

Multiple Constraints and Non-regular Solution in Deep Declarative Network

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Except where otherwise indicated, this thesis is my own original work.

Suikei Wang
22 September 2020

to my parents, yyy (yyy is the people you want to dedicated this thesis to.)

Acknowledgments

The past two years at the Australian National University have been an invaluable experience for me. When I started my Master of Machine Learning and Computer Vision at the beginning of 2019, I could barely understand lectures, knew little about the country, and had never heard of the term "convex optimization". It is unbelievable that I have been doing a research project on this topic for a whole year. ANU has the top tier research group in this realm and how honored I am to be a postgraduate student here.

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I would like to thank Dylan Campbell and Miaomiao Liu – another two giants of the Australian Centre for Robotic Vision – for offering my supervision and being my second examiner on my thesis. Dylan

Abstract

Put your abstract here.

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Introduction

1.1 Motivation

Deep learning models composed with multiple parametrized processing layers can learn different levels of features and representations of data through the directed graph structure.

Put your introduction here. You could use `\fix{ABCDEFG.}` to leave your comments, see the box at the left side.

You have to
rewrite your
thesis!!!

1.2 Thesis Outline

How many chapters you have? You may have Chapter 2, Chapter ??, Chapter ??, Chapter 6, and Chapter 7.

1.3 Contribution

Part I

Deep Declarative Network: Multiple Constrained Declarative Nodes

An Overview of Numerical Optimization

In this chapter, we aim to provide readers with an overview of numerical optimization. We begin with the theory of optimization (Section 2.1), from the existence of optimizers, to the optimality conditions for both unconstrained and constrained problems with duality. As the theoretical background of optimization, this field provides a solid solution for the algorithm.

We then formally define the optimization of unconstrained and constrained problems in Section 2.2 and describe the general regular solution for these problems based on the gradient calculation.

Next, we discuss briefly the bi-level optimization, which is a lower-level optimization problem embedded within an upper-level problem sharing the same variables. (Section 2.3). Finally, we give a summary of the numerical optimization in constrained problems in Section 2.4.

2.1 Theory of Optimization

2.1.1 Existence of Optimizers

In optimization, a basic question is to determine the existence of a global minimizer for a given function f . There are several sufficient conditions on f to guarantee the existence, and the optimizer falls in the feasible set of solutions. For a feasible set, some related definitions are following:

Definition 2.1. A subset $\Omega \in \mathbb{R}^n$ is called

- *bounded* if there is a constant $R > 0$ such that $\|x\| \leq R$ for all $x \in \Omega$
- *closed* if the limit point of any convergent sequence in Ω always lies in Ω
- *compact* if any sequence $\{x_k\}$ in Ω contains a subsequence that converges to a point in Ω

The following result gives a characterization of compact sets in \mathbb{R} . When we find the minimum or maximum solution for the problem, there exists a lower bound

or upper bound but not necessarily an optimal solution. Therefore, we have some additional requirements.

Firstly, we give the definition of compact sets in Lemma 2.2. [Oman, 2017] gives a brief proof.

Lemma 2.2 (Bolzano-Weierstrass theorem). A subset Ω in \mathbb{R}^n is *compact* if and only if it is bounded and closed.

We also assume that the function f is continuous and " $+\infty$ at infinity". More precisely, $f(x) \rightarrow +\infty$ if $|x| \rightarrow +\infty$. Such a function is called *inf-compact* or *coercive*. [Nocedal and Wright, 2006] Then the problem can be restricted to a bounded set and existence of a global minimum x^* is guaranteed: a continuous function has a minimum on a compact set. This theorem is defined as follows and the proof is given in Appendix A.1.1.

Theorem 2.3. [Nocedal and Wright, 2006] If f is a continuous function defined on a compact set Ω in \mathbb{R} , then f has a global minimizer x^* on Ω i.e. there exists $x^* \in \Omega$ such that $f(x^*) \leq f(x)$ for all $x \in \Omega$

More general, based on the definition of coercive function f , we can give following theorem. Proof is given in Appendix A.1.2.

Theorem 2.4. [Nocedal and Wright, 2006] If $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is a continuous coercive function, then f has at least one global minimizer.

Theorem 2.4 requires the continuity of f which is somewhat restrictive for applications. However, we can replace it by the lower semi-continuity of f which is a rather weaker condition.

Definition 2.5. Let $f : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{\pm\infty\}$. Then f is called *lower semi-continuous* at a point $x_0 \in \mathbb{R}^n$ if for any sequence $f(x_k)$ converging to x_0 here holds $f(x_0) \leq \lim_{k \rightarrow \infty} f(x_k)$. f is called *lower semi-continuous* if f is lower semi-continuous at every point.

Recall our assumptions on function f , it is a continuous function, which is always lower semi-continuous. However, lower semi-continuous functions are not necessarily continuous. For instance, a binary function equals to 0 when $x \leq 0$ and equals to 1 when $x > 0$ is not continuous at $x_0 = 0$. However, since it is greater than 0 for all x and $f(0) = 0$, we have $f(0) = 0 \leq \liminf_{x \rightarrow 0} f(x)$ and it is lower semi-continuous at $x_0 = 0$.

The theorem of the existence of the optimizer of lower semi-continuous function is given as follows and the proof is given in Appendix A.1.3

Theorem 2.6. [Nocedal and Wright, 2006] Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a lower semi-continuous function. If f has a nonempty, compact sublevel set $D := \{x \in \mathbb{R}^n : f(x) \leq \alpha\}$, then f achieves a global minimizer on \mathbb{R}

Also, we introduce the definition of convex function and convex set which are important in regular optimization problems.

Definition 2.7. A function f is convex when

$$f(\alpha x + (1 - \alpha)y) \leq \alpha f(x) + (1 - \alpha)f(y) \quad \text{for all } x, y, \text{ and } \alpha \in]0, 1[$$

A set $C \subset \mathbb{R}^n$ is convex when

$$\alpha x + (1 - \alpha)y \in C \quad \text{for all } x, y \text{ in } C, \text{ and } \alpha \in]0, 1[$$

The problem we are going to discuss in this part is convex and regular, which means its gradient can be computed and the solution exists. However, although the existence of the optimizer is sufficient, for different problems, the optimality conditions are different. In the next two sections, we will give necessary and sufficient conditions for both unconstrained and constrained problems.

2.1.2 Optimality Conditions for Unconstrained Problems

Firstly, we consider the unconstrained minimization problem

$$\min_{x \in \mathbb{R}^n} f(x), \tag{2.1}$$

where f is given function on \mathbb{R}^n .

In order to determine the minimizer, it is important to understand what can happen at a minimizer, and at what condition a point must be a minimizer. Now we have to recognize the optimum point. There are two necessary conditions and one sufficient condition given below [Nocedal and Wright, 2006]. The proof is given in Appendix A.2.1.

Theorem 2.8. Necessary and Sufficient Conditions. Let $f : \Omega \rightarrow \mathbb{R}$ be a function defined on a set $\Omega \subset \mathbb{R}^n$ and let x^* be an interior point of Ω that is a local minimizer of f .

Necessary conditions:

- (NC1) If f is differentiable at x^* , then x^* is a critical point of f , i.e. $\nabla f(x^*) = 0$.
- (NC2) If f is twice continuous differentiable on Ω , then the Hessian $\nabla^2 f(x^*)$ is positive semidefinite.

Sufficient condition (SC1): if x^* is such that $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ is positive definite, then x^* is a local minimum. (i.e. $f(x) \geq f(x^*)$ for x close to x^*)

Any point satisfying (NC1) as the minimizer of f is called a *critical* or *stationary* point of f . In the objective function f is convex, (NC1) is also the sufficient condition for the global minimum of the solution.

Let us see an example of unconstrained minimization problem. Supposed we have to determine the minimization of function

$$f(x, y) = x^4 - 4xy + y^4$$

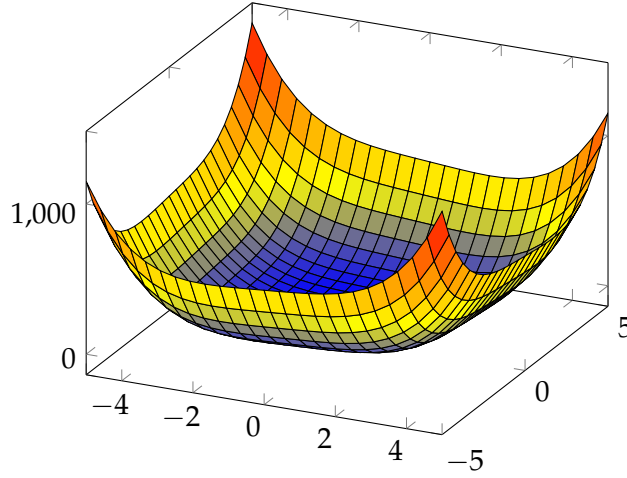


Figure 2.1: Function Graph of $f(x, y) = x^4 - 4xy + y^4$

From the definition of function f , it is clear that f is continuous. Then we can expand f by writing

$$f(x, y) = (x^4 + y^4) \left(1 - \frac{4xy}{x^4 + y^4} \right)$$

we can see f is coercive. Also, we give the plotting graph of function f in Figure 2.1. Therefore f has global minimizers which are critical points. Now according to (NC1), we can find the global minimizer through solving the derivative of f equaling to zero:

$$0 = \nabla f(x, y) = \begin{pmatrix} 4x^3 - 4y \\ -4x + 4y^3 \end{pmatrix}$$

Thus, $y = x^3$ and $x = y^3$. Consequently $y = y^9$, i.e.

$$0 = y - y^9 = y(1 - y^8) = y(1 - y^4)(1 + y^4) = y(1 - y)(1 + y)(1 + y^2)(1 + y^4)$$

This implies $y = 0, 1, -1$. Thus f has three critical points $(0, 0), (1, 1), (-1, -1)$. Then we can evaluate f as these points since they may be local minimizer:

$$f(0, 0) = 0, \quad f(1, 1) = -2, \quad f(-1, -1) = -2$$

It achieves the same global minimum value on $(1, 1)$ and $(-1, -1)$. Therefore, they are both global minimizers of f .

From this example, we verify that through (NC1), we can find the global minimizer. However, not all continuous functions with critical points have any maximizer or minimizer. If the function goes to infinity along its axes or a line, it does not have any maximizer or minimizer although it has a critical point. The condition of the minimizer as the critical point is that the function f should be a convex function with continuous first partial derivatives.

Let us move to the sufficient condition (SC1). The result obtained under this theorem is best possible for general functions. Specifically, for a convex function f is defined on a convex set $\Omega \subset \mathbb{R}^n$, any local minimizer of f is also a global minimizer. Moreover, if a function f is strictly convex, it has at most one global minimizer.

2.1.3 Optimality Conditions for Constrained Problems

A general formulation for constrained optimization problems is as follows:

$$\begin{aligned} & \text{minimize } f(x) \\ & \text{subject to } \begin{cases} c_i(x) = 0 & \text{for } i = 1, \dots, m_e, \\ c_i(x) \leq 0 & \text{for } i = m_e + 1, \dots, m \end{cases} \end{aligned} \quad (2.2)$$

where f and c_i are smooth real-valued functions on \mathbb{R}^n , and m_e and m are nonnegative integers with $m_e < m$. We set

$$\mathbb{E} := \{1, \dots, m_e\} \quad \text{and} \quad \mathbb{I} := \{m_e + 1, \dots, m\}$$

as index sets of equality constraints and inequality constraints, respectively. Here, f is so-called the objective function, and $c_i, i \in \mathbb{E}$ and \mathbb{I} are equality constraints and inequality constraints respectively.

To solve the optimization problem (2.2), we define the feasible set of it to be

$$\mathbb{F} := \{x \in \mathbb{R}^n : c_i(x) = 0 \text{ for } i \in \mathbb{E} \text{ and } c_i(x) \leq 0 \text{ for } i \in \mathbb{I}\}$$

Any point $x \in \mathbb{F}$ is called a feasible point of (2.2) and we call (2.2) infeasible if $\mathbb{F} = \emptyset$. Also, in this feasible set, a feasible point $x^* \in \mathbb{F}$ is called a local minimizer of (2.2) if it is the minimum solution in a neighborhood (strict local minimizer if it is the only one minimum solution). The definition of the global minimizer and strict global minimizer are similar, whose neighborhood is the whole feasible set.

Let us move to the constraints in this problem. For equality constraints, they are strictly equivalent. However, for inequality constraints, there are some exceptions. Let x^* be a local minimizer of (2.2). If there is an index $i \in \mathbb{I}$ such that $c_i(x^*) < 0$, then, x^* is still the local minimizer of the problem obtained by deleting i -th constraint. In this situation, we say that the i -th constraint is inactive at x^* since it does not have any effect on the solution.

2.1.4 Duality**2.2 Unconstrained and Constrained Optimization****2.2.1 Unconstrained Optimization****2.2.2 Equality Constrained Optimization****2.2.3 Inequality Constrained Optimization****2.3 Bi-level Optimization****2.4 Summary**

Summary what you discussed in this chapter, and mention the story in next chapter. Readers should roughly understand what your thesis takes about by only reading words at the beginning and the end (Summary) of each chapter.

Deep Declarative Network

Same as the last chapter, introduce the motivation and the high-level picture to readers, and introduce the sections in this chapter.

3.1 Notation

3.2 An Overview of Deep Declarative Network

3.2.1 Structure

3.2.2 Declarative Nodes

3.3 Learning

3.4 Back-propagation Through Declarative Nodes

3.4.1 Unconstrained

3.4.2 Equality Constrained

3.4.3 Inequality Constrained

3.5 Experiments

3.5.1 Platform

3.5.2 Implementation Details

3.5.3 Experimental Results

3.5.4 Analysis: Is the Gradient Always Converged?

3.6 Summary

Same as the last chapter, summary what you discussed in this chapter and be the bridge to next chapter. s

The Future of Declarative Nodes

Same as the last chapter, introduce the motivation and the high-level picture to readers, and introduce the sections in this chapter.

4.1 Summary

Same as the last chapter, summary what you discussed in this chapter and be the bridge to the next chapter.

Part II

Deep Declarative Network: Non-regular Solution

Solution of Deep Declarative Nodes

5.1 Software platform

5.2 Hardware platform

Table 5.1 shows how to include tables and Figure 5.1 shows how to include codes.

Architecture	Pentium 4	Atom D510	i7-2600
Model	P4D 820	Atom D510	Core i7-2600
Technology	90nm	45nm	32nm
Clock	2.8GHz	1.66GHz	3.4GHz
Cores \times SMT	2×2	2×2	4×2
L2 Cache	1MB \times 2	512KB \times 2	256KB \times 4
L3 Cache	none	none	8MB
Memory	1GB DDR2-400	2GB DDR2-800	4GB DDR3-1066

Table 5.1: Processors used in our evaluation.

```
1 int main(void)
2 {
3     printf("Hello_World\n");
4     return 0;
5 }
```

(a)

```
1 void main(String[] args)
2 {
3     System.out.println("Hello_World");
4 }
```

(b)

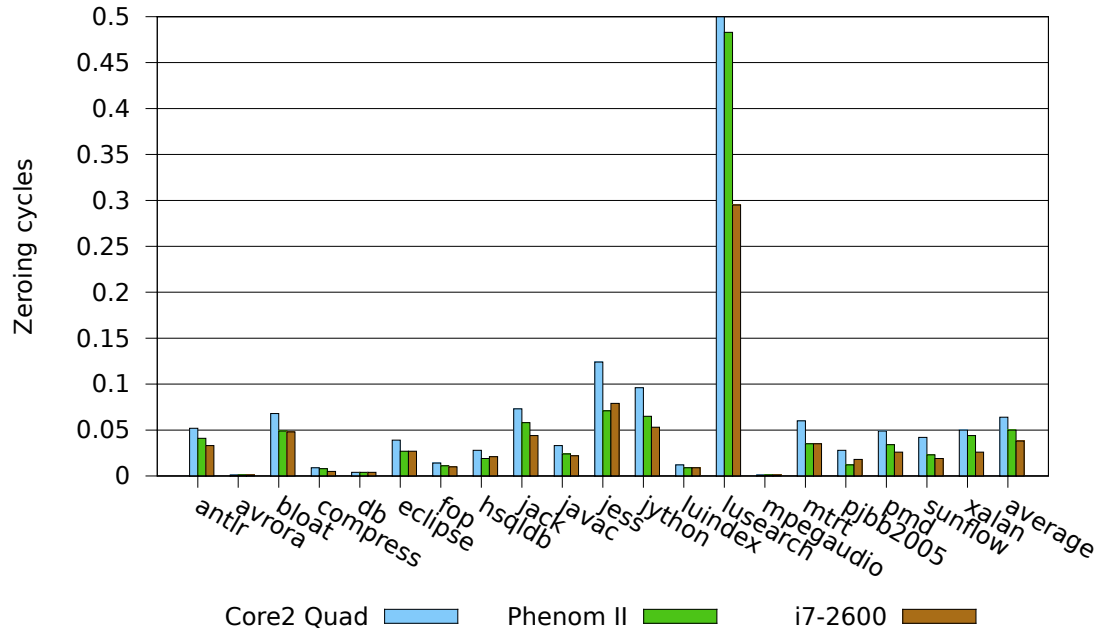
Figure 5.1: Hello world in Java and C.

Results

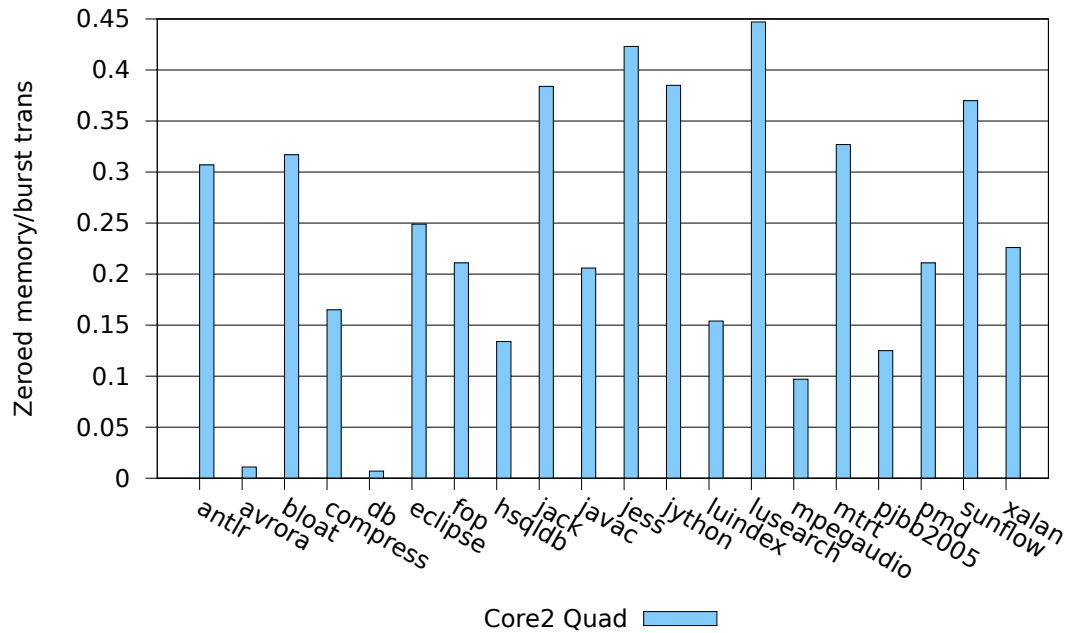
6.1 Direct Cost

Here is the example to show how to include a figure. Figure 6.1 includes two subfigures (Figure 6.1(a), and Figure 6.1(b));

6.2 Summary



(a) Fraction of cycles spent on zeroing



(b) BytesZeroed / BytesBurstTransactionsTransferred

Figure 6.1: The cost of zero initialization

Conclusion

Summary your thesis and discuss what you are going to do in the future in Section 7.1.

7.1 Future Work

Good luck.

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Appendix

A Theory of Optimization

A.1 Existence of Optimizers

A.1.1 Proof of Theorem 2.3

Proof. Let

$$m := \inf\{f(x) : x \in \Omega\}$$

By the definition of m we may pick a sequence $\{x_k\} \subset \Omega$ with $f(x_k) \rightarrow m$ as $k \rightarrow \infty$. Because Ω is compact, we can extract a convergent subsequence $\{x_{k_j}\}$ from $\{x_k\}$. Let $x^* \in \Omega$ denote the limit point of $\{x_{k_j}\}$. Since f is continuous, $f(x^*) = \lim_{j \rightarrow \infty} f(x_{k_j}) = m$. Thus m is finite and x^* is a global minimizer of f on Ω .

When $\Omega = \mathbb{R}^n$, we need to impose conditions on f at infinity to guarantee the existence of a global minimizer. \square

A.1.2 Proof of Theorem 2.4

Proof. Let $m := \inf\{f(x) : x \in \mathbb{R}^n\}$, and take a sequence $\{x_k\}$ such that

$$f(x_k) \rightarrow m \quad \text{as } k \rightarrow \infty.$$

Since f is coercive, $\{x_k\}$ must be bounded; otherwise it has a subsequence $\{x_{k_j}\}$ with $\|x_{k_j}\| \rightarrow \infty$ as $j \rightarrow \infty$, and hence $m = \lim_{j \rightarrow \infty} f(x_{k_j}) = +\infty$, a contradiction. Thus there is $r > 0$ such that

$$\{x_k\} \subset \{x \in \mathbb{R}^n : \|x_k\| \leq r\}.$$

Because $\{x \in \mathbb{R}^n : \|x\| \leq r\}$ is compact, $\{x_k\}$ has a convergent subsequence $\{x_{k_j}\}$ with $x_{k_j} \rightarrow x^*$ as $j \rightarrow \infty$. In view of the continuity of f , we have

$$f(x^*) = \lim_{j \rightarrow \infty} f(x_{k_j}) = m$$

Therefore m is finite and f achieves its minimum on \mathbb{R}^n at x^* □

A.1.3 Proof of Theorem 2.6

Proof. We may assume that $\alpha > f_* := \inf \{f(x) : x \in \mathbb{R}^n\}$. Let $\{x_k\}$ be a minimizing sequence for f , i.e.

$$f(x_k) \rightarrow f_* \quad \text{as } k \rightarrow \infty$$

Then there is an N such that $f(x_k) \leq \alpha$ for all $k \geq N$, that is, $x_k \in D$ for all $k \geq N$. Since D is compact, $\{x_k\}_{k=N}^\infty$ has a convergent subsequence $\{x_{k_j}\}$ with $x_{k_j} \rightarrow x_* \in D$ as $j \rightarrow \infty$. In view of the lower semi-continuity of f , we have

$$f(x_*) \leq \lim_{j \rightarrow \infty} f(x_{k_j}) = f_*$$

By the definition of f_* we must have $f(x_*) = f_*$. Therefore f achieves its minimum on \mathbb{R} at x_* . □

A.2 Optimality Conditions for Unconstrained Problems

A.2.1 Proof of Theorem 2.8

Proof. (NC1): First recall that for any $v \in \mathbb{R}^n$ there holds

$$v^T \nabla f(x^*) = D_v f(x^*) = \lim_{t \searrow 0} \frac{f(x^* + tv) - f(x^*)}{t}.$$

Since x^* is a local minimizer, we have

$$f(x^* + tv) - f(x^*) \geq 0 \quad \text{for small } |t|.$$

Therefore

$$v^T \nabla f(x^*) \geq 0 \quad \text{for all } v \in \mathbb{R}^n.$$

In particular this implies $(-v)^T \nabla f(x^*) \geq 0$ and thus

$$v^T \nabla f(x^*) \leq 0 \quad \text{for all } v \in \mathbb{R}^n.$$

Therefore $v^T \nabla f(x^*) = 0$ for all $v \in \mathbb{R}^n$. Taking $v = \nabla f(x^*)$ gives $\|\nabla f(x^*)\|^2 = 0$ which shows that $\nabla f(x^*) = 0$ □

Proof. (NC2): Recall that for any $v \in \mathbb{R}^n$ and small $t > 0$ there is $0 < s < 1$ such that

$$f(x^* + tv) = f(x^*) + tv^T \nabla f(x^*) + \frac{1}{2} t^2 v^T \nabla^2 f(x^* + stv) v.$$

Since x^* is a local minimizer of f , we have $f(x^* + tv) \geq f(x^*)$ and $\nabla f(x^*) = 0$ by (NC1). Therefore

$$\frac{1}{2} t^2 v^T \nabla^2 f(x^* + stv) v = f(x^* + tv) - f(x^*) \geq 0.$$

This implies that

$$v^T \nabla^2 f(x^* + stv) v \geq 0.$$

Taking $t \rightarrow 0$ gives

$$v^T \nabla^2 f(x^*) v \geq 0 \quad \text{for all } v \in \mathbb{R}^n$$

i.e. $\nabla^2 f(x^*)$ is semi-definite. □

Proof. (SC1): Since $\nabla^2 f(x)$ is continuous and $\nabla^2 f(x^*) \geq 0$, we can find $r > 0$ such that

$$B_r(x^*) \subset \Omega \quad \text{and} \quad \nabla^2 f(x) > 0 \text{ for all } x \in B_r(x^*).$$

By Taylor's formula we have

$$f(x) = f(x^*) + \nabla f(x^*) \cdot (x - x^*) + \frac{1}{2} (x - x^*)^T \nabla^2 f(\hat{x}) (x - x^*)$$

where $\hat{x} := x^* + t(x - x^*)$ for some $0 < t < 1$. It is clear that $\hat{x} \in B_r(x^*)$ and hence $\nabla^2 f(\hat{x}) > 0$ which implies that

$$(x - x^*)^T \nabla^2 f(\hat{x}) (x - x^*) > 0 \quad \text{for } x \neq x^*$$

Consequently

$$f(x) > f(x^*) + \nabla f(x^*) \cdot (x - x^*)$$

for all $x \in B_r(x^*)$ with $x \neq x^*$. Since $\nabla f(x^*) = 0$, we can obtain $f(x) > f(x^*)$ for all $x \in B_r(x^*)$ with $x \neq x^*$. □