $||u-v||_{\infty} \le 0.01$, we have $||\exp(u)-\exp(v)||_2 \le ||\exp(u)||_2 \cdot 2||u-v||_{\infty}$

Proof. For all the other facts we omit the details. We will only prove the last fact. We have

$$\| \exp(u) - \exp(v) \|_{2} = \| \exp(u) \circ (\mathbf{1}_{n} - \exp(v - u)) \|_{2}$$

$$\leq \| \exp(u) \|_{2} \cdot \| \mathbf{1}_{n} - \exp(v - u) \|_{\infty}$$

$$\leq \| \exp(u) \|_{2} \cdot 2 \| u - v \|_{\infty},$$

where the 1st step follows from definition of \circ operation and $\exp()$, the 2nd step follows from $||u \circ v||_2 \le ||u||_{\infty} \cdot ||v||_2$, the 3rd step follows from $|\exp(x) - 1| \le 2x$ for all $x \in (0, 0.1)$.

4.4 Basic Matrix Norm Bounds

Fact 4.4. For matrices U, V, we have

- $\bullet \|U^{\top}\| = \|U\|$
- $||U|| \ge ||V|| ||U V||$
- $||U + V|| \le ||U|| + ||V||$
- $\bullet \ \|U \cdot V\| \le \|U\| \cdot \|V\|$
- If $U \leq \alpha \cdot V$, then $||U|| \leq \alpha \cdot ||V||$
- For scalar $\alpha \in \mathbb{R}$, we have $\|\alpha \cdot U\| \leq |\alpha| \cdot \|U\|$
- For any vector v, we have $||Uv||_2 \le ||U|| \cdot ||v||_2$.
- Let $u, v \in \mathbb{R}^n$ denote two vectors, then we have $||uv^{\top}|| \le ||u||_2 ||v||_2$

4.5 Basic PSD

Fact 4.5. Let $u, v \in \mathbb{R}^n$, We have:

- $\bullet \ uu^{\top} \leq ||u||_2^2 \cdot I_n.$
- $\operatorname{diag}(u) \leq ||u||_2 \cdot I_n$
- $\operatorname{diag}(u \circ u) \leq ||u||_2^2 \cdot I_n$
- $uv^{\top} + vu^{\top} \leq uu^{\top} + vv^{\top}$
- $uv^{\top} + vu^{\top} \succeq -(uu^{\top} + vv^{\top})$
- $\bullet \ (v \circ u)(v \circ u)^{\top} \preceq \|v\|_{\infty}^{2} u u^{\top}$

4.6 Basic Derivative Rules

Fact 4.6. Let f be a differentiable function.

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 4.7 (Rules of differentiation). Let f denote a differentiable function. For all $n, i \in \mathbb{Z}_+$, we have

- Sum rule 1. $\frac{\mathrm{d}}{\mathrm{d}t} \sum_{l=1}^{n} f(x_l) = \sum_{l=1}^{n} \frac{\mathrm{d}}{\mathrm{d}t} f(x_i)$
- Sum rule 2. $\frac{\mathrm{d}}{\mathrm{d}x_i} \sum_{l=1}^n f(x_l) = \frac{\mathrm{d}}{\mathrm{d}x_i} f(x_i)$
- Chain rule. $\frac{d}{dx_i}f(g(x_i)) = f'(g(x_i)) \cdot g'(x_i)$
- Difference rule. $\frac{d}{dx_i}(f(x_i) g(x_i)) = \frac{d}{dx_i}f(x_i) \frac{d}{dx_i}g(x_i)$
- Product rule. $\frac{d}{dx_i}(f(x_i)g(x_i)) = f'(x_i)g(x_i) + f(x_i)g'(x_i)$
- Constant multiple rule. For any $x \neq y$, $\frac{d}{dx_i}(y_i \cdot f(x_i)) = y_i \cdot \frac{d}{dx_i}f(x_i)$

4.7 Regularization

Definition 4.8. Given matrix $A \in \mathbb{R}^{n \times d}$. For a given vector $w \in \mathbb{R}^n$, let $W = \operatorname{diag}(w)$. We define $L_{\operatorname{reg}} : \mathbb{R}^d \to \mathbb{R}$ as follows

$$L_{\text{reg}}(x) := 0.5 \|WAx\|_2^2$$

Lemma 4.9 (Folklore, see [LSZ23] as an example). For a given vector $w \in \mathbb{R}^n$, let W = diag(w). Let $L_{\text{reg}} : \mathbb{R}^d \to \mathbb{R}$ be defined as Definition 4.8.

Then, we have

• The gradient is

$$\frac{\mathrm{d}L_{\mathrm{reg}}}{\mathrm{d}x} = A^{\top}W^2Ax$$

• The Hessian is

$$\frac{\mathrm{d}^2 L_{\mathrm{reg}}}{\mathrm{d}x^2} = A^{\top} W^2 A$$

5 Softmax Regression Loss

In this section, we provide detailed computation for $\nabla L_{\rm exp}$ and $\nabla^2 L_{\rm exp}$. In Section 5.1, we define f(x) and $\alpha(x)$ to simplify the computation for $\nabla L_{\rm exp}$ and $\nabla^2 L_{\rm exp}$. In Section 5.2, we compute $\nabla L_{\rm exp}$ step by step. In Section 5.3, we define the gradient of Loss function and also prove the Lipschitz property for gradient. In Section 5.4-5.8, we compute $\nabla^2 L_{\rm exp}$ step by step. To be specific, in Section 5.4, we compute $\nabla^2 \exp(Ax)$; in Section 5.5, we compute $\nabla^2 \alpha(x)$; in Section 5.6, we compute $\nabla^2 \alpha(x)^{-1}$; in Section 5.7, we compute $\nabla^2 f(x)$; in Section 5.8, we compute $\nabla^2 L_{\rm exp}$. In Section 5.9, we provide some result to aid the computation in Section 5.10. In Section 5.10, we split $\nabla^2 L_{\rm exp}$ into several low rank matrices and diagonal matrices.

5.1 Definitions

We define function softmax f as follows

Definition 5.1 (Function f). Given a matrix $A \in \mathbb{R}^{n \times d}$. Let $\mathbf{1}_n$ denote a length-n vector that all entries are ones. We define prediction function $f : \mathbb{R}^d \to \mathbb{R}^n$ as follows

$$f(x) := \langle \exp(Ax), \mathbf{1}_n \rangle^{-1} \cdot \exp(Ax).$$

Then we have

Lemma 5.2. Let $f: \mathbb{R}^d \to \mathbb{R}^n$ be defined as Definition 5.1, then we have for all $x \in \mathbb{R}^d$,

- $||f(x)||_2 \le ||f(x)||_1 \le 1$.
- $0 \leq f(x)f(x)^{\top} \leq I_n$.
- For any vector b, $0 \leq (b \circ f(x))(b \circ f(x))^{\top} \leq \|b\|_{\infty}^2 f(x)f(x)^{\top} \leq \|b\|_{\infty}^2 I_n$
- For any vector b, diag $(b \circ b) \leq ||b||_{\infty}^{2} I_{n}$
- $0 \leq \operatorname{diag}(f(x)) \leq ||f(x)||_{\infty} I_n \leq ||f(x)||_2 I_n$.

• $0 \leq \operatorname{diag}(f(x) \circ f(x)) \leq ||f(x)||_{\infty}^{2} I_{n} \leq ||f(x)||_{2} I_{n}$.

Proof. The proofs are very straightforward, so we omitted the details here.

Definition 5.3 (Loss function L_{\exp}). Given a matrix $A \in \mathbb{R}^{n \times d}$ and a vector $b \in \mathbb{R}^n$. We define loss function $L_{\exp} : \mathbb{R}^d \to \mathbb{R}$ as follows

$$L_{\exp}(x) := 0.5 \cdot \|\langle \exp(Ax), \mathbf{1}_n \rangle^{-1} \exp(Ax) - b\|_2^2$$

For convenient, we define two helpful notations α and c

Definition 5.4 (Normalized coefficients). We define $\alpha : \mathbb{R}^d \to \mathbb{R}$ as follows

$$\alpha(x) := \langle \exp(Ax), \mathbf{1}_n \rangle.$$

Then, we can rewrite f(x) (see Definition 5.1) and $L_{\text{exp}}(x)$ (see Definition 5.3) as follows

- $f(x) = \alpha(x)^{-1} \cdot \exp(Ax)$.
- $L_{\exp}(x) = 0.5 \cdot \|\alpha(x)^{-1} \cdot \exp(Ax) b\|_2^2$.
- $L_{\exp}(x) = 0.5 \cdot ||f(x) b||_2^2$.

Definition 5.5. We define function $c : \mathbb{R}^d \in \mathbb{R}^n$ as follows

$$c(x) := f(x) - b.$$

Then we can rewrite $L_{\text{exp}}(x)$ (see Definition 5.3) as follows

• $L_{\exp}(x) = 0.5 \cdot ||c(x)||_2^2$.

5.2 Gradient

Lemma 5.6 (Gradient). If the following conditions hold

- Given matrix $A \in \mathbb{R}^{n \times d}$ and a vector $b \in \mathbb{R}^n$.
- Let $\alpha(x)$ be defined in Definition 5.4.
- Let f(x) be defined in Definition 5.1.
- Let c(x) be defined in Definition 5.5.
- Let $L_{\exp}(x)$ be defined in Definition 5.3.

For each $i \in [d]$, we have

• *Part 1.*

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

• Part 2.

$$\frac{\mathrm{d}\langle \exp(Ax), \mathbf{1}_n \rangle}{\mathrm{d}x_i} = \langle \exp(Ax), A_{*,i} \rangle$$

• Part 3.

$$\frac{\mathrm{d}\alpha(x)^{-1}}{\mathrm{d}x_i} = -\alpha(x)^{-1} \cdot \langle f(x), A_{*,i} \rangle$$

• Part 4.

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x_i} = \frac{\mathrm{d}c(x)}{\mathrm{d}x_i} = -\langle f(x), A_{*,i} \rangle \cdot f(x) + f(x) \circ A_{*,i}$$

• Part 5.

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

• Part 6. For each $j \neq i$

$$\frac{\mathrm{d}\langle f(x), A_{*,i}\rangle}{\mathrm{d}x_i} = -\langle f(x), A_{*,i}\rangle \cdot \langle f(x), A_{*,j}\rangle + \langle f(x), A_{*,i}\circ A_{*,j}\rangle$$

• Part 7.

$$\frac{\mathrm{d}L_{\exp}(x)}{\mathrm{d}x_i} = A_{*,i}^{\top} \cdot (f(x)(f(x) - b)^{\top} f(x) + \mathrm{diag}(f(x))(f(x) - b))$$

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

$$\frac{d(\exp(Ax))_i}{dx_i} = \exp(Ax)_i \cdot \frac{d(Ax)_i}{dx_i}$$
$$= \exp(Ax)_i \cdot \frac{(Adx)_i}{dx_i}$$
$$= \exp(Ax)_i \cdot A_{*,i}$$

where the 1st step follows from simple algebra, the 2nd step follows from Fact 4.6, the 3rd step follows from simple algebra.

Thus, we have

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

Proof of Part 2. It trivially follows from arguments in Part 1. **Proof of Part 3.**

$$\frac{d\alpha(x)^{-1}}{dx_i} = \frac{d\langle \exp(Ax), \mathbf{1}_n \rangle^{-1}}{dx_i}$$

$$= -1 \cdot \langle \exp(Ax), \mathbf{1}_n \rangle^{-1-1} \cdot \frac{d}{dx_i} (\langle \exp(Ax), \mathbf{1}_n \rangle)$$

$$= -\langle \exp(Ax), \mathbf{1}_n \rangle^{-2} \langle \exp(Ax), A_{*,i} \rangle$$

$$= -\alpha(x)^{-1} \langle f(x), A_{*,i} \rangle$$

where the 1st step follows from $\frac{\mathrm{d}y^z}{\mathrm{d}x} = z \cdot y^{z-1} \frac{\mathrm{d}y}{\mathrm{d}x}$, the 2nd step follows from results in Part 2.

Proof of Part 4.

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x_{i}} = \frac{\mathrm{d}\langle \exp(Ax), \mathbf{1}_{n} \rangle^{-1} \exp(Ax)}{\mathrm{d}x_{i}}$$

$$= \exp(Ax) \cdot \frac{\mathrm{d}}{\mathrm{d}x_{i}} (\langle \exp(Ax), \mathbf{1}_{n} \rangle^{-1}) + \langle \exp(Ax), \mathbf{1}_{n} \rangle^{-1} \cdot \frac{\mathrm{d}}{\mathrm{d}x_{i}} \exp(Ax)$$

$$= -\langle \exp(Ax), \mathbf{1}_{n} \rangle^{-2} \cdot \langle \exp(Ax), A_{*,i} \rangle \cdot \exp(Ax)$$

$$+ \langle \exp(Ax), \mathbf{1}_{n} \rangle^{-1} \cdot \exp(Ax) \circ A_{*,i}$$

$$= -\langle f(x), A_{*,i} \rangle \cdot f(x) + f(x) \circ A_{*,i}$$

where the 1st step follows from Definition of f, 2nd step follows from differential chain rule, the 3rd step follows from the result from Part 2 and Part 3, the forth step follows from definition of f (see Definition 5.1).

Proof of Part 5

$$\frac{\mathrm{d}\langle f(x), A_{*,i}\rangle}{\mathrm{d}x_i} = A_{*,i}^{\top} \frac{\mathrm{d}f(x)}{\mathrm{d}x_i}$$

$$= A_{*,i}^{\top} (-\langle f(x), A_{*,i}\rangle \cdot f(x) + f(x) \circ A_{*,i})$$

$$= -\langle f(x), A_{*,i}\rangle \cdot A_{*,i}^{\top} f(x) + A_{*,i}^{\top} f(x) \circ A_{*,i}$$

$$= -\langle f(x), A_{*,i}\rangle^2 + \langle f(x), A_{*,i} \circ A_{*,i}\rangle$$

where the 1st step follows from extracting $A_{*,i}$, the 2nd step follows from result of Part 4, the 3rd step follows from simple algebra, the last step follows from simple algebra.

Proof of Part 6.

$$\frac{\mathrm{d}\langle f(x), A_{*,i}\rangle}{\mathrm{d}x_{j}} = A_{*,i}^{\top} \frac{\mathrm{d}f(x)}{\mathrm{d}x_{j}}$$

$$= A_{*,i}^{\top}(-\langle f(x), A_{*,j}\rangle \cdot f(x) + f(x) \circ A_{*,j})$$

$$= -\langle f(x), A_{*,j}\rangle \cdot A_{*,i}^{\top}f(x) + A_{*,i}^{\top}f(x) \circ A_{*,j}$$

$$= -\langle f(x), A_{*,j}\rangle \langle f(x), A_{*,i}\rangle + \langle A_{*,i}, f(x) \circ A_{*,j}\rangle$$

$$= -\langle f(x), A_{*,i}\rangle \cdot \langle f(x), A_{*,j}\rangle + \langle f(x), A_{*,i} \circ A_{*,j}\rangle$$

where the 1st step follows from extracting $A_{*,i}$, the 2nd step follows from result of Part 4, the 3rd step follows from simple algebra, the 4th step follows from simple algebra, the last step follows from simple algebra.

Proof of Part 7.

$$\frac{\mathrm{d}L_{\exp}(x)}{\mathrm{d}x_{i}} = \frac{\mathrm{d}}{\mathrm{d}x_{i}}(0.5 \cdot ||f(x) - b||_{2}^{2})$$

$$= (f(x) - b)^{\top} \frac{\mathrm{d}}{\mathrm{d}x_{i}}(f(x) - b)$$

$$= (f(x) - b)^{\top} (-\langle f(x), A_{*,i} \rangle \cdot f(x) + f(x) \circ A_{*,i})$$

$$= A_{*,i}^{\top} f(x) (f(x) - b)^{\top} f(x) + (f(x) - b)^{\top} f(x) \circ A_{*,i}$$

$$= A_{*,i}^{\top} f(x) (f(x) - b)^{\top} f(x) + A_{*,i}^{\top} f(x) \circ (f(x) - b)$$

$$= A_{*,i}^{\top} (f(x) (f(x) - b)^{\top} f(x) + \mathrm{diag}(f(x)) (f(x) - b))$$

where the 1st step follows from the definition of f, the 2nd step follows from $\frac{d||y||_2^2}{dx} = 2y^{\top}\frac{dy}{dx}$, the 3rd step follows from the result in Part 4, the forth step follows from simple algebra, the 5th step step follows from simple algebra, and the last step follows from simple algebra.

5.3 Definition of Gradient

In this section, we use g(x) to denote the gradient of $L_{\exp}(x)$.

Definition 5.7. If the following conditions hold

- Let $L_{\exp}(x)$ be defined as Definition 5.3.
- Let c(x) be defined as Definition 5.5.
- Let f(x) be defined as Definition 5.1.

We define $g(x) \in \mathbb{R}^d$ as follows

$$g(x) := \underbrace{A^{\top}}_{d \times n} \cdot \left(\underbrace{f(x)}_{n \times 1} \underbrace{\langle c(x), f(x) \rangle}_{\text{scalar}} + \underbrace{\operatorname{diag}(f(x))}_{n \times n} \underbrace{c(x)}_{n \times 1} \right)$$

Equivalently, for each $i \in [d]$, we define

$$g(x)_i := \underbrace{\langle A_{*,i}, f(x) \rangle}_{\text{scalar}} \cdot \underbrace{\langle c(x), f(x) \rangle}_{\text{scalar}} + \underbrace{\langle A_{*,i}, f(x) \circ c(x) \rangle}_{\text{scalar}}.$$

Lemma 5.8. If the following conditions hold

- Let $g_1: \mathbb{R}^d \to \mathbb{R}^n$ be defined as $g_1(x) := f(x)\langle c(x), f(x) \rangle$
- Let $g_2: \mathbb{R}^d \to \mathbb{R}^n$ be defined as $g_2(x) := \operatorname{diag}(f(x))c(x)$
- Let R_f be parameter such that

$$- ||f(x) - f(y)||_2 \le R_f \cdot ||x - y||_2$$
$$- ||c(x) - c(y)||_2 \le R_f \cdot ||x - y||_2$$

• Let $R_{\infty} \in (0,2]$ be parameter such that

$$R_{\infty} := \max\{\|f(x)\|_{2}, \|f(y)\|_{2}, \|c(x)\|_{2}, \|c(y)\|_{2}\}$$

We can show

• Part 1.

$$||g_1(x) - g_1(y)||_2 \le 3R_f R_\infty^2 ||x - y||_2$$

• Part 2.

$$||g_2(x) - g_2(x)||_2 \le 2R_f R_\infty ||x - y||_2$$

• Part 3.

$$||g_1(x) + g_2(x) - g_1(y) - g_2(y)||_2 \le 8R_f R_\infty ||x - y||_2$$

• Part 4.

$$||g(x) - g(y)||_2 \le 8 \cdot ||A|| \cdot R_f \cdot R_\infty ||x - y||_2$$

Proof. **Proof of Part 1.** We can show

$$||g_1(x) - g_1(y)||_2 = ||f(x)\langle c(x), f(x)\rangle - f(y)\langle c(y), f(y)\rangle||_2$$

$$\leq ||f(x)\langle c(x), f(x)\rangle - f(y)\langle c(x), f(x)\rangle||_2$$

$$+ ||f(y)\langle c(x), f(x)\rangle - f(y)\langle c(y), f(x)\rangle||_2$$

$$+ ||f(y)\langle c(y), f(x)\rangle - f(y)\langle c(y), f(y)\rangle||_2$$

where the 1st step follows from the definition of g_1 , the 2nd step follows from adding some terms $-f(y)\langle c(x), f(x)\rangle + f(y)\langle c(x), f(x)\rangle - f(y)\langle c(y), f(x)\rangle + f(y)\langle c(y), f(x)\rangle$ and $||a+b||_2 \le ||a||_2 + ||b||_2$ (Fact 4.3).

For the first term, we have

$$||f(x)\langle c(x), f(x)\rangle - f(y)\langle c(x), f(x)\rangle||_{2} \le ||f(x) - f(y)||_{2} \cdot |\langle c(x), f(x)\rangle|$$

$$\le ||f(x) - f(y)||_{2} \cdot ||c(x)||_{2} \cdot ||f(x)||_{2}$$

$$\le R_{f} \cdot ||x - y||_{2} \cdot ||c(x)||_{2} \cdot ||f(x)||_{2}$$

where the 1st step follows from $\|\alpha a\|_2 \leq |\alpha| \|a\|_2$ (Fact 4.3), the 2nd step follows from $\langle a, b \rangle \leq \|a\|_2 \|b\|_2$ (Fact 4.3), the 3rd step follows from the definition of R_f .

For the second term, we have

$$||f(y)\langle c(x), f(x)\rangle - f(y)\langle c(y), f(x)\rangle||_{2} \le ||f(y)||_{2} \cdot ||\langle c(x) - c(y), f(x)\rangle|$$

$$\le ||f(y)||_{2} \cdot ||c(x) - c(y)||_{2} \cdot ||f(x)||_{2}$$

$$\le ||f(y)||_{2} \cdot R_{f} \cdot ||x - y||_{2} \cdot ||f(x)||_{2}$$

where the 1st step follows from $\|\alpha a\|_2 \leq |\alpha| \|a\|_2$ (Fact 4.3), the 2nd step follows from $\langle a, b \rangle \leq \|a\|_2 \|b\|_2$ (Fact 4.3), the 3rd step follows from the definition of R_f .

For the third term, we have

$$||f(y)\langle c(y), f(x)\rangle - f(y)\langle c(y), f(y)\rangle||_{2} \le ||f(y)||_{2} \cdot ||\langle c(y), f(x) - f(y)\rangle||_{2}$$

$$\le ||f(y)||_{2} \cdot ||c(y)||_{2} \cdot ||f(x) - f(y)||_{2}$$

$$\le ||f(y)||_{2} \cdot ||c(y)||_{2} \cdot R_{f} \cdot ||x - y||_{2}$$

the 2nd step follows from $\langle a, b \rangle \leq ||a||_2 ||b||_2$ (Fact 4.3), the 3rd step follows from the definition of R_f .

Combining three terms together, we complete the proof.

Proof of Part 2.

We have

$$\|\operatorname{diag}(f(x))c(x) - \operatorname{diag}(f(y))c(y)\|_{2}$$

$$\leq \|\operatorname{diag}(f(x))c(x) - \operatorname{diag}(f(x))c(y)\|_{2} + \|\operatorname{diag}(f(x))c(y) - \operatorname{diag}(f(y))c(y)\|_{2}$$

this step follows from adding terms $-\operatorname{diag}(f(x))c(y) + \operatorname{diag}(f(x))c(y)$. For the first term, we have

$$\|\operatorname{diag}(f(x))c(x) - \operatorname{diag}(f(x))c(y)\|_{2} \leq \|f(x)\|_{\infty} \cdot \|c(x) - c(y)\|_{2}$$

$$\leq \|f(x)\|_{2} \cdot \|c(x) - c(y)\|_{2}$$

$$\leq \|f(x)\|_{2} \cdot R_{f} \cdot \|x - y\|_{2}$$

where the 1st step follows from $||Aa|| \leq ||A|| ||a||_2$ where $A \in \mathbb{R}^{n \times d}$, $b \in \mathbb{R}^{d \times 1}$ (Fact 4.4) and $||\operatorname{diag}(a)|| \leq ||a||_{\infty}$, the 2nd step follows from $||a||_{\infty} \leq ||a||_2$, the 3rd step follows from the definition of R_f .

For the second term, we have

$$\|\operatorname{diag}(f(x))c(y) - \operatorname{diag}(f(y))c(y)\|_{2} \le \|f(x) - f(y)\|_{2} \cdot \|c(y)\|_{2}$$

$$\le R_{f} \cdot \|x - y\|_{2} \cdot \|c(y)\|_{2}$$

where the 1st step follows from $\operatorname{diag}(a) + \operatorname{diag}(b) = \operatorname{diag}(a+b)$, $||Ab|| \leq ||A|| ||b||_2$ where $A \in \mathbb{R}^{n \times d}$, $b \in \mathbb{R}^{d \times 1}$ and $||\operatorname{diag}(a)|| \leq ||a||_{\infty} \leq ||a||_2$, the 2nd step follows from the definition of R_f . Combining two terms together, then we complete the proof.

Proof of Part 3.

It follows from combining Part 1 and Part 2.

Proof of Part 4.

It follows from Part 3.

5.4 Hessian Calculations: Step 1, Hessian of $\exp(Ax)$

Lemma 5.9 (Hessian of $\exp(Ax)$). If the following condition holds

• Given a matrix $A \in \mathbb{R}^{n \times d}$.

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

• Part 1.

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

• Part 2.

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

Proof. Proof of Part 1.

$$\frac{\mathrm{d}^2(\exp(Ax))}{\mathrm{d}x_i^2} = \frac{\mathrm{d}}{\mathrm{d}x_i} \left(\frac{\mathrm{d}(\exp(Ax))}{\mathrm{d}x_i}\right)$$

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

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

$$= A_{*,i} \circ \exp(Ax) \circ A_{*,i}$$

where the 1st step is an expansion of the Hessian, the 2nd step follows from the differential chain rule, the 3rd step extracts the matrix $A_{*,i}$ with constant entries out of the derivative, and the last step also follows from the chain rule.

Proof of Part 2.

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

where the 1st step is an expansion of the Hessian, the 2nd and 3rd steps follow from the differential chain rule, the 3rd step follows from simple algebra.

5.5 Hessian Calculations: Step 2, Hessian of $\alpha(x)$

Lemma 5.10. If the following conditions hold

• Let $\alpha(x)$ be defined as Definition 5.4.

Then, we have

• Part 1.

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

• Part 2.

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

Proof. Proof of Part 1.

$$\frac{\mathrm{d}^2 \alpha(x)}{\mathrm{d}x_i^2} = \frac{\mathrm{d}}{\mathrm{d}x_i} \left(\frac{\mathrm{d}}{\mathrm{d}x_i} \langle \exp(Ax), \mathbf{1}_n \rangle \right)$$

$$= \frac{\mathrm{d}}{\mathrm{d}x_i} \left(\langle \exp(Ax) \circ A_{*,i}, \mathbf{1}_n \rangle \right)$$

$$= \langle A_{*,i} \circ \exp(Ax) \circ A_{*,i}, \mathbf{1}_n \rangle$$

$$= \langle \exp(Ax), A_{*,i} \circ A_{*,i} \rangle$$

where the 1st step follows from the expansion of hessian, the 2nd step follows from Part 3 of Lemma 5.6, the 3rd step follows from simple algebra, and the last step follows from Fact 4.1.

Proof of Part 2.

$$\frac{\mathrm{d}^2 \alpha(x)}{\mathrm{d}x_i \mathrm{d}x_j} = \frac{\mathrm{d}}{\mathrm{d}x_j} (\frac{\mathrm{d}}{\mathrm{d}x_i} \langle \exp(Ax), \mathbf{1}_n \rangle)$$

$$= \frac{\mathrm{d}}{\mathrm{d}x_j} (\langle \exp(Ax) \circ A_{*,i}, \mathbf{1}_n \rangle)$$

$$= \langle A_{*,j} \circ \exp(Ax) \circ A_{*,i}, \mathbf{1}_n \rangle$$

$$= \langle \exp(Ax), A_{*,i} \circ A_{*,j} \rangle$$

where the 1st step follows from the expansion of hessian, the 2nd step follows from Part 2 of Lemma 5.6, the 3rd step follows from simple algebra, the last step follows from Fact 4.1.

5.6 Hessian Calculations: Step 3, Hessian of $\alpha(x)^{-1}$

Lemma 5.11 (Hessian of $\alpha(x)^{-1}$). If the following conditions hold

- Let $\alpha(x)$ be defined as Definition 5.4
- Let f(x) be defined in Definition 5.1.

We have

• Part 1.

$$\frac{\mathrm{d}^{2}\alpha(x)^{-1}}{\mathrm{d}x_{i}^{2}} = 2\alpha(x)^{-1} \cdot \langle f(x), A_{*,i} \rangle^{2} - \alpha(x)^{-1} \cdot \langle f(x), A_{*,i} \circ A_{*,i} \rangle$$
$$= 2\alpha(x)^{-1} A_{*,i}^{\top} f(x) f(x)^{\top} A_{*,i} - A_{*,i}^{\top} \operatorname{diag}(f(x)) A_{*,i}$$

• Part 2.

$$\frac{\mathrm{d}^{2}\alpha(x)^{-1}}{\mathrm{d}x_{i}\mathrm{d}x_{j}} = 2\alpha(x)^{-1}\langle f(x), A_{*,i}\rangle\langle f(x), A_{*,j}\rangle - \alpha(x)^{-1}\langle f(x), A_{*,i} \circ A_{*,j}\rangle$$
$$= 2\alpha(x)^{-1}A_{*,i}^{\top}f(x)f(x)^{\top}A_{*,j} - A_{*,i}^{\top}\operatorname{diag}(f(x))A_{*,j}$$

Proof. Proof of Part 1.

$$\frac{\mathrm{d}^2 \alpha(x)^{-1}}{\mathrm{d}x_i^2} = \frac{\mathrm{d}}{\mathrm{d}x_i} \left(\frac{\mathrm{d}}{\mathrm{d}x_i} \alpha(x)^{-1} \right)
= \frac{\mathrm{d}}{\mathrm{d}x_i} \left(-\alpha(x)^{-1} \langle f(x), A_{*,i} \rangle \right)
= -\left(\frac{\mathrm{d}}{\mathrm{d}x_i} \alpha(x)^{-1} \right) \cdot \langle f(x), A_{*,i} \rangle - \alpha(x)^{-1} \frac{\mathrm{d}}{\mathrm{d}x_i} \langle f(x), A_{*,i} \rangle
= 2\alpha(x)^{-1} \langle f(x), A_{*,i} \rangle^2 - \alpha(x)^{-1} \langle f(x), A_{*,i} \rangle \wedge A_{*,i} \rangle$$

where the 1st step follows from the expansion of hessian, the 2nd step follows from Part 3 of Lemma 5.6, the 3rd step follows from differential chain rule, the 4th step follows from simple algebra, the last step follows from Fact 4.1.

Proof of Part 2.

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

$$= \frac{\mathrm{d}}{\mathrm{d}x_{j}} \left(-\alpha(x)^{-1}\langle f(x), A_{*,i}\rangle\right)$$

$$= -\left(\frac{\mathrm{d}}{\mathrm{d}x_{j}}\alpha(x)^{-1}\right) \cdot \langle f(x), A_{*,i}\rangle - \alpha(x)^{-1} \frac{\mathrm{d}}{\mathrm{d}x_{j}}\langle f(x), A_{*,i}\rangle$$

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

where the 1st step follows from the expansion of hessian, the 2nd step follows from Part 3 of Lemma 5.6, the 3rd step follows from differential chain rule, the 4th step follows from basic differential rule, the 5th step step follows from simple algebra, the last step follows from Fact 4.1. \square

5.7 Hessian Calculations: Step 4, Hessian of f(x)

Lemma 5.12 (Hessian of f(x)). If the following conditions hold

- Let $f(x) = \langle \exp(Ax), \mathbf{1}_n \rangle^{-1} \exp(Ax)$ (see Definition 5.1). Then, we have
- Part 1.

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

• Part 2.

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

Proof. Proof of Part 1.

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

$$= \frac{\mathrm{d}}{\mathrm{d}x_i} \left(-\langle f(x), A_{*,i} \rangle \cdot f(x) + f(x) \circ A_{*,i} \right)$$

$$= 2\langle f(x), A_{*,i} \rangle^2 \cdot f(x) - \langle f(x), A_{*,i} \circ A_{*,i} \rangle \cdot f(x)$$

$$- 2\langle f(x), A_{*,i} \rangle f(x) \circ A_{*,i} + A_{*,i} \circ f(x) \circ A_{*,i}$$

where the 1st step follows from the expansion of hessian, the 2nd step follows from Part 4 of Lemma 5.6 and differential chain rule.

Proof of Part 2.

$$\frac{\mathrm{d}^2 f(x)}{\mathrm{d}x_i \mathrm{d}x_j}$$

$$= \frac{\mathrm{d}}{\mathrm{d}x_j} \left(\frac{\mathrm{d}}{\mathrm{d}x_i} f(x) \right)$$

$$= \frac{\mathrm{d}}{\mathrm{d}x_j} \left(-\langle f(x), A_{*,i} \rangle \cdot f(x) + f(x) \circ A_{*,i} \right)$$

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

$$- \langle f(x), A_{*,i} \rangle f(x) \circ A_{*,j} - \langle f(x), A_{*,j} \rangle f(x) \circ A_{*,i} + A_{*,i} \circ f(x) \circ A_{*,j}$$

where the 1st step follows from the expansion of hessian, the 2nd step follows from Part 4 of Lemma 5.6, the 3rd step follows from differential chain rule.

5.8 Hessian Calculations: Step 5, Hessian of $L_{\text{exp}}(x)$

Lemma 5.13 (Hessian of $L_{\exp}(x)$). We define

- $B_1(x) \in \mathbb{R}^{n \times n}$ such that $A_{*,i}^{\top} B_1(x) A_{*,i} := (-\langle f(x), A_{*,i} \rangle f(x) + f(x) \circ A_{*,i})^{\top} \cdot (-\langle f(x), A_{*,i} \rangle f(x)) + f(x) \circ A_{*,i})$
- $B_2(x) \in \mathbb{R}^{n \times n}$ such that

$$A_{*,i}^{\top} B_2(x) A_{*,j} := c^{\top} \cdot (2\langle f(x), A_{*,i} \rangle \langle f(x), A_{*,j} \rangle f(x) - \langle f(x), A_{*,i} \circ A_{*,j} \rangle f(x) - \langle f(x), A_{*,i} \rangle f(x) \circ A_{*,j} - \langle f(x), A_{*,j} \rangle f(x) \circ A_{*,i} + A_{*,i} \circ f(x) \circ A_{*,j})$$

Then we have

• Part 1.

$$\frac{\mathrm{d}^2 L}{\mathrm{d}x_i^2} = A_{*,i}^{\top} B_1(x) A_{*,i} + A_{*,i}^{\top} B_2(x) A_{*,i}$$

• Part 2.

$$\frac{\mathrm{d}^2 L}{\mathrm{d} x_i \mathrm{d} x_j} = A_{*,i}^{\top} B_1(x) A_{*,j} + A_{*,i}^{\top} B_2(x) A_{*,j}$$

Proof. Proof of Part 1.

$$\frac{\mathrm{d}^{2}L}{\mathrm{d}x_{i}^{2}} = \frac{\mathrm{d}}{\mathrm{d}x_{i}} \left(\frac{\mathrm{d}L}{\mathrm{d}x_{i}} \right)
= \frac{\mathrm{d}}{\mathrm{d}x_{i}} \left((f(x) - b)^{\top} \left(-\langle f(x) \circ A_{*,i}, \mathbf{1}_{n} \rangle f(x) \right) + f(x) \circ A_{*,i} \right)
= \left(-\langle f(x), A_{*,i} \rangle f(x) + f(x) \circ A_{*,i} \right)^{\top} \right) \cdot \left(-\langle f(x), A_{*,i} \rangle f(x) \right) + f(x) \circ A_{*,i} \right)
+ c^{\top} \cdot \left(2\langle f(x), A_{*,i} \rangle^{2} f(x) - \langle f(x), A_{*,i} \circ A_{*,j} \rangle f(x) - 2\langle f(x), A_{*,i} \rangle f(x) \circ A_{*,i} + A_{*,i} \circ f(x) \circ A_{*,i} \right)
= A_{*,i}^{\top} B_{1}(x) A_{*,i} + A_{*,i}^{\top} B_{2}(x) A_{*,i}$$

where the 1st step follows from the expansion of hessian, the 2nd step follows from differential chain rule.

Proof of Part 2.

$$\frac{\mathrm{d}^{2}L}{\mathrm{d}x_{i}\mathrm{d}x_{j}} = \frac{\mathrm{d}}{\mathrm{d}x_{j}} \left(\frac{\mathrm{d}L}{\mathrm{d}x_{i}}\right)
= \frac{\mathrm{d}}{\mathrm{d}x_{j}} \left((f(x) - b)^{\top} \left(-\langle f(x), A_{*,i} \rangle f(x) \right) + f(x) \circ A_{*,i} \right)
= \left(-\langle f(x), A_{*,j} \rangle f(x) + f(x) \circ A_{*,j} \right)^{\top} \cdot \left(-\langle f(x), A_{*,i} \rangle f(x) \right) + f(x) \circ A_{*,i} \right)
+ c^{\top}
\cdot \left(2\langle f(x), A_{*,i} \rangle \langle f(x), A_{*,j} \rangle f(x) - \langle f(x), A_{*,i} \circ A_{*,j} \rangle f(x) - \langle f(x), A_{*,i} \rangle f(x) \circ A_{*,j} \right)
- \langle f(x), A_{*,j} \rangle f(x) \circ A_{*,i} + A_{*,i} \circ f(x) \circ A_{*,j} \right)
= A_{*,i}^{\top} B_{1}(x) A_{*,j} + A_{*,i}^{\top} B_{2}(x) A_{*,j}$$

where the 1st step follows from the expansion of hessian, the 2nd step follows from differential chain rule, the 3rd step is a simplification of step 2 by applying notations α (Definition 5.4) and c (Definition 5.5).

5.9 Helpful Lemma

The goal of this section to prove Lemma 5.14. We remark that in this lemma, we can replace f(x) by any vector. However, for easy of presentation, we use f(x).

Lemma 5.14. For any length-n vector $c \in \mathbb{R}^n$ and any vector $f(x) \in \mathbb{R}^n$, we have

• Part 1.

$$c^{\top}(A_{*,i} \circ f(x) \circ A_{*,j}) = A_{*,i}^{\top} \underbrace{\operatorname{diag}(c \circ f(x))}_{n \times n} A_{*,j}$$

• Part 2.

$$c^{\top} f(x) \langle f(x), A_{*,i} \rangle \langle f(x), A_{*,j} \rangle = A_{*,i}^{\top} \underbrace{f(x)}_{n \times 1} \underbrace{\langle c, f(x) \rangle}_{\text{scalar}} \underbrace{f(x)}_{1 \times n}^{\top} A_{*,j}$$

• Part 3.

$$c^{\top} \langle f(x), A_{*,i} \circ A_{*,j} \rangle f(x) = A_{*,i}^{\top} \underbrace{\operatorname{diag}(\langle c, f(x) \rangle f(x))}_{n \times n} A_{*,j}$$

• Part 4.

$$c^{\top}\langle f(x), A_{*,j}\rangle f(x) \circ A_{*,i} = A_{*,i}^{\top}\underbrace{(c \circ f(x))}_{n \times 1}\underbrace{f(x)^{\top}}_{1 \times n}A_{*,j}$$

• Part 5.

$$c^{\top}\langle f(x), A_{*,i}\rangle f(x) \circ A_{*,j} = A_{*,i}^{\top}\underbrace{f(x)}_{n\times 1}\underbrace{(f(x)\circ c)^{\top}}_{1\times n}A_{*,j}$$

• Part 6.

$$(\langle f(x), A_{*,j} \rangle f(x))^{\top} f(x) \circ A_{*,i} = A_{*,i} \underbrace{(f(x) \circ f(x))}_{n \times 1} \underbrace{f(x)}_{1 \times n} A_{*,j}$$

• Part 7.

$$(f(x) \circ A_{*,i})^{\top} (f(x) \circ A_{*,j}) = A_{*,i}^{\top} \underbrace{\operatorname{diag}(f(x) \circ f(x))}_{n \times n} A_{*,j}$$

• Part 8.

$$(\langle f(x), A_{*,j} \rangle f(x))^{\top} (\langle f(x), A_{*,i} \rangle f(x)) = A_{*,i}^{\top} \underbrace{f(x)}_{n \times 1} \underbrace{\langle f(x), f(x) \rangle}_{\text{scalar}} \underbrace{f(x)}_{1 \times n}^{\top} A_{*,j}$$

• Part 9.

$$(f(x) \circ A_{*,i})^{\top} (f(x) \circ A_{*,j}) = A_{*,i}^{\top} \operatorname{diag}(f(x) \circ f(x)) A_{*,j}$$

Proof. Proof of Part 1.

$$c^{\top}(A_{*,i} \circ f(x) \circ A_{*,j}) = A_{*,i}^{\top}(c \circ f(x) \circ A_{*,j})$$
$$= A_{*,i}^{\top} \operatorname{diag}(c \circ f(x)) \circ A_{*,i}$$

where the 1st step follows from Fact 4.2, the 2nd step follows from Fact 4.2.

Proof of Part 2.

$$c^{\top} f(x) \langle f(x), A_{*,i} \rangle \langle f(x), A_{*,j} \rangle = \langle c, f(x) \rangle \langle f(x), A_{*,i} \rangle \langle f(x), A_{*,j} \rangle$$
$$= A_{*,i}^{\top} f(x) \langle c, f(x) \rangle \langle f(x) \rangle^{\top} A_{*,j}$$

where the 1st step follows from $a^{\top}b = \langle a, b \rangle$ (Fact 4.1), the 2nd step follows from $\langle a, b \rangle = a^{\top}b$ (Fact 4.1).

Proof of Part 3.

$$c^{\top} \langle f(x), A_{*,i} \circ A_{*,j} \rangle f(x) = c^{\top} (f(x))^{\top} A_{*,i} \circ A_{*,j} f(x)$$

$$= A_{*,i}^{\top}(f(x))^{\top}c \circ A_{*,j}f(x)$$

$$= A_{*,i}^{\top}\langle f(x), c \rangle \circ A_{*,j}f(x)$$

$$= A_{*,i}^{\top}\operatorname{diag}(\langle f(x), c \rangle)f(x)A_{*,j}$$

where the 1st step follows from $\langle a, b \rangle = a^{\top}b$ (Fact 4.1), the 2nd step follows from Fact 4.2, the 3rd step follows from $a^{\top}b = \langle a, b \rangle$ (Fact 4.1), the last step follows from Fact 4.2.

Proof of Part 4.

$$c^{\top} \langle f(x), A_{*,j} \rangle f(x) \circ A_{*,i} = c^{\top} (f(x))^{\top} A_{*,j} f(x) \circ A_{*,i}$$
$$= A_{*,i}^{\top} (f(x))^{\top} A_{*,j} f(x) \circ c$$
$$= A_{*,i}^{\top} (f(x) \circ c) (f(x))^{\top} A_{*,j}$$

where the 1st step follows from $\langle a, b \rangle = a^{\top}b$ (Fact 4.1), the 2nd step follows from Fact 4.2, the 3rd step follows from $f(x)^{\top}A_{*,j} = \langle f(x), A_{*,j} \rangle$ (Fact 4.1) is a scalar.

Proof of Part 5.

$$c^{\top} \langle f(x), A_{*,i} \rangle f(x) \circ A_{*,j} = (f(x))^{\top} A_{*,i} c^{\top} f(x) \circ A_{*,j}$$

$$= (f(x))^{\top} A_{*,i} A_{*,j}^{\top} f(x) \circ c$$

$$= (f(x))^{\top} A_{*,i} (f(x) \circ c)^{\top} A_{*,j}$$

$$= A_{*,i}^{\top} f(x) (f(x) \circ c)^{\top} A_{*,j}$$

where the 1st step follows from $\langle a, b \rangle = a^{\top}b$ (Fact 4.1), the 2nd step follows from Fact 4.2, the 3rd step follows from $a^{\top}b = b^{\top}a$ (Fact 4.1), the last step follows from $a^{\top}b = b^{\top}a$ (Fact 4.1).

Proof of Part 6

$$(\langle f(x), A_{*,j} \rangle f(x))^{\top} f(x) \circ A_{*,i} = A_{*,i}^{\top} f(x) \circ \langle f(x), A_{*,j} \rangle f(x)$$

$$= A_{*,i}^{\top} f(x) \circ (f(x))^{\top} A_{*,j} f(x)$$

$$= A_{*,i}^{\top} f(x) \circ f(x) (f(x))^{\top} A_{*,j}$$

where the 1st step follows from Fact 4.2, the 2nd step follows from $\langle a,b\rangle=a^{\top}b$ (Fact 4.1), the 3rd step follows from $f(x)^{\top}A_{*,j}=\langle f(x),A_{*,j}\rangle$ is a scalar (Fact 4.1).

Proof of Part 7.

$$(f(x) \circ A_{*,i})^{\top} (f(x) \circ A_{*,j}) = \langle f(x) \circ A_{*,i}, f(x) \circ A_{*,j} \rangle$$

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

$$= (f(x) \circ f(x))^{\top} (A_{*,i} \circ A_{*,j})$$

$$= A_{*,i}^{\top} (f(x) \circ f(x) \circ A_{*,j})$$

$$= A_{*,i}^{\top} \operatorname{diag}(f(x) \circ f(x)) A_{*,j}$$

where the 1st step follows from $a^{\top}b = \langle a, b \rangle$ (Fact 4.1), the 2nd step follows from Fact 4.1, the 3rd step follows from $\langle a, b \rangle = a^{\top}b$ (Fact 4.1), the 4th step follows from Fact 4.2, the last step follows from Fact 4.2.

Proof of Part 8.

$$(\langle f(x), A_{*,j} \rangle f(x))^{\top} (\langle f(x), A_{*,i} \rangle f(x)) = \langle f(x), A_{*,j} \rangle f(x)^{\top} (\langle f(x), A_{*,i} \rangle f(x))$$

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

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

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

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

$$= A_{*,i}^{\top} f(x) \langle f(x), f(x) \rangle f(x)^{\top} A_{*,j}$$

where the 1st step follows from $a^{\top}b = b^{\top}a$ (Fact 4.1), the 2nd step follows from $\langle a,b\rangle = a^{\top}b$ (Fact 4.1), the 3rd step follows from $a^{\top}b = b^{\top}a$ (Fact 4.1), the 4th step follows from $A_{*,i}^{\top}f(x) = \langle A_{*,i}, f(x)\rangle$ is a scalar (Fact 4.1), the 5th step step follows from $f(x)^{\top}A_{*,j} = \langle f(x), A_{*,j}\rangle$ is a scalar (Fact 4.1), the last step follows from $a^{\top}b = \langle a,b\rangle$ (Fact 4.1).

Proof of Part 9.

$$(f(x) \circ A_{*,i})^{\top} (f(x) \circ A_{*,j}) = \langle f(x) \circ A_{*,i}, f(x) \circ A_{*,j} \rangle$$

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

$$= (f(x) \circ f(x))^{\top} (A_{*,i} \circ A_{*,j})$$

$$= A_{*,i}^{\top} (f(x) \circ f(x)) \circ A_{*,j})$$

$$= A_{*,i}^{\top} \operatorname{diag}(f(x) \circ f(x)) A_{*,j}$$

where the 1st step follows from $a^{\top}b = \langle a,b \rangle$ (Fact 4.1), the 2nd step follows from Fact 4.1, the 3rd step follows from $\langle a,b \rangle = a^{\top}b$ (Fact 4.1), the 4th step follows from Fact 4.2, the last step follows from Fact 4.2.

5.10 Decomposing $B_1(x)$, $B_2(x)$ and B(x) into Low Rank Plus Diagonal

Lemma 5.15 (Rewriting $B_1(x)$ and $B_2(x)$). If the following conditions hold

- Given matrix $A \in \mathbb{R}^{n \times d}$.
- Let f(x) be defined as Definition 5.1.
- Let c(x) be defined as Definition 5.5.
- Let $B(x) = B_1(x) + B_2(x)$.

Then, we can show that

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

$$B_{1}(x) = \underbrace{\langle f(x), f(x) \rangle}_{\text{scalar}} \cdot \underbrace{f(x)}_{n \times 1} \underbrace{f(x)}_{1 \times n}^{\top} + \underbrace{\text{diag}(f(x) \circ f(x))}_{n \times n \text{ diagonal matrix}} + \underbrace{(f(x) \circ f(x))}_{n \times 1} \cdot \underbrace{f(x)}_{1 \times n}^{\top} + \underbrace{(f(x) \circ f(x))}_{n \times 1} \cdot \underbrace{f(x)}_{1 \times n}^{\top}$$

- In summary, $B_1(x) \in \mathbb{R}^{n \times n}$ is constructed by three rank-1 matrices and a diagonal matrix.

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

$$B_{2}(x) = \underbrace{2\langle c(x), f(x) \rangle}_{\text{scalar}} \cdot \underbrace{f(x)}_{n \times 1} \underbrace{f(x)}_{1 \times n}^{\top} + \underbrace{\langle c(x), f(x) \rangle}_{\text{scalar}} \cdot \underbrace{\text{diag}(f(x))}_{n \times n} + \underbrace{\text{diag}(c(x) \circ f(x))}_{n \times n} \underbrace{\text{diagonal matrix}}_{n \times n} + \underbrace{\text{diag}(c(x) \circ f(x))}_{n \times n}$$

$$- \underbrace{(c(x) \circ f(x))}_{n \times 1} \underbrace{f(x)}_{1 \times n}^{\top} - \underbrace{f(x)}_{n \times 1} \underbrace{(f(x) \circ c(x))}_{1 \times n}^{\top}$$

- In summary, $B_2(x) \in \mathbb{R}^{n \times n}$ is constructed by three rank-1 matrices and two diagonal matrices.
- Part 3. For $B(x) \in \mathbb{R}^{n \times n}$, we have

$$B(x) = \underbrace{\langle 3f(x) - 2b, f(x) \rangle}_{\text{scalar}} \cdot \underbrace{f(x)}_{n \times 1} \underbrace{f(x)}_{1 \times n}^{\top} + \underbrace{\langle f(x) - b, f(x) \rangle}_{\text{scalar}} \cdot \underbrace{\text{diag}(f(x))}_{n \times n \text{ diagonal matrix}} + \underbrace{\text{diag}((2f(x) - b) \circ f(x))}_{n \times n \text{ diagonal matrix}} + \underbrace{(b \circ f(x))}_{n \times 1} \cdot \underbrace{f(x)}_{1 \times n}^{\top} + \underbrace{f(x)}_{n \times 1} \cdot \underbrace{(b \circ f(x))}_{1 \times n}^{\top}$$

- In summary, $B(x) \in \mathbb{R}^{n \times n}$ is constructed by three rank-1 matrices and two diagonal matrices.

Proof. Proof of Part 1. $B_1(x)$.

For $B_1(x)$, we have:

$$A_{*,i}^{\top}B_{1}(x)A_{*,j} = (-\langle f(x), A_{*,j}\rangle f(x) + f(x) \circ A_{*,j})^{\top} \cdot (-\langle f(x), A_{*,i}\rangle f(x)) + f(x) \circ A_{*,i}))$$

$$= (-(\langle f(x), A_{*,j}\rangle f(x))^{\top} + (f(x) \circ A_{*,j})^{\top}) \cdot (-\langle f(x), A_{*,i}\rangle f(x)) + f(x) \circ A_{*,i}))$$

$$= (\langle f(x), A_{*,j}\rangle f(x))^{\top} \langle f(x), A_{*,i}\rangle f(x) + (f(x) \circ A_{*,j})^{\top} (f(x) \circ A_{*,i}))$$

$$- (\langle f(x), A_{*,j}\rangle f(x))^{\top} (f(x) \circ A_{*,i}) - (f(x) \circ A_{*,j})^{\top} \langle f(x), A_{*,i}\rangle f(x)$$

$$= A_{*,i}^{\top} f(x) \langle f(x), f(x)\rangle f(x)^{\top} A_{*,j} + A_{*,i}^{\top} \operatorname{diag}(f(x) \circ f(x)) A_{*,j}$$

$$- A_{*,i}^{\top} (f(x) \circ f(x)) f(x)^{\top} A_{*,j} - A_{*,i}^{\top} (f(x) \circ f(x))^{\top} f(x) A_{*,j}$$

$$(1)$$

where the 1st step follows from the definition of $B_1(x)$, the 2nd step follows from $(A + B)^{\top} = A^{\top} + B^{\top}$, the 3rd step follows from simple algebra, the last step follows from Lemma 5.14.

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

$$B_1(x) = \langle f(x), f(x) \rangle \cdot f(x) f(x)^\top + \operatorname{diag}(f(x) \circ f(x))$$
$$+ (f(x) \circ f(x)) f(x)^\top + f(x) (f(x) \circ f(x))^\top$$

Proof of Part 2. $B_2(x)$.

For $B_2(x) \in \mathbb{R}^{n \times n}$, we have:

$$A_{*,i}^{\top} B_2(x) A_{*,j} = c(x)^{\top} \cdot (2\langle f(x), A_{*,i} \rangle \langle f(x), A_{*,j} \rangle f(x) - \langle f(x), A_{*,i} \circ A_{*,j} \rangle f(x) - \langle f(x), A_{*,i} \rangle f(x) \circ A_{*,j}$$

$$-\langle f(x), A_{*,i} \rangle f(x) \circ A_{*,i} + A_{*,i} \circ f(x) \circ A_{*,i} \rangle$$

Thus, we can rewrite $B_2(x)$ as

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

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

$$- \langle f(x), A_{*,j}\rangle f(x) \circ A_{*,i} + A_{*,i} \circ f(x) \circ A_{*,j})$$

$$= 2c(x)^{\top} \langle f(x), A_{*,i}\rangle\langle f(x), A_{*,j}\rangle f(x) - c(x)^{\top} \langle f(x), A_{*,i} \circ A_{*,j}\rangle f(x) + c(x)^{\top} A_{*,i} \circ f(x) \circ A_{*,j}$$

$$- c(x)^{\top} \langle f(x), A_{*,i}\rangle f(x) \circ A_{*,j} - c(x)^{\top} \langle f(x), A_{*,j}\rangle f(x) \circ A_{*,i}$$

$$= 2A_{*,i}^{\top} f(x)\langle c(x), f(x)\rangle f(x)^{\top} A_{*,j} - A_{*,i}^{\top} \operatorname{diag}(\langle c(x), f(x)\rangle f(x)) A_{*,j} + A_{*,i}^{\top} \operatorname{diag}(c(x) \circ f(x)) A_{*,j}$$

$$- A_{*,i}^{\top} f(x)\langle f(x) \circ c\rangle^{\top} A_{*,j} - A_{*,i} \langle c(x) \circ f(x)\rangle f(x)^{\top} A_{*,j}$$

$$(2)$$

where the 1st step follows from definition of $B_2(x)$, the 2nd step follows from simple algebra, the 3rd step follows from simple algebra, the last step follows from Lemma 5.14.

By extracting $A_{*,i}^{\top}$ and $A_{*,j}$, we have

$$B_2(x) = 2\langle c, f(x)\rangle f(x)f(x)^{\top} + \operatorname{diag}(\langle c, f(x)\rangle f(x)) + \operatorname{diag}(c \circ f(x))$$
$$- (c(x) \circ f(x))f(x)^{\top} - f(x)(c(x) \circ f(x))^{\top}$$

Proof of Part 3. B(x)

We define

$$B_{1,1}(x) := \langle f(x), f(x) \rangle \cdot f(x) f(x)^{\top}$$

$$B_{1,2}(x) := \operatorname{diag}(f(x) \circ f(x))$$

$$B_{1,3}(x) := (f(x) \circ f(x)) f(x)^{\top}$$

$$B_{1,4}(x) := f(x) (f(x) \circ f(x))^{\top}$$

Thus, we have:

$$B_1(x) = B_{1,1}(x) + B_{1,2}(x) + B_{1,3}(x) + B_{1,4}(x)$$

Similarly, we define

$$B_{2,1}(x) := 2\langle c, f(x) \rangle f(x) f(x)^{\top}$$

$$B_{2,2}(x) := \operatorname{diag}(\langle c, f(x) \rangle f(x))$$

$$B_{2,3}(x) := \operatorname{diag}(c \circ f(x))$$

$$B_{2,4}(x) := -(c(x) \circ f(x)) f(x)^{\top}$$

$$B_{2,5}(x) := -f(x) (c(x) \circ f(x))^{\top}$$

Thus, we have:

$$B_2(x) = B_{2,1}(x) + B_{2,2}(x) + B_{2,3}(x) + B_{2,4}(x) + B_{2,5}(x)$$

Merge $B_{1,1}(x)$ and $B_{2,1}(x)$:

$$B_{1,1}(x) + B_{2,1}(x) = \langle f(x), f(x) \rangle \cdot f(x) f(x)^{\top} + 2 \langle c(x), f(x) \rangle f(x) f(x)^{\top}$$

= $\langle 3f(x) - 2b, f(x) \rangle f(x) f(x)^{\top}$

Maintain $B_{2,2}(x)$ itself:

$$B_{2,2}(x) = \operatorname{diag}(\langle f(x) - b, f(x) \rangle f(x))$$
$$= \langle f(x) - b, f(x) \rangle \operatorname{diag}(f(x))$$

Merge $B_{1,2}(x)$ and $B_{2,3}(x)$:

$$B_{1,2}(x) + B_{2,3}(x) = \operatorname{diag}((f(x) - b) \circ f(x)) + \operatorname{diag}(f(x) \circ f(x))$$
$$= \operatorname{diag}((2f(x) - b) \circ f(x))$$

Merge $B_{1,3}(x)$ and $B_{2,4}(x)$:

$$B_{1,3}(x) + B_{2,4}(x) = (f(x) \circ f(x))f(x)^{\top} - ((f(x) - b) \circ f(x))f(x)^{\top}$$

= $(f(x) \circ f(x) - f(x) \circ f(x) + b \circ f(x))f(x)^{\top}$
= $(b \circ f(x))f(x)^{\top}$

Merge $B_{1,4}(x)$ and $B_{2,5}(x)$:

$$B_{1,4}(x) + B_{2,5}(x) = f(x)(f(x) \circ f(x))^{\top} - f(x)((f(x) - b) \circ f(x))^{\top}$$

= $f(x)(f(x)^{\top} \circ f(x)^{\top} - f(x)^{\top} \circ f(x)^{\top} + b^{\top} \circ f(x)^{\top})$
= $f(x)(b \circ f(x))^{\top}$

By combining all the above equations, we have

$$B(x) = \underbrace{\langle 3f(x) - 2b, f(x) \rangle f(x) f(x)^{\top}}_{B_{1,1} + B_{2,1}} + \underbrace{\langle f(x) - b, f(x) \rangle \operatorname{diag}(f(x))}_{B_{2,2}} + \underbrace{\operatorname{diag}((2f(x) - b) \circ f(x))}_{B_{1,2} + B_{2,3}} + \underbrace{(b \circ f(x)) f(x)^{\top}}_{B_{1,3} + B_{2,4}} + \underbrace{f(x)(b \circ f(x))^{\top}}_{B_{1,4} + B_{2,5}}$$

Thus, we complete the proof.

6 Hessian is Positive Definite

In this section, we prove that $\nabla^2 L \succeq 0$ and thus L is convex. In Section 6.1, we find the lower bound of B(x). To be specific, we split B(x) into several terms and find their lower bounds separately. In Section 6.2, we use the result of Section 6.1 to prove that lower bound of $\nabla^2 L \succeq 0$ and thus L is convex.

6.1 PSD Lower Bound

For convenient, we define B(x)

Definition 6.1. We define B(x) as follows

$$B(x) := \langle 3f(x) - 2b, f(x) \rangle f(x) f(x)^{\top}$$
$$+ (b \circ f(x)) f(x)^{\top} + f(x) (b \circ f(x))^{\top}$$
$$+ \langle f(x) - b, f(x) \rangle \cdot \operatorname{diag}(f(x))$$
$$+ \operatorname{diag}((2f(x) - b) \circ f(x))$$

Further, we define

$$B_{\text{rank}}(x) := \underbrace{\langle 3f(x) - 2b, f(x) \rangle f(x) f(x)^{\top}}_{:=B_{\text{rank}}^{1}(x)} + \underbrace{\langle b \circ f(x) \rangle f(x)^{\top} + f(x) \langle b \circ f(x) \rangle^{\top}}_{:=B_{\text{diag}}^{2}(x)} + \underbrace{\langle f(x) - b, f(x) \rangle \cdot \operatorname{diag}(f(x))}_{:=B_{\text{diag}}^{1}(x)} + \underbrace{\operatorname{diag}(\langle 2f(x) - b \rangle \circ f(x))}_{:=B_{\text{diag}}^{2}(x)}$$

Lemma 6.2. If the following conditions hold

- $||f(x)||_1 = 1$ (see Definition 5.1).
- Let $B(x) \in \mathbb{R}^{n \times n}$ be defined as Definition 6.1.
- Let $f(x) > \mathbf{0}_n$.
- Let $b \geq \mathbf{0}_n$.
- Let B_{rank}^1 , B_{rank}^2 be defined as Definition 6.1.
- Let B_{diag}^1 , B_{diag}^2 be defined as Definition 6.1.

Then we have

• Part 1.

$$-0.5\|b\|_2^2 \cdot f(x)f(x)^{\top} \preceq B_{\mathrm{rank}}^1(x) \preceq (3\|f(x)\|_2^2) \cdot f(x)f(x)^{\top}$$

• Part 2.

$$-(1 + ||b||_{\infty}^{2}) \cdot f(x)f(x)^{\top} \leq B_{\text{rank}}^{2}(x) \leq (1 + ||b||_{\infty}^{2}) \cdot f(x)f(x)^{\top}$$

• Part 3.

$$-0.25||b||_2^2 \cdot \operatorname{diag}(f(x)) \leq B_{\operatorname{diag}}^1 \leq (||f(x)||_2^2) \cdot \operatorname{diag}(f(x))$$

• Part 4.

$$-0.5 \cdot \operatorname{diag}(b \circ b) \preceq B^2_{\operatorname{diag}} \preceq 2 \cdot \operatorname{diag}(f(x) \circ f(x))$$

• Part 5. If $||b||_1 \le 1$ and $||f(x)||_1 \le 1$, then we have

$$-4I_n \leq B(x) \leq 8I_n$$

Proof. Recall that in Definition 6.1, we split B(x) into four terms

$$B(x) = B_{\text{rank}}^1 + B_{\text{rank}}^2 + B_{\text{diag}}^1 + B_{\text{diag}}^2,$$

where B_{rank}^{i} and B_{diag}^{i} are defined as

$$B_{\text{rank}}^{1} := \langle 3f(x) - 2b, f(x) \rangle f(x) f(x)^{\top},$$

$$B_{\text{rank}}^{2} := (b \circ f(x)) f(x)^{\top} + f(x) (b \circ f(x))^{\top},$$

$$B_{\text{diag}}^{1} := \langle f(x) - b, f(x) \rangle \operatorname{diag}(f(x)),$$

$$B_{\text{diag}}^{2} := \operatorname{diag}(f(x) \circ (2f(x) - b)).$$

Proof of B_{rank}^1 .

On one hand, we can lower bound the coefficient, we have

$$\begin{split} \langle 3f(x) - 2b, f(x) \rangle &\geq 2 \langle f(x) - b, f(x) \rangle \\ &= 2 \langle f(x) - b, f(x) \rangle + 0.5 \|b\|_2^2 - 0.5 \|b\|_2^2 \\ &= 0.5 \|2f(x) - b\|_2^2 - 0.5 \|b\|_2^2 \\ &\geq -0.5 \|b\|_2^2. \end{split}$$

Thus,

$$B_{\text{rank}}^1 \succeq -0.5 \|b\|_2^2 f(x) f(x)^{\top}.$$

On the other hard, we have

$$\langle 3f(x) - 2b, f(x) \rangle = 3||f(x)||_2^2 - 2\langle b, f(x) \rangle$$

 $\leq 3||f(x)||_2^2$

Thus,

$$B_{\text{rank}}^1 \leq 3 \|f(x)\|_2^2 \cdot f(x) f(x)^\top.$$

Proof of $B_{\text{rank}}^2(x)$. On one hand, we have

$$B_{\text{rank}}^{2}(x) \succeq -(b \circ f(x))^{\top} (b \circ f(x)) - f(x) f(x)^{\top}$$

= - (\|b\|_{\infty}^{2} + 1) \cdot f(x) f(x)^{\tau},

where the 1st step follows from Fact 4.5, , the last step follows from Fact 4.5. On the other hand, we have

$$B_{\text{rank}}^{2}(x) \leq (b \circ f(x))^{\top} (b \circ f(x)) + f(x) f(x)^{\top}$$
$$\leq (\|b\|_{\infty}^{2} + 1) \cdot f(x) f(x)^{\top}$$

where the 1st step follows from Fact 4.5, the 2nd step follows from Fact 4.5.

Proof of $B^1_{\text{diag}}(x)$.

For the coefficient, we have

$$\langle f(x) - b, f(x) \rangle = \langle f(x) - b, f(x) \rangle + \frac{1}{4} ||b||_2^2 - \frac{1}{4} ||b||_2^2$$

$$= \|f(x) - \frac{1}{2}b\|_2^2 - \frac{1}{4}\|b\|_2^2$$

$$\geq -\frac{1}{4}\|b\|_2^2$$

Thus, we have

$$B_{\operatorname{diag}}^1 \succeq -\frac{1}{4} \|b\|_2^2 \cdot \operatorname{diag}(f(x)).$$

We can show

$$\langle f(x) - b, f(x) \rangle = ||f(x)||_2^2 - \langle b, f(x) \rangle$$

$$\leq ||f(x)||_2^2$$

We have,

$$B_{\mathrm{diag}}^2 \leq (\|f(x)\|_2^2) \cdot \mathrm{diag}(f(x))$$

Proof of $B^2_{\text{diag}}(x)$. For the third term, we have

$$B_{\text{diag}}^2 = \operatorname{diag}(f(x) \circ (2f(x) - b) + \frac{1}{2}b \circ b) - \frac{1}{2}\operatorname{diag}(b \circ b)$$

$$\succeq -\frac{1}{2}\operatorname{diag}(b \circ b)$$

$$\succeq -\frac{1}{2}||b||_2^2 I_n$$

where the 1st step follows from simple algebra, the 2nd step follows from simple algebra, the last step follows from Fact 4.5.

Proof of B(x). It trivially follows from

$$||f(x)||_1 \le 1, ||b||_1 \le 1$$

and using Lemma 5.2 and Fact 4.5

$$\max\{f(x)f(x)^{\top}, \operatorname{diag}(f(x)), \operatorname{diag}(f(x)\circ f(x)), \operatorname{diag}(b\circ b)\} \leq I_n.$$

6.2Lower bound on Hessian

The goal of this section is to prove Lemma 6.3.

Lemma 6.3. If the following conditions hold

- Given matrix $A \in \mathbb{R}^{n \times d}$.
- Let $L_{\exp}(x)$ be defined as Definition 5.3.
- Let $L_{reg}(x)$ be defined as Definition 4.8.
- Let $L(x) = L_{\text{exp}}(x) + L_{\text{reg}}(x)$.

- Let $W = \operatorname{diag}(w) \in \mathbb{R}^{n \times n}$. Let $W^2 \in \mathbb{R}^{n \times n}$ denote the matrix that i-th diagonal entry is $w_{i,i}^2$.
- \bullet Let $\sigma_{\min}(A)$ denote the minimum singular value of A.
- Let l > 0 denote a scalar.

Then, we have

• Part 1. If all $i \in [n]$, $w_i^2 \ge 4 + l/\sigma_{\min}(A)^2$, then

$$\frac{\mathrm{d}^2 L}{\mathrm{d}x^2} \succeq l \cdot I_d$$

• Part 2. If all $i \in [n], w_i^2 \ge 100 + l/\sigma_{\min}(A)^2$, then

$$(1 - 1/10) \cdot (B(x) + W^2) \le W^2 \le (1 + 1/10) \cdot (B(x) + W^2)$$

Proof. By applying Lemma 5.13 and Lemma 5.15, we have

$$\frac{\mathrm{d}^2 L_{\mathrm{exp}}}{\mathrm{d}x^2} = A^{\top} B(x) A$$

where

$$B(x) \succeq -4I_n \tag{3}$$

Also, it's trivial that

$$\frac{\mathrm{d}^2 L}{\mathrm{d}x^2} = \frac{\mathrm{d}^2 L_{\text{reg}}}{\mathrm{d}x^2} + \frac{\mathrm{d}^2 L_{\text{exp}}}{\mathrm{d}x^2} \tag{4}$$

Thus, by applying Lemma 4.9, Eq. (4) can be written as

$$\frac{\mathrm{d}^2 L}{\mathrm{d}x^2} = A^{\top} B(x) A + A^{\top} W^2 A$$
$$= A^{\top} (B(x) + W^2) A$$

Let

$$D = B(x) + W^2$$

Then, $\frac{\mathrm{d}^2 L}{\mathrm{d}x^2}$ can be rewrite as

$$\frac{\mathrm{d}^2 L}{\mathrm{d}x^2} = A^{\top} D A$$

Now, we can bound D as follows

$$D \succeq -4I_n + w_{\min}^2 I_n$$
$$= (-4 + w_{\min}^2) I_n$$
$$\succeq \frac{l}{\sigma_{\min}(A)^2} I_n$$

where the 3rd step follows from $w_{\min}^2 \ge 4 + l/\sigma_{\min}(A)^2$, the last step follows from simple algebra. Since D is positive definite, then we have

$$A^{\top}DA \succeq \sigma_{\min}(D) \cdot \sigma_{\min}(A)^2 I_d \succeq l \cdot I_d$$

Thus, Hessian is positive definite forever and thus the function is convex.

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. In Section 7.2, we prove that some basic terms satisfy the property of Lipschitz. In Section 7.3, we provide a sketch of how we find the bound of $\|\nabla^2 L(x) - \nabla^2 L(y)\|$, to be specific, we split $\|\nabla^2 L(x) - \nabla^2 L(y)\|$ into 8 terms and state that all these terms can be bound by using $\|f(x) - f(y)\|$. In Section 7.4, we use $\|f(x) - f(y)\|$ to bound the first term. In Section 7.5, we use $\|f(x) - f(y)\|$ to bound the second term. In Section 7.6, we use $\|f(x) - f(y)\|$ to bound the third term. In Section 7.7, we use $\|f(x) - f(y)\|$ to bound the fifth term. In Section 7.9, we use $\|f(x) - f(y)\|$ to bound the sixth term. In Section 7.10, we use $\|f(x) - f(y)\|$ to bound the seventh term. In Section 7.11, we use $\|f(x) - f(y)\|$ to bound the last term.

7.1 Main Result

Lemma 7.1. If the following condition holds

- Let $H(x) = \frac{\mathrm{d}^2 L}{\mathrm{d}x^2}$
- Let R > 2
- $||x||_2 \le R, ||y||_2 \le R$
- $||A(x-y)||_{\infty} < 0.01$
- $||A|| \leq R$
- $||b||_2 < R$
- $\langle \exp(Ax), \mathbf{1}_n \rangle \geq \beta$ and $\langle \exp(Ay), \mathbf{1}_n \rangle \geq \beta$

Then we have

$$||H(x) - H(y)|| \le \beta^{-2} n^{1.5} \exp(20R^2) \cdot ||x - y||_2$$

Proof.

$$||H(x) - H(y)||$$

$$\leq ||A|| \cdot (2||G_1|| + ||G_2|| + \dots + ||G_8||) ||A||$$

$$\leq R^2 \cdot (2||G_1|| + ||G_2|| + \dots + ||G_8||)$$

$$\leq R^2 \cdot 100R \cdot ||f(x) - f(y)||_2$$

$$\leq R^2 \cdot 100R \cdot \beta^{-2} n^{1.5} \exp(3R^2) ||x - y||_2$$

$$\leq \beta^{-2} n^{1.5} \exp(20R^2) ||x - y||_2$$

where the 1st step follows definition of G_i and matrix spectral norm, the 2nd step follows from $||A|| \leq R$, the 3rd step follows from Lemma 7.3, the 4th step follows from Lemma 7.2, and the last step follows from simple algebra.

7.2 A Core Tool: Lipschitz Property for Several Basic Functions

Lemma 7.2. If the following conditions hold

- Let $A \in \mathbb{R}^{n \times d}$
- Let $b \in \mathbb{R}^n$ satisfy that $||b||_1 \le 1$
- Let $\beta \in (0, 0.1)$
- Let R > 4
- Let $x, y \in \mathbb{R}^d$ satisfy $||A(x-y)||_{\infty} < 0.01$
- $||A|| \leq R$
- $\langle \exp(Ax), \mathbf{1}_n \rangle \geq \beta$
- $\langle \exp(Ay), \mathbf{1}_n \rangle \geq \beta$
- Let $R_f := \beta^{-2} n^{1.5} \exp(3R^2)$
- Let $\alpha(x)$ be defined as Definition 5.4
- Let c(x) be defined as Definition 5.5
- Let f(x) be defined as Definition 5.1
- Let g(x) be defined as Definition 5.7

We have

- $Part \ 0. \ \|\exp(Ax)\|_2 \le \sqrt{n}\exp(R^2)$
- Part 1. $\|\exp(Ax) \exp(Ay)\|_2 \le 2\sqrt{n}R\exp(R^2) \cdot \|x y\|_2$
- Part 2. $|\alpha(x) \alpha(y)| \le \sqrt{n} \cdot \|\exp(Ax) \exp(Ay)\|_2$
- Part 3. $|\alpha(x)^{-1} \alpha(y)^{-1}| \le \beta^{-2} \cdot |\alpha(x) \alpha(y)|$
- Part 4. $||f(x) f(y)||_2 \le R_f \cdot ||x y||_2$
- Part 5. $||c(x) c(y)||_2 \le R_f \cdot ||x y||_2$
- Part 6. $||g(x) g(y)||_2 \le 16 \cdot R \cdot R_f \cdot ||x y||_2$

Proof. Proof of Part 0.

We can show that

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

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

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

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

where the first step follows from Fact 4.3, the second step follows from Fact 4.3, the third step follows from Fact 4.3, and the last step follows from $||A|| \le R$ and $||x||_2 \le R$.

Proof of Part 1. We have

$$\|\exp(Ax) - \exp(Ay)\|_{2} \leq \|\exp(Ax)\|_{2} \cdot 2\|A(y-x)\|_{\infty}$$

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

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

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

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

where the 1st step follows from $||A(y-x)||_{\infty} < 0.01$ and Fact 4.3, the 2nd step follows from Part 0, the 3rd step follows from Fact 4.3, the 4th step follows from Fact 4.4, the last step follows from $||A|| \le R$.

Proof of Part 2.

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

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

where the 1st step follows from the definition of $\alpha(x)$, the 2nd step follows from Cauchy-Schwarz inequality (Fact 4.3).

Proof of Part 3.

We can show that

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

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

where the 1st step follows from simple algebra, the 2nd step follows from $\alpha(x), \alpha(y) \geq \beta$.

Proof of Part 4.

We can show that

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

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

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

where the 1st step follows from the definition of f(x) and $\alpha(x)$, the 2nd step follows from triangle inequality, the 3rd step follows from $\|\alpha A\| \leq |\alpha| \|A\|$ (Fact 4.4).

For the first term in the above, we have

$$\alpha(x)^{-1} \| \exp(Ax) - \exp(Ay) \|_{2} \le \beta^{-1} \| \exp(Ax) - \exp(Ay) \|_{2}$$
$$\le \beta^{-1} \cdot 2\sqrt{n} R \exp(R^{2}) \cdot \|x - y\|_{2}$$
(5)

where the 1st step follows from $\alpha(x) \geq \beta$, the 2nd step follows from Part 1.

For the second term in the above, we have

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

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

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

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

$$= \beta^{-2} \cdot 2n^{1.5} R \exp(2R^{2}) \|x - y\|_{2}$$
(6)

where the 1st step follows from the result of **Part 3**, the 2nd step follows from **Part 0**, the 3rd step follows from the result of **Part 2**, the 4th step follows from **Part 1**, and the last step follows from simple algebra.

Combining Eq. (5) and Eq. (6) together, we have

$$||f(x) - f(y)||_{2} \le \beta^{-1} \cdot 2\sqrt{n}R \exp(R^{2}) \cdot ||x - y||_{2} + \beta^{-2}2n^{1.5}R \exp(2R^{2})||x - y||_{2}$$

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

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

where the 1st step follows from the bound of the first term and the second term, the 2nd step follows from $\beta^{-1} \ge 1$ and n > 1 trivially, the 3rd step follows from simple algebra.

Proof of Part 5. We have

$$||c(x) - c(y)||_2 = ||f(x) - f(y)||_2 \le R_f \cdot ||x - y||_2,$$

the first step follows from the definition of c(x), the last step follows from **Part 4** and definition of R_f . **Proof of Part 6.**

Using Lemma 5.8, we have

$$||g(x) - g(y)||_2 \le 8||A||R_f \cdot 2||x - y||_2$$

$$\le 18RR_f \cdot ||x - y||_2,$$

where the second step follows from $||A|| \leq R$.

Thus, we complete the proof.

7.3 Summary of Eight Steps

Lemma 7.3. If the following conditions hold

- $G_1 = ||f(x)||_2^2 f(x) f(x)^\top ||f(y)||_2^2 f(y) f(y)^\top$
- $G_2 = \langle f(x), b \rangle f(x) f(x)^{\top} \langle f(y), b \rangle f(y) f(y)^{\top}$
- $G_3 = \langle f(x), f(x) \rangle \operatorname{diag}(f(x)) \langle f(y), f(y) \rangle \operatorname{diag}(f(y))$
- $G_4 = \langle f(x), b \rangle \operatorname{diag}(f(x)) \langle f(y), b \rangle \operatorname{diag}(f(y))$
- $G_5 = \operatorname{diag}(f(x) \circ (f(x) b)) \operatorname{diag}(f(y) \circ (f(y) b))$
- $G_6 = \operatorname{diag}(f(x) \circ f(x)) \operatorname{diag}(f(y) \circ f(y))$
- $G_7 = f(x)(f(x) \circ b)^{\top} f(y)(f(y) \circ b)^{\top}$
- $G_8 = (f(x) \circ b)f(x)^{\top} (f(y) \circ b)f(y)^{\top}$

We have

$$||G_1|| + \sum_{i=1}^{8} ||G_i|| \le 100R \cdot ||f(x) - f(y)||_2$$

Proof. The proof directly follows from applying Lemma 7.4, Lemma 7.5, Lemma 7.6, Lemma 7.7, Lemma 7.8, Lemma 7.9, Lemma 7.10, Lemma 7.11.

7.4 Lipschitz Calculations: Step 1. Lipschitz for Matrix Function $||f(x)||_2^2 f(x) f(x)^{\top}$

Lemma 7.4. If the following condition holds

•
$$G_1 = ||f(x)||_2^2 f(x) f(x)^\top - ||f(y)||_2^2 f(y) f(y)^\top$$

Then

$$||G_1|| \le 4||f(x) - f(y)||_2$$

Proof. We define

$$G_{1,1} := \langle f(x), f(x) \rangle f(x) f(x)^{\top} - \langle f(x), f(y) \rangle f(x) f(x)^{\top}$$

$$G_{1,2} := \langle f(x), f(y) \rangle f(x) f(x)^{\top} - \langle f(y), f(y) \rangle f(x) f(x)^{\top}$$

$$G_{1,3} := \langle f(y), f(y) \rangle f(x) f(x)^{\top} - \langle f(y), f(y) \rangle f(y) f(x)^{\top}$$

$$G_{1,4} := \langle f(y), f(y) \rangle f(y) f(x)^{\top} - \langle f(y), f(y) \rangle f(y) f(y)^{\top}$$

We have

$$G_1 = G_{1,1} + G_{1,2} + G_{1,3} + G_{1,4}$$

Let us only prove for $G_{1,1}$, the others are similar,

$$||G_{1,1}|| \le |\langle f(x), f(x) - f(y) \rangle| \cdot ||f(x)f(x)^{\top}||$$

$$\le ||f(x)||_2 \cdot ||f(x) - f(y)||_2 \cdot ||f(x)f(x)^{\top}||$$

$$= ||f(x)||_2 \cdot ||f(x) - f(y)||_2 \cdot ||f(x)||_2^2$$

$$\le ||f(x) - f(y)||_2$$

where the 1st step follows from Fact 4.4, the 2nd step follows from $|\langle a,b\rangle| \leq ||a||_2 ||b||_2$ (Fact 4.3), the 3rd step follows from $aa^{\top} \leq ||a||_2^2 I_n$ (Fact 4.3), the last step follows from $||f(x)||_2 \leq ||f(x)||_1 \leq 1$ (Lemma 5.2).

It is obvious that for each $i \in [4]$, we have

$$||G_{1,i}|| \le ||f(x) - f(y)||_2 \max\{||f(x)||_2, ||f(y)||_2\}^3$$

$$\le ||f(x) - f(y)||_2$$

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

7.5 Lipschitz Calculations: Step 2. Lipschitz for Matrix Function $\langle f(x), b \rangle f(x) f(x)^{\top}$

Lemma 7.5. If the following condition holds

•
$$G_2 := \langle f(x), b \rangle f(x) f(x)^{\top} - \langle f(y), b \rangle f(y) f(y)^{\top}$$

Then we have

$$||G_2|| \le 3||f(x) - f(y)||_2 \cdot ||b||_2$$

Proof. We define

$$G_{2,1} := \langle f(x), b \rangle f(x) f(x)^{\top} - \langle f(x), b \rangle f(y) f(x)^{\top}$$

$$G_{2,2} := \langle f(x), b \rangle f(y) f(x)^{\top} - \langle f(x), b \rangle f(y) f(y)^{\top}$$

$$G_{2,3} := \langle f(x), b \rangle f(y) f(y)^{\top} - \langle f(y), b \rangle f(y) f(y)^{\top}$$

Then it's apparent that

$$G_2 = G_{2,1} + G_{2,2} + G_{2,3}$$

Since $G_{2,1}, G_{2,2}, G_{2,3}$ are similar, we only have to bound $||G_{2,1}||$:

$$||G_{2,1}|| = ||\langle f(x), b \rangle f(x) f(x)^{\top} - \langle f(x), b \rangle f(y) f(x)^{\top}||$$

$$= ||\langle f(x), b \rangle (f(x) - f(y)) f(x)^{\top}||$$

$$\leq |\langle f(x), b \rangle| \cdot ||(f(x) - f(y)) f(x)^{\top}||$$

$$\leq |\langle f(x), b \rangle| \cdot ||f(x) - f(y)||_{2} \cdot ||f(x)||_{2}$$

$$\leq ||f(x)||_{2}^{2} \cdot ||b||_{2} ||f(x) - f(y)||_{2}$$

$$\leq ||f(x) - f(y)||_{2} \cdot ||b||_{2}$$

where the 1st step follows from the definition of $G_{2,1}$, the 2nd step follows from simple algebra, the 3rd step follows from Fact 4.4, the 4th step follows from $||ab^{\top}|| \le ||a||_2 ||b||_2$ (Fact 4.4), the 5th step follows from $\langle a,b\rangle \le ||a||_2 ||b||_2$ (Fact 4.3), the last step follows from $||f(x)||_2 \le ||f(x)||_1 \le 1$.

Thus, we have

$$||G_2|| \le 3||f(x) - f(y)|||b||_2$$

7.6 Lipschitz Calculations: Step 3. Lipschitz for Matrix Function $f(x)f(x)^{\top} \operatorname{diag}(f(x))$

Lemma 7.6. If the following condition holds

•
$$G_3 := \langle f(x), f(x) \rangle \operatorname{diag}(f(x)) - \langle f(y), f(y) \rangle \operatorname{diag}(f(y))$$

Then we have

$$||G_3|| \le 3||f(x) - f(y)||_2$$

Proof. We define

$$G_{3,1} := \langle f(x), f(x) \rangle \operatorname{diag}(f(x)) - \langle f(x), f(y) \rangle \operatorname{diag}(f(x))$$

$$G_{3,2} := \langle f(x), f(y) \rangle \operatorname{diag}(f(x)) - \langle f(x), f(y) \rangle \operatorname{diag}(f(y))$$

$$G_{3,3} := \langle f(x), f(y) \rangle \operatorname{diag}(f(y)) - \langle f(y), f(y) \rangle \operatorname{diag}(f(y))$$

Thus, it's trivial that

$$G_3 = G_{3,1} + G_{3,2} + G_{3,3}$$

Since $G_{3,1}, G_{3,2}, G_{3,3}$ are similar, we only need to bound $||G_{3,1}||$:

$$||G_{3,1}|| = ||\langle f(x), f(x)\rangle \operatorname{diag}(f(x)) - \langle f(x), f(y)\rangle \operatorname{diag}(f(x))||$$

$$= \|\langle f(x), f(x) - f(y) \rangle \operatorname{diag}(f(x)) \|$$

$$\leq \|f(x)^{\top}\|_{2} \|f(x) - f(y)\|_{2} \|\operatorname{diag}(f(x))\|$$

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

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

where the 1st step follows from the definition of $G_{3,1}$, the 2nd step follows from simple algebra, the 3rd step follows from $\|\alpha A\| \leq |\alpha| \|A\|$ (Fact 4.4), $\langle a,b\rangle \leq \|a\|_2 \|b\|_2$ (Fact 4.3), and $\|ab\| \leq \|a\| \|b\|$ (Fact 4.4), the 4th step follows from $\|\operatorname{diag}(f(x))\| = \|f(x)\|_2$, the last step follows from $\|f(x)\|_2 \leq \|f(x)\|_1 \leq 1$ (Fact 4.3).

Thus, we have

$$||G_8|| = ||G_{8,1} + G_{8,2} + G_{3,3}||$$

$$\leq ||G_{8,1}|| + ||G_{8,2}|| + ||G_{3,3}||$$

$$= 3||f(x) - f(y)||_2$$

where the 1st step follows from the definition of G_3 , the 2nd step follows from Fact 4.4, the last step follows from the bound of $||G_{3,1}||, ||G_{3,2}||$ and $||G_{3,3}||$.

7.7 Lipschitz Calculations: Step 4. Lipschitz for Matrix Function $\langle f(x), b \rangle \operatorname{diag}(f(x))$

Lemma 7.7. If the following condition holds

•
$$G_4 := \langle f(x), b \rangle \operatorname{diag}(f(x)) - \langle f(y), b \rangle \operatorname{diag}(f(y))$$

Then we have

$$||G_4|| < 2||f(x) - f(y)||_2 ||b||_2$$

Proof. We define:

$$G_{4,1} := \langle f(x), b \rangle \operatorname{diag}(f(x)) - \langle f(y), b \rangle \operatorname{diag}(f(x))$$

$$G_{4,2} := \langle f(y), b \rangle \operatorname{diag}(f(x)) - \langle f(y), b \rangle \operatorname{diag}(f(y))$$

Thus, it's trivial that

$$G_4 = G_{4,1} + G_{4,2}$$

Since $G_{4,1}$ and $G_{4,2}$ are similar, we only need to bound $||G_{4,1}||$:

$$||G_{4,1}|| = ||\langle f(x), b \rangle \operatorname{diag}(f(x)) - \langle f(y), b \rangle \operatorname{diag}(f(x))||$$

$$= ||b^{\top}(f(x) - f(y)) \operatorname{diag}(f(x))||$$

$$\leq ||b^{\top}||_{2}||f(x) - f(y)||_{2}||\operatorname{diag}(f(x))||$$

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

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

where the 1st step follows from the definition of $G_{4,1}$, the 2nd step follows from simple algebra, the 3rd step follows from $||ab|| \le ||a|| ||b||$ (Fact 4.4) and , the 4th step follows from $||\operatorname{diag}(x)|| \le ||x||_{\infty} \le ||x||_{2}$ (Fact 4.3), the last step follows from $||f(x)||_{2} \le ||f(x)||_{1} \le 1$ (Fact 4.3).

Thus, we have

$$||G_4|| = ||G_{4,1} + G_{4,2}||$$

$$\leq ||G_{4,1}|| + ||G_{4,2}||$$

$$= 2||f(x) - f(y)||_2 \cdot ||b||_2$$

where the 1st step follows from the definition of G_4 , the 2nd step follows from Fact 4.4, the last step follows from the bound of $||G_{4,1}||$ and $||G_{4,2}||$.

7.8 Lipschitz Calculations: Step 5. Lipschitz for Matrix Function $\operatorname{diag}(f(x) \circ (f(x) - b))$

Lemma 7.8. If the following condition holds

•
$$G_5 := \operatorname{diag}(f(x) \circ (f(x) - b)) - \operatorname{diag}(f(y) \circ (f(y) - b))$$

Then we have

$$||G_5|| \le 2||f(x) - f(y)||_2 + ||f(x) - f(y)|| \cdot ||b||_2$$

Proof. We define:

$$G_{5,1} := \operatorname{diag}(f(x) \circ (f(x) - b)) - \operatorname{diag}(f(x) \circ (f(y) - b))$$

$$G_{5,2} := \operatorname{diag}(f(x) \circ (f(y) - b)) - \operatorname{diag}(f(y) \circ (f(y) - b))$$

Then, it's trivial that

$$G_5 = G_{5,1} + G_{5,2}$$

Bound $||G_{5,1}||$:

$$||G_{5,1}|| = ||\operatorname{diag}(f(x) \circ (f(x) - b)) - \operatorname{diag}(f(x) \circ (f(y) - b))||$$

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

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

$$\leq ||f(x)||_2||f(x) - f(y)||_2$$

$$\leq ||f(x) - f(y)||_2$$

where the 1st step follows from the definition of $G_{5,1}$, the 2nd step follows from Fact 4.2, the 3rd step follows from $||ab|| \le ||a|| ||b||$ (Fact 4.4), the 4th step follows from $||\operatorname{diag}(a)|| \le ||a||_{\infty} \le ||a||_{2}$ (Fact 4.3), the last step follows from $||f(x)||_{2} \le ||f(x)||_{1} \le 1$.

Bound $||G_{5,2}||$:

$$||G_{5,2}|| = ||\operatorname{diag}(f(x) \circ (f(y) - b)) - \operatorname{diag}(f(y) \circ (f(y) - b))||$$

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

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

$$\leq ||f(x) - f(y)||_2 ||f(y)||_2 + ||f(x) - f(y)||_2 ||b||_2$$

$$\leq ||f(x) - f(y)||_2 + ||f(x) - f(y)||_2 ||b||_2$$

where the 1st step follows from the definition of $G_{5,2}$, the 2nd step follows from Fact 4.2, the 3rd step follows from Fact 4.4, the 4th step follows from $\|\operatorname{diag}(a)\| \leq \|a\|_{\infty} \leq \|a\|_{2}$ (Fact 4.3), the last step follows from $\|f(x)\|_{2} \leq \|f(x)\|_{1} \leq 1$.

Thus, we have

$$||G_5|| = ||G_{5,1} + G_{5,2}||$$

$$\leq ||G_{5,1}|| + ||G_{5,2}||$$

$$\leq 2||f(x) - f(y)||_2 + ||f(x) - f(y)||_2 \cdot ||b||_2$$

where the 1st step follows from the definition of G_5 , the 2nd step follows from Fact 4.2, the 3rd step follows from the bound of $||G_{5,1}||$ and $||G_{5,2}||$.

7.9 Lipschitz Calculations: Step 6. Lipschitz for Matrix Function $\operatorname{diag}(f(x) \circ f(x))$

Lemma 7.9. If the following condition holds

•
$$G_6 := \operatorname{diag}(f(x) \circ f(x)) - \operatorname{diag}(f(y) \circ f(y))$$

Then we have

$$||G_6|| \le 2||f(x) - f(y)||_2$$

Proof. We define:

$$G_{6,1} := \operatorname{diag}(f(x) \circ f(x)) - \operatorname{diag}(f(x) \circ f(y))$$

$$G_{6,2} := \operatorname{diag}(f(x) \circ f(y)) - \operatorname{diag}(f(y) \circ f(y))$$

Then, it's trivial that

$$G_6 = G_{6,1} + G_{6,2}$$

Since, $G_{6,1}$ and $G_{6,2}$ are similar, we only need to bound $||G_{6,1}||$:

$$||G_{6,1}|| = ||\operatorname{diag}(f(x) \circ f(x)) - \operatorname{diag}(f(x) \circ f(y))||$$

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

$$\leq ||f(x)||_2 ||f(x) - f(y)||_2$$

$$\leq ||f(x) - f(y)||$$

where the 1st step follows from the definition of $G_{6,1}$, the 2nd step follows from Fact 4.2, the 3rd step follows from $||ab|| \le ||a|| ||b||$ (Fact 4.4) and $||\operatorname{diag}(a)|| \le ||a||_{\infty} \le ||a||_2$ (Fact 4.3), the last step follows from $||f(x)||_2 \le ||f(x)||_1 \le 1$.

Thus, we have

$$||G_6|| = ||G_{6,1} + G_{6,2}||$$

$$\leq ||G_{6,1}|| + ||G_{6,2}||$$

$$= 2||f(x) - f(y)||_2$$

where the 1st step follows from the definition of G_6 , the 2nd step follows from Fact 4.4, the last step follows from the bound of $||G_{6,1}||$ and $||G_{6,2}||$.

7.10 Lipschitz Calculations: Step 7. Lipschitz for Matrix Function $f(x)(f(x) \circ b)^{\top}$

Lemma 7.10. If the following condition holds

•
$$G_7 := f(x)(f(x) \circ b)^{\top} - f(y)(f(y) \circ b)^{\top}$$

Then, we have

$$||G_7|| \le 2||f(x) - f(y)||_2 \cdot ||b||_2$$

Proof. We define:

$$G_{7,1} := f(x)(f(x) \circ b)^{\top} - f(x)(f(y) \circ b)^{\top}$$

$$G_{7,2} := f(x)(f(y) \circ b)^{\top} - f(y)(f(y) \circ b)^{\top}$$

Since $G_{7,1}$ and $G_{7,2}$ are similar, we only need to bound $||G_{7,1}||$:

$$||G_{7,1}|| = ||f(x)(f(x) \circ b)^{\top} - f(x)(f(y) \circ b)^{\top}||$$

$$= ||f(x)((f(x) - f(y)) \circ b)^{\top}||$$

$$\leq ||f(x)||_2 ||(f(x) - f(y)) \circ b||_2$$

$$\leq ||f(x) - f(y)||_2 ||b||_2$$

where the 1st step follows from the definition of $G_{7,1}$, the 2nd step follows from simple algebra, the 3rd step follows from $||ab^{\top}|| \le ||a||_2 ||b||_2$ (Fact 4.4) and $||a^{\top}||_2 = ||a||_2$, the last step follows from $||a \circ b||_2 \le ||a||_\infty ||b|| \le ||a||_2 ||b||_2$ (Fact 4.3) and $||f(x)||_2 \le ||f(x)||_1 \le 1$.

Thus, we have

$$||G_7|| = ||G_{7,1} + G_{7,2}||$$

$$\leq ||G_{7,1}|| + ||G_{7,2}||$$

$$= 2||f(x) - f(y)||_2 \cdot ||b||_2$$

where the 1st step follows from the definition of G_7 , the 2nd step follows from Fact 4.4, the last step follows from the bound of $||G_{7,1}||$ and $||G_{7,2}||$.

7.11 Lipschitz Calculations: Step 8. Lipschitz for Matrix Function $(f(x) \circ b) f(x)^{\top}$

Lemma 7.11. If the following condition holds

•
$$G_8 := (f(x) \circ b)f(x)^{\top} - (f(y) \circ b)f(y)^{\top}$$

Then we have

$$||G_8|| \le 2||f(x) - f(y)||_2 \cdot ||b||_2$$

Proof. We define:

$$G_{8,1} := (f(x) \circ b) f(x)^{\top} - (f(x) \circ b) f(y)^{\top}$$

$$G_{8,2} := (f(x) \circ b) f(y)^{\top} - (f(y) \circ b) f(y)^{\top}$$

Then, it's trivial that

$$G_8 = G_{8,1} + G_{8,2}$$

Since $G_{8,1}$ and $G_{8,2}$ are similar, we only need to bound $||G_{8,1}||$:

$$||G_{8,1}|| = ||(f(x) \circ b)f(x)^{\top} - (f(x) \circ b)f(y)^{\top}||$$

$$= ||(f(x) \circ b)(f(x) - f(y))^{\top}||$$

$$\leq ||f(x) \circ b||_{2} ||f(x) - f(y)||_{2}$$

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

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

where the 1st step follows from the definition of $G_{8,1}$, the 2nd step follows from simple algebra, the 3rd step follows from $||ab^{\top}|| \leq ||a||_2 ||b||_2$ (Fact 4.4), the 4th step follows from $||a \circ b||_2 \leq ||a||_{\infty} ||b|| \leq ||a||_2 ||b||_2$ (Fact 4.3), the last step follows from $||f(x)||_2 \leq ||f(x)||_1 \leq 1$ (Lemma 5.2).

Thus, we have

$$||G_8|| = ||G_{8,1} + G_{8,2}||$$

$$\leq ||G_{8,1}|| + ||G_{8,2}||$$

$$= 2||f(x) - f(y)||_2 \cdot ||b||_2$$

where the 1st step follows from the definition of G_8 , the 2nd step follows from Fact 4.4, the last step follows from the bound of $||G_{8,1}||$ and $||G_{8,2}||$.

8 Approximate Newton Method

In this section, we provide an approximate version of the newton method for convex optimization. In Section 8.1, we state some assumptions of the traditional newton method and the exact update rule of the traditional algorithm. In Section 8.2, 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 [LSZ23] to analyze the approximate newton method. In Section 8.3, we prove a lower bound on β . In Section 8.4, we prove an upper bound on M.

8.1 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 8.1 ((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

$$r_0 M \le 0.1 l$$

We define gradient and Hessian as follows

Definition 8.2 (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 8.3 (Exact update of the Newton method).

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

8.2 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 8.4 (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,

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

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 8.5 ([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

$$(1 - \epsilon_0)A^{\mathsf{T}}DA \preceq A^{\mathsf{T}}\widetilde{D}A \preceq (1 + \epsilon_0)A^{\mathsf{T}}DA.$$

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, LSZ23], we consider the following.

Definition 8.6 (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 8.7 (Iterative shrinking Lemma, Lemma 6.9 on page 32 of [LSZ23]). If the following condition hold

- Loss Function L is (l, M)-good (see Definition 8.1).
- Let $\epsilon_0 \in (0, 0.1)$ (see Definition 8.4).
- 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 8.7, we will need the following induction hypothesis lemma. This is very standard in the literature, see [LSZ23].

Lemma 8.8 (Induction hypothesis, Lemma 6.10 on page 34 of [LSZ23]). For each $i \in [t]$, we define $r_i := ||x_i - x^*||_2$. If the following condition hold

- $\epsilon_0 = 0.01$ (see Definition 8.4 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 8.1 for M)

Then we have

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

8.3 Lower bound on β

Lemma 8.9. 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

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

$$\ge \exp(-||Ax||_{\infty})$$

$$\ge \exp(-||Ax||_2)$$

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

the 1st step follows from simple algebra, the 2nd step follows from definition of ℓ_{∞} norm, the 3rd step follows from Fact 4.3.

8.4 Upper bound on M

Lemma 8.10. 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 7.1)

Then, we have

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

Proof. It follows from Lemma 8.9.

9 Main Result

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Algorithm 1 Here, we present our main algorithm in an informal way.
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```
1: procedure IterativeSoftmaxRegression(A \in \mathbb{R}^{n \times d}, b \in \mathbb{R}^{n}, w \in \mathbb{R}^{n}, \epsilon, \delta) > Theorem 9.1
           We choose x_0 (suppose it satisfies Definition 8.1)
           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:
                 \widetilde{D} \leftarrow \text{SUBSAMPLE}(D, A, \epsilon_1 = \Theta(1), \delta_1 = \delta/T)
 6:
                                                                                                                                               ▶ Lemma 8.5
                 g \leftarrow A^{\top}(f(x_t)\langle c(x_t), f(x_t)\rangle + \operatorname{diag}(f(x_t))c(x_t))\widetilde{H} \leftarrow A^{\top}\widetilde{D}A
 7:
 8:
                 x_{t+1} \leftarrow x_t + \widetilde{H}^{-1}q
 9:
           end for
10:
11:
           \widetilde{x} \leftarrow x_{T+1}
           return \tilde{x}
12:
13: end procedure
```

Theorem 9.1. Suppose we have matrix $A \in \mathbb{R}^{n \times d}$, and vectors $b, w \in \mathbb{R}^n$. And we have the following

- Define $f(x) := \langle \exp(Ax), \mathbf{1}_n \rangle^{-1} \exp(Ax)$.
- Define x^* as the optimal solution of

$$\min_{x \in \mathbb{R}^d} 0.5 ||f(Ax) - b||_2^2 + 0.5 ||\operatorname{diag}(w)Ax||_2^2$$

for which,

- $-g(x^*) = \mathbf{0}_d.$
- $\|x^*\|_2 \le R.$
- Define $R \ge 10$ be a positive scalar.
- It holds that $||A|| \le R$
- It holds that $b \geq \mathbf{0}_n$, and $||b||_1 \leq 1$.
- It holds that $w_i^2 \ge 100 + l/\sigma_{\min}(A)^2$ for all $i \in [n]$
- It holds that $M = n^{1.5} \exp(30R^2)$.
- Let x_0 denote an initial point for which it holds that $M||x_0 x^*||_2 \le 0.1l$.

Then for any 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 denote the exponent of matrix multiplication. Currently $\omega \approx 2.373$ [Wil12, LG14, AW21].

Proof. It follows from combining Lemma 6.3, Lemma 8.8, Lemma 8.5, Lemma 7.1 and Lemma 8.7.

Proof of Upper bound on M.

It follows from Lemma 8.10.

Proof of Hessian is PD.

This follows from Lemma 6.3.

Proof of Hessian is Lipschitz.

This follows from Lemma 7.1.

Proof of Cost per iteration.

This follows from Lemma 8.5.

Proof of Convergence per Iteration.

By Lemma 8.7, we have

$$||x_k - x^*||_2 \le 0.4 \cdot ||x_{k-1} - x^*||_2.$$

Proof of Number of Iterations. After T iterations, we have

$$||x_T - x^*||_2 \le 0.4^T \cdot ||x_0 - x^*||_2$$

By choice of T, we get the desired bound. The failure probability is following from union bound over T iterations.

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