APM462: Nonlinear Optimization

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1 Preliminaries

1.1 Mean Value Theorems and Taylor Approximations.

Definition 1.1. Let $f : S \subseteq \mathbb{R}^n \to \mathbb{R}$, the **gradient** of f at $x \in S$, if exists, is a vector $\nabla f(x) \in \mathbb{R}^n$ characterized by the property

$$\lim_{v \to 0} \frac{f(x+v) - f(x) - \nabla f(x) \cdot v}{||v||} = 0 \tag{1.1}$$

Theorem 1.1 (The First Order Mean Value Theorem)**.** Let $f \in C^1(\mathbb{R}^n, \mathbb{R})$, then for any $x, v \in \mathbb{R}^n$, there exists some $\theta \in (0,1)$ such that

$$f(x+v) = f(x) + \nabla f(x + \theta v) \cdot v \tag{1.2}$$

Proof. Let $x, v \in \mathbb{R}^n$, define $g(t) := f(x+tv) \in C^1(\mathbb{R}, \mathbb{R})$.
By the mean value theorem on $\mathbb{R}^{\mathbb{R}}$, there exists $\theta \in (0,1)$ such that $g(0+1) = g(0) + g'(\theta)(1-0)$, that is, $f(x+v) = f(x) + g'(\theta)$. Note that $g'(\theta) = \nabla f(x + \theta v) \cdot v$. ■

Proposition 1.1 (The First Order Taylor Approximation)**.** Let $f \in C^1(\mathbb{R}^n, \mathbb{R})$, then

$$f(x+v) = f(x) + \nabla f(x) \cdot v + o(||v||) \tag{1.3}$$

that is

$$\lim_{||v|| \to 0} \frac{f(x+v) - f(x) - \nabla f(x) \cdot v}{||v||} = 0 \tag{1.4}$$

Proof. By the mean value theorem, $\exists \theta \in (0,1)$ such that $f(x+v) - f(x) = \nabla f(x + \theta v) \cdot v$.
The limit becomes $\lim_{||v|| \to 0} \frac{[\nabla f(x+\theta v) - \nabla f(x)] \cdot v}{||v||} = \lim_{||v|| \to 0; x+\theta v \to x} \frac{[\nabla f(x+\theta v) - \nabla f(x)] \cdot v}{||v||}$.
Since $f \in C^1$, $\lim_{x+\theta v \to x} \nabla f(x+\theta v) = \nabla f(x)$.
And $\frac{v}{||v||}$ is a unit vector, and every component of it is bounded, as the result, the limit of inner product vanishes instead of explodes. ■

Theorem 1.2 (The Second Order Mean Value Theorem)**.** Let $f : \mathbb{R}^n \to \mathbb{R}$ be a C^2 function, then for any $x, v \in \mathbb{R}^n$, there exists $\theta \in (0,1)$ satisfying

$$f(x+v) = f(x) + \nabla f(x) \cdot v + \frac{1}{2} v^T \nabla^2 f(x + \theta v) v \tag{1.5}$$

Proposition 1.2 (The Second Order Taylor Approximation)**.** Let $f : C^2(\mathbb{R}^n, \mathbb{R})$ function, and $x, v \in \mathbb{R}^n$, then

$$f(x+v) = f(x) + \nabla f(x) \cdot v + \frac{1}{2} v^T \nabla^2 f(x + \theta v) v + o(||v||^2) \tag{1.6}$$

that is

$$\lim_{||v|| \to 0} \frac{f(x+v) - f(x) - \nabla f(x) \cdot v - \frac{1}{2} v^T \nabla^2 f(x) v}{||v||^2} = 0 \tag{1.7}$$

Proof. By the second mean value theorem, there exists $\theta \in (0,1)$ such that the limit is equivalent to

$$\lim_{||v|| \to 0} \frac{1}{2} \left(\frac{v}{||v||} \right)^T \left[\nabla^2 f(x + \theta v) - \nabla^2 f(x) \right] \frac{v}{||v||} \tag{1.8}$$

Since $f \in C^2$, the limit of $[H_f(x+\theta v) - H_f(x)]$ is in fact $\mathbf{0}_{n \times n}$. And every component of unit vector $\frac{v}{||v||}$ is bounded, the quadratic form converges to zero as an immediate result. ■

It is often noted that the gradient at a particular $x_0 \in dom(f) \subseteq \mathbb{R}^n$ gives the direction f increases most rapidly. Let $x_0 \in dom(f)$, and v be a unit vector representing a *feasible direction* of change. That is, there exists $\delta > 0$ such that $x_0 + tv \in dom(f)\ \forall t \in [0, \delta)$. Then the rate of change of f along feasible direction v can be written as

$$\left.\frac{d}{dt}\right|_{t=0} f(x_0 + tv) = \nabla f(x_0) \cdot v = ||\nabla f(x_0)||\ ||v|| \cos(\theta) \tag{1.9}$$

where $\theta = \angle(v, \nabla f(x_0)$. And the derivative is maximized when $\theta = 0$, that is, when v and ∇f point the same direction.

1.2 Implicit Function Theorem

Theorem 1.3 (Implicit Function Theorem)**.** Let $f : C^1(\mathbb{R}^{n+1}, \mathbb{R})$, let $(a, b) \in \mathbb{R}^n \times \mathbb{R}$ such that $f(a, b) = 0$. If $\nabla f(a, b) \neq 0$, then $\{(x, y) \in \mathbb{R}^n \times \mathbb{R} : f(x, y) = 0\}$ is locally a graph of a function $g : \mathbb{R}^n \to \mathbb{R}$.

Remark 1.1. $\nabla f(x_0) \perp$ level set of f near x_0.

2 Convexity

2.1 Terminologies

Definition 2.1. Set $\Omega \subseteq \mathbb{R}^n$ is **convex** if and only if

$$\forall x_1, x_2 \in \Omega,\ \lambda \in [0, 1],\ \lambda x_1 + (1 - \lambda)x_2 \in \Omega \tag{2.1}$$

Definition 2.2. A function $f : \Omega \subseteq \mathbb{R}^n \to \mathbb{R}$ is **convex** if and only if Ω is convex, and

$$\forall x_1, x_2 \in \Omega,\ \lambda \in [0, 1],\ f\left(\lambda x_1 + (1 - \lambda)x_2\right) \leq \lambda f(x_1) + (1 - \lambda)f(x_2) \tag{2.2}$$

Definition 2.3. A function $f : \Omega \subseteq \mathbb{R}^n \to \mathbb{R}$ is **strictly convex** if and only if Ω is convex and

$$\forall x_1, x_2 \in \Omega,\ \lambda \in (0, 1),\ f\left(\lambda x_1 + (1 - \lambda)x_2\right) < \lambda f(x_1) + (1 - \lambda)f(x_2) \tag{2.3}$$

2.2 Basic Properties of Convex Functions

Definition 2.4. A function $f : \Omega \to \mathbb{R}$ is **concave** if and only if $-f$ is **convex**.

Proposition 2.1. Properties of convex functions:

(i) If f_1, f_2 are convex on Ω, so is $f_1 + f_2$;

(ii) If f is convex on Ω, then for any $a > 0$, af is also convex on Ω;

(iii) Any **sub-level/lower contour set** of a convex function f

$$\mathcal{L}(c) := \{x \in \mathbb{R}^n : f(x) \leq c\} \tag{2.4}$$

is convex.

Proof of (iii). Let $c \in \mathbb{R}$, and $x_1, x_2 \in SL(c)$. Let $s \in [0, 1]$. Since $x_1, x_2 \in \mathcal{L}(c)$, and $f(\cdot)$ is convex, $f(sx_1 + (1 - s)x_2) \leq sf(x_1) + (1 - s)f(x_2) \leq sc + (1 - s)c = c$. Which implies $sx_1 + (1 - s)x_2 \in \mathcal{L}(c)$. ■

Example 2.1. ℓ_2 norm $f(x) : \mathbb{R}^n \to \mathbb{R} := ||x||_2$ is convex.

Proof. Note that for any $u, v \in \mathbb{R}^n$, by triangle inequality, $||u - (-v)|| \leq ||u - 0|| + ||0 - (-v)|| = ||u|| + ||v||$. Consequently, let $u, v \in \mathbb{R}^n$ and $s \in [0,1]$, then $||su + (1-s)v|| \leq ||su|| + ||(1-s)v|| = s||u|| + (1-s)||v||$. Therefore, $||\cdot||$ is convex. ■

Proposition 2.2. Any norm function $||\cdot||$ defined on a vector space $\mathcal{X}(\mathbb{R})$ is convex.

Proof. The proof follows the defining properties of norm,

$$||\lambda x + (1-\lambda)y|| \leq ||\lambda x|| + ||(1-\lambda)y|| \tag{2.5}$$

$$= \lambda||x|| + (1-\lambda)||y|| \tag{2.6}$$

■

2.3 Characteristics of C^1 Convex Functions

Theorem 2.1 (C^1 criterions for convexity)**.** Let $f \in C^1$, then f is convex on a convex set Ω <u>if and only if</u>

$$\forall x, y \in \Omega,\ \ f(y) \geq f(x) + \nabla f(x) \cdot (y - x) \tag{2.7}$$

that is, *the linear approximation is never an overestimation of value of f.*

Proof. ($\Longrightarrow$) Suppose f is convex on a convex set Ω. Then $f(sy + (1-s)x) \leq sf(y) + (1-s)f(x)$ for every $x, y \in \Omega$ and $s \in [0,1]$, which implies, for every $s \in (0,1]$:

$$\frac{f(sy + (1-s)x) - f(x)}{s} \leq f(y) - f(x) \tag{2.8}$$

By taking the limit of $s \to 0$,

$$\lim_{s \to 0} \frac{f(x + s(y-x)) - f(x)}{s} \leq f(y) - f(x) \tag{2.9}$$

$$\Longrightarrow \left.\frac{d}{ds}\right|_{s=0} f(x + s(y-x)) \leq f(y) - f(x) \tag{2.10}$$

$$\Longrightarrow \nabla f(x) \cdot (y - x) \leq f(y) - f(x) \tag{2.11}$$

($\Longleftarrow$) Let $x_0, x_1 \in \Omega$, let $s \in [0,1]$. Define $x^* := sx_0 + (1-s)x_1$, then

$$f(x_0) \geq f(x^*) + \nabla f(x^*) \cdot (x_0 - x^*) \tag{2.12}$$

$$\Longrightarrow f(x_0) \geq f(x^*) + \nabla f(x^*) \cdot [(1-s)(x_0 - x_1)] \tag{2.13}$$

Similarly,

$$f(x_1) \geq f(x^*) + \nabla f(x^*) \cdot (x_1 - x^*) \tag{2.14}$$

$$\Longrightarrow f(x_1) \geq f(x^*) + \nabla f(x^*) \cdot [s(x_1 - x_0)] \tag{2.15}$$

Therefore, $sf(x_0) + (1-s)f(x_1) \geq f(x^*)$. ■

Theorem 2.2 (C^2 criterion for convexity)**.** $f \in C^2$ is a convex function on a convex set $\Omega \subseteq \mathbb{R}^n$ <u>if and only if</u> $\nabla^2 f(x) \succcurlyeq 0$ (i.e. positive semidefinite) for all $x \in \Omega$.

Corollary 2.1. When f is defined on $\mathbb{R}$, the C^2 criterion becomes $f''(x) \geq 0$.

Proof. ($\Longleftarrow$) Suppose $\nabla^2 f(x) \succcurlyeq 0$ for every $x \in \Omega$, let $x, y \in \Omega$. By the second order MVT,

$$f(y) = f(x) + \nabla f(x) \cdot (y - x) + \frac{1}{2}(y - x)^T \nabla^2 f(x + s(y - x))(y - x) \text{ for some } s \in [0, 1] \tag{2.16}$$

$$\implies f(y) \geq f(x) + \nabla f(x) \cdot (y - x) \tag{2.17}$$

So f is convex by the C^1 criterion of convexity.
($\Longrightarrow$) Let $v \in \mathbb{R}^n$. Suppose, for contradiction, that for some $x \in \Omega$, $\nabla^2 f(x) \not\succcurlyeq 0$.
If such $x \in \partial\Omega$, note that $v^T \nabla^2 f(\cdot) v$ is continuous because $f \in C^2$, then there exists $\varepsilon > 0$ such that $\forall x' \in V_\varepsilon(x) \cap \Omega^{int},\ v^T \nabla^2 f(x') v < 0$.
Hence, one may assume with loss of generality that such $x \in \Omega^{int}$.
Because $x \in \Omega^{int}$, exists $\varepsilon' > 0$, such that $V_{\varepsilon'}(x) \subseteq \Omega^{int}$.
Define $\hat{v} := \frac{v}{\sqrt{\varepsilon'}}$, then for every $s \in [0, 1]$, $\hat{v}^T \nabla^2 f(x + s\hat{v})\hat{v} < 0$.
Let $y = x + \hat{v}$, by the mean value theorem,

$$f(y) = f(x) + \nabla f(x) \cdot (y - x) + \frac{1}{2}(y - x)^T \nabla^2 f[x + s(y - x)](y - x) \tag{2.18}$$

for some $s \in [0, 1]$.
This implies $f(y) < f(x) + \nabla f(x) \cdot (y - x)$, which contradicts the C^1 criterion for convexity. ■

2.4 Minimum and Maximum of Convex Functions

Theorem 2.3. Let $\Omega \subseteq \mathbb{R}^n$ be a convex set, and $f : \Omega \to \mathbb{R}$ is a convex function. Let

$$\Gamma := \left\{ x \in \Omega : f(x) = \min_{x \in \Omega} f(x) \right\} \equiv \operatorname*{argmin}_{x \in \Omega} f(x) \tag{2.19}$$

If $\Gamma \neq \varnothing$, then

(i) Γ is convex;

(ii) any local minimum of f is the global minimum.

Proof (i). Let $x, y \in \Gamma$, $s \in [0, 1]$, then $sx + (1 - s)y \in \Omega$ because Ω is convex. Since f is convex, $f(sx + (1 - s)y) \leq sf(x) + (1 - s)f(y) = \min_{x \in \Omega} f(x)$. The inequality must be equality since it would contradicts the fact that $x, y \in \Gamma$. Therefore, $sx + (1 - s)y \in \Gamma$. ■

Proof (ii). Let $x \in \Omega$ be a local minimizer for f, but assume, for contradiction, it is not a global minimizer. That is, there exists some other y such that $f(y) < f(x)$. Since f is convex,

$$f(x + t(y - x)) = f((1 - t)x + ty) \leq (1 - t)f(x) + tf(y) < f(x) \tag{2.20}$$

for every $t \in (0, 1]$. Therefore, for every $\varepsilon > 0$, there exists $t^* \in (0, 1]$ such that $x + t^*(y - x) \in V_\varepsilon(x)$ and $f(x + t^*(y - x)) < f(x)$, this contradicts the fact that x is a local minimum. ■

Theorem 2.4. Let $\Omega \subseteq \mathbb{R}^n$ be a <u>convex and compact</u> set, and $f : \Omega \to \mathbb{R}$ is a <u>convex</u> function. Then

$$\max_{x \in \Omega} f(x) = \max_{x \in \partial\Omega} f(x) \tag{2.21}$$

Proof. As we assumed, Ω is closed, therefore $\partial\Omega \subseteq \Omega$. Hence, $\max_{x \in \Omega} f \geq \max_{x \in \partial\Omega} f$.
Suppose, for contradiction, $\max_{x \in \Omega} f > \max_{x \in \partial\Omega} f$, then $x^* := \operatorname{argmax}_{x \in \Omega} f \in \Omega^{int}$.
Then we can construct a straight line through x^* and intersects $\partial\Omega$ at two points, $y_1, y_2 \in \partial\Omega$, such that

$x^* = sy_1 + (1-s)y_2$ for some $s \in (0,1)$. Further, since f is convex, $\max_{x\in\Omega} f(x) = f(x^*) \le sf(y_1) + (1-s)f(y_2) \le s\max_{\partial\Omega} f + (1-s)\max_{\partial\Omega} f = \max_{\partial\Omega} f$, which leads to a contradiction.
Therefore, $\max_{x\in\Omega} f = \max_{x\in\partial\Omega} f$. ■

Proposition 2.3. For $p, g > 1$ satisfying $\frac{1}{p} + \frac{1}{g} = 1$,

$$|ab| \le \frac{1}{p}|a|^p + \frac{1}{g}|b|^g \tag{2.22}$$

Proof.

$$\begin{aligned}
(-\log)|ab| &= (-\log)|a| + (-\log)|b| && (2.23)\\
&= \frac{1}{p}(-\log)|a|^p + \frac{1}{g}(-\log)|b|^p && (2.24)\\
(\because (-\log) \text{ is convex}) \quad &\ge (-\log)\left(\frac{1}{p}|a|^p + \frac{1}{g}|b|^p\right) && (2.25)
\end{aligned}$$

And since $(-\log)$ is monotonically decreasing,

$$|ab| \le \frac{1}{p}|a|^p + \frac{1}{g}|b|^p \tag{2.26}$$

■

Corollary 2.2.

$$|ab| \le \frac{|a|^2 + |b|^2}{2} \tag{2.27}$$

3 Finite Dimensional Optimization

3.1 Unconstraint Optimization

Theorem 3.1 (Extreme Value Theorem)**.** Let $f : \mathbb{R}^n \to \mathbb{R}$ is continuous and $K \subseteq \mathbb{R}^n$ be a compact set, then the minimization problem $\min_{x\in K} f(x)$ has a solution.

Remark 3.1. $f : \Omega \to \mathbb{R}$ is convex does not imply f is continuous.

Proposition 3.1. A convex function f defined on a convex open set is continuous.

Proof. Let $f : \Omega \to \mathbb{R}$ be a convex function, where $\Omega \subseteq \mathbb{R}^n$ is open. TODO: *Is this true?* ■

Proposition 3.2. A convex function f defined on an open interval in $\mathbb{R}$ is continuous.

Proof. See homework 1. The proof involves squeeze theorem. ■

Proof of EVT.. Let $f : K \to \mathbb{R}$ be a continuous function defined on a compact set K.
WLOG, we only prove the existence of $\min f$, since the existence of max can be easily proven by applying the exact same argument on $-f$.
That is, we claim the infimum of $f(K)$ is attained within K.
Because K is compact, the continuity of f implies $f(K)$ is compact.
By the completeness axiom of $\mathbb{R}$, $m := \inf_{x\in K} f(x)$ is well-defined. There exists a sequence $(x_i) \subseteq K$, such that $(f(x_i)) \to m$. Because K is compact, there exists a subsequence (x_{ik}) of (x_i) converges to some limit $x^* \in K$.

Since f is continuous, $(f(x_{ik})) \to f(x^*)$, which is a subsequence of the convergent sequence $(f(x_i))$, and they must converge to the same limit. Hence, $f(x^*) = m$, and the infimum is attained at $x^* \in K$. ■

Theorem 3.2 (Heine–Borel)**.** Let $K \subseteq \mathbb{R}^n$, then the following are equivalent:

(i) K is compact (every open cover of K has a finite sub-cover);

(ii) K is closed and bounded;

(iii) Every sequence in K has a convergent subsequence converges to a point in K.

Proposition 3.3. Let $\{h_i\}$ and $\{g_i\}$ be sets of continuous functions on $\mathbb{R}^n$, the the set of all points in $\mathbb{R}^n$ that satisfy

$$\begin{cases} h_i(x) = 0 \ \forall i \\ g_j(x) \leq 0 \ \forall j \end{cases} \tag{3.1}$$

is a closed set. Moreover, if the qualified set is also bounded, then it is compact.

Proof. For every equality constraint h_i, it can be represented as the conjunction of two inequality constraint, namely $h_i^\alpha(x) := -h_i(x) \leq 0 \wedge h_i^\beta(x) := h_i(x) \leq 0$. Then the constraint collection is equivalent to

$$\begin{cases} h_i^\alpha(x) \leq 0 \ \forall i \\ h_i^\beta(x) \leq 0 \ \forall i \\ g_j(x) \leq 0 \ \forall j \end{cases} \tag{3.2}$$

The subset of $\mathbb{R}^n$ qualified by each individual constraint is closed by the property of continuous functions (i.e. a continuous function's pre-image of closed set is closed). And the intersection of arbitrarily many closed sets is closed. ■

Remark 3.2. Computer algorithms for solving minimization problems try to construct a sequence of (x_i) such that $f(x_i)$ decreases to $\min f$ rapidly.

The optimization problems investigated in this section can be formulated as

$$\min_{x \in \Omega} f(x) \tag{3.3}$$

where $\Omega \subseteq \mathbb{R}^n$. Typically, for simplicity, Ω are often $\mathbb{R}^n$, an open subset of R^n, or the closure of some open subset of $\mathbb{R}^n$.

Everything above minimization discussed in this section is applicable to maximization as well using the proposition below.

Proposition 3.4. When $\Omega = \mathbb{R}^n$, the unconstrained minimization has the following properties

(i) $\operatorname{argmax} f = \operatorname{argmin}(-f)$;

(ii) $\max f = -\min(-f)$

Proof. Immediate by applying definitions of maximum and minimum. ■

Definition 3.1. A function $f : \Omega \to \mathbb{R}$ has **local minimum** at $x_0 \in \Omega$ if

$$\exists \varepsilon > 0 \ s.t. \ \forall x \in V_\varepsilon(x_0) \cap \Omega, \ f(x_0) \leq f(x) \tag{3.4}$$

f attains **strictly local minimum** at x_0 if

$$\exists \varepsilon > 0 \; s.t. \; \forall x \in V_\varepsilon(x_0) \cap \Omega \backslash \{x_0\} \; f(x_0) < f(x) \tag{3.5}$$

f attains **global minimum** at x_0 if

$$\forall x \in \Omega \; f(x_0) \leq f(x) \tag{3.6}$$

f attains **strict global minimum** at x_0 if

$$\forall x \in \Omega \backslash \{x_0\} \; f(x_0) < f(x) \tag{3.7}$$

Note that strict global minimum is always unique.

Theorem 3.3 (Necessary Condition for Local Minimum)**.** Let $C^1 \ni f : \Omega \to \mathbb{R}$, let $x_0 \in \Omega$ be a local minimum of f, then for every *feasible direction* v at x_0,

$$\nabla f(x_0) \cdot v \geq 0 \tag{3.8}$$

This theorem serves as the primary defining property of local minimum.

Definition 3.2. For $x_0 \in \Omega \subseteq \mathbb{R}^n$, $v \in \mathbb{R}^n$ is a **feasible direction** at x_0 if

$$\exists \overline{s} > 0 \; s.t. \; \forall s \in [0, \overline{s}], x_0 + sv \in \Omega \tag{3.9}$$

Proof of Necessary Condition. Let $x_0 \in \Omega$ be a local minimum, and let v be a Define auxiliary function $g(s) := f(x + sv)$. And since g attains minimum at $s = 0$, there exists some $\overline{s} > 0$ such that

$$g(s) - g(0) \geq 0 \; \forall s \in [0, \overline{s}] \tag{3.10}$$

Therefore

$$g'(0) := \lim_{s \to 0} \frac{g(s) - g(0)}{s - 0} \geq 0 \tag{3.11}$$

The alternative form of derivative can be derived using chain rule as

$$g'(0) = \nabla f(x + sv) \cdot v \mid_{s=0} = \nabla f(x) \cdot v \tag{3.12}$$

By combing the two identities above, $\nabla f(x) \cdot v \geq 0$. ■

Alternative Proof of Necessary Condition (not that rigorous). The prove is almost immediate, if there exists a feasible direction v^* such that $\nabla f(x_0) \cdot v^* < 0$, for every $\varepsilon > 0$, one can construct $x' := x^* + sv^*$ with sufficiently small s so that $x' \in V_\varepsilon(x^*) \cap \Omega$ and $f(x') < f(x^*)$. ■

Corollary 3.1. When Ω is open, then x_0 is a local minimum $\implies \nabla f(x_0) = 0$.

Proof. Since Ω is open, any sufficiently small $v \neq 0$ such that both v and $-v$ are feasible directions at x_0, applying the necessary condition on both v and $-v$ provides the equality. ■

Theorem 3.4 (Second Order Necessary Condition for Local Minimum)**.** Let $C^2 \ni f : \Omega \to \mathbb{R}$, let $x_0 \in \Omega$ be a local minimum of f, then for every non-zero feasible direction v at x_0,

(i) $\nabla f(x_0) \cdot v \geq 0$;

(ii) $\nabla f(x_0) \cdot v = 0 \implies v^T \nabla^2 f(x_0) v \geq 0$.

Proof. Let x_0 be a local minimum and v be a feasible direction at Ω, and $s \in (0, \overline{s}]$. The first statement is the immediate result of the first order necessary condition. Now suppose $\nabla f(x_0) = 0$, by the Taylor's theorem,

$$0 \leq f(x_0 + sv) - f(x_0) = s \nabla f(x_0) \cdot v + \frac{s^2}{2} v^T \nabla^2 f(x_0) v + o(s^2) \tag{3.13}$$

$$= \frac{s^2}{2} v^T \nabla^2 f(x_0) v + o(s^2) \tag{3.14}$$

Since $s^2 > 0$, divide both sides by s^2 and take limit,

$$\lim_{s \to 0} \frac{f(x_0 + sv) - f(x_0)}{s^2} = \lim_{s \to 0} \left\{ \frac{1}{2} v^T \nabla^2 f(x_0) v + \frac{o(s^2)}{s^2} \right\} \tag{3.15}$$

$$= \frac{1}{2} v^T \nabla^2 f(x_0) v + \lim_{s \to 0} \frac{o(s^2)}{s^2} \tag{3.16}$$

$$= \frac{1}{2} v^T \nabla^2 f(x_0) v \geq 0 \tag{3.17}$$

■

Example 3.1. $f(x, y) = x^2 - xy + y^2 - 3y : \Omega = \mathbb{R}^2 \to \mathbb{R}$. Then at $(x_0, y_0) = (1, 2)$,

$$\nabla f(x_0, y_0) = (2x_0 - y, -x_0 + 2y_0 - 3) = (0, 0) \tag{3.18}$$

$$\nabla^2 f(x_0, y_0) = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \succcurlyeq 0 \tag{3.19}$$

Definition 3.3. Let $A \in \mathbb{R}^{n \times n}$, A is

(i) **Positive definite** (denoted as $A \succ 0$) if $x^T A x > 0 \ \forall x \neq 0$, if and only if all eigenvalues $\lambda_i > 0$;

(ii) **Positive Semi-definite** (denoted as $A \succcurlyeq 0$) if $x^T A x \geq \ \forall x \in \mathbb{R}^n$, if and only if all eigenvalues $\lambda_i \geq 0$.

Theorem 3.5 (Sylvester's Criterion)**.** Let $A \in \mathbb{R}^{n \times n}$ be a Hermitian matrix (i.e. $A = \overline{A^T})$[1], then

1. $A \succ 0 \iff$ all *leading principal minors* have positive determinants;
2. $A \succcurlyeq 0 \iff$ all leading principal minors have non-negative determinants.

Theorem 3.6 (Second Order Sufficient Condition for Interior Local Minima)**.** Let $f : C^2(\Omega, \mathbb{R})$, for some $x_0 \in \Omega$, if

(i) $\nabla f(x_0) = 0$,

(ii) *(and)* $\nabla^2 f(x_0) \succ 0$.

then x_0 is a <u>strictly local minimizer</u>.

Lemma 3.1. Suppose $\nabla^2 f(x_0)$ is positive definite, then

$$\exists \ a > 0 \ s.t. \ v^T \nabla^2 f(x_0) v \geq a||v||^2 \quad \forall v \tag{3.20}$$

That is, the quadratic form of a positive definite matrix is bounded away from zero.

[1] $\overline{A^T}$ denotes the complex conjugate of the transpose, a matrix with *real entries* is Hermitian if and only if it is symmetric.

Proof of the Lemma. Recall that a squared matrix Q is called **orthogonal** when every column and row of it is an orthogonal unit vector. So that for every orthogonal matrix Q, $Q^TQ = I$, which implies $Q^T = Q^{-1}$. Further, note that

$$||Qv||^2 = (Qv)^T(Qv) = v^TQ^TQv = ||v||^2 \tag{3.21}$$

$$\implies ||Qv|| = ||v|| \ \forall v \in \mathbb{R}^n \tag{3.22}$$

Let $v \in \mathbb{R}^n$, consider the eigenvector decomposition of $\nabla^2 f(x_0)$, let w satisfy $v = Qw$:

$$Q^T\nabla^2 f(x_0)Q = \text{diag}(\lambda_1, \cdots, \lambda_n) \tag{3.23}$$

$$\implies v^T\nabla^2 f(x_0)v = (Qw)^T\nabla^2 f(x_0)(Qw) \tag{3.24}$$

$$= w^TQ^T\nabla^2 f(x_0)Qw \tag{3.25}$$

$$= w^T\text{diag}(\lambda_1, \cdots, \lambda_n)w \tag{3.26}$$

$$= \lambda_1 w_1^2 + \cdots + \lambda_n w_n^2 \tag{3.27}$$

Let $a := \min\{\lambda_1, \cdots, \lambda_n\}$,

$$... \geq a||w||^2 = a||Q^Tv||^2 = a||v||^2 \tag{3.28}$$

■

Proof of the Theorem. Let $x \in \Omega$, suppose $\nabla f(x_0) = 0$ and $\nabla^2 f(x_0) \succcurlyeq 0$. By the second order Taylor approximation,

$$f(x_0 + v) - f(x_0) = \nabla f(x_0)^Tv + \frac{1}{2}v^T\nabla^2 f(x_0)v + o(||v||^2) \tag{3.29}$$

$$= \frac{1}{2}v^T\nabla^2 f(x_0)v + o(||v||^2) \tag{3.30}$$

$$\geq \frac{a}{2}||v||^2 + o(||v||^2) \text{ for some } a > 0 \tag{3.31}$$

$$= ||v||^2\left(\frac{a}{2} + \frac{o(||v||^2)}{||v||}\right) \tag{3.32}$$

$$> 0 \ \text{ for sufficiently small } v \tag{3.33}$$

Therefore, $f(x_0) < f(x) \ \forall x \in V_\varepsilon(x_0)$. ■

3.2 Equality Constraints: Lagrangian Multiplier

3.2.1 Tangent Space to a (Hyper) Surface at a Point

Definition 3.4. A **surface** $\mathcal{M} \subseteq \mathbb{R}^n$ is defined as

$$\mathcal{M} := \{x \in \mathbb{R}^n : h_i(x) = 0 \ \forall i\} \tag{3.34}$$

where h_i are all C^1 functions.

Definition 3.5. A **differentiable curve** on a surface $\mathcal{M}$ is a C^1 function mapping from $(-\varepsilon, \varepsilon)$ to $\mathcal{M}$. *Remark: in previous calculus courses, differentiable curves are often referred to as parameterizations.*

Let $x(s)$ be a differentiable curve on $\mathcal{M}$ passes through $x_0 \in \mathcal{M}$, re-parameterize it so that $x(0) = x_0$.

Then vector

$$v := \frac{d}{ds}\bigg|_{s=0} x(s) \tag{3.35}$$

touches $\mathcal{M}$ *tangentially.*

Definition 3.6. Any vector v generated by some differentiable curve on $\mathcal{M}$ and takes above form is a **tangent vector** on $\mathcal{M}$ through x_0.

Definition 3.7. The **tangent space** to $\mathcal{M}$ at x_0 is defined to be the set of all tangent vectors:

$$T_{x_0}\mathcal{M} := \left\{ v \in \mathbb{R}^n : v := \frac{d}{ds}\bigg|_{s=0} x(s) \text{ for some } x \in C^1((-\varepsilon, \varepsilon), \mathcal{M}) \ s.t. \ x(0) = x_0 \right\} \tag{3.36}$$

Example 3.2. Define

$$\mathcal{M} := \left\{ x \in \mathbb{R}^2 : ||x||_2 = 1 \right\} \tag{3.37}$$

By defining C^1 functions $g(x) := ||x||_2^2 - 1$, $\mathcal{M}$ is a surface. The tangent space of $\mathcal{M}$ at x_0 is

$$T_{x_0}\mathcal{M} = \{ v \in \mathbb{R}^n : \langle v, x_0 \rangle = 0 \} \tag{3.38}$$

Definition 3.8. Let $\mathcal{M}$ be a surface defined using C^1 functions, a point $x_0 \in \mathcal{M}$ is a **regular point** of the constraints if

$$\{ \nabla h_1(x_0), \cdots, \nabla h_k(x_0) \} \tag{3.39}$$

are linearly independent.
Remark: if there is only one constraint h, then x_0 is regular if and only if $\nabla h(x_0) \neq 0$.

Notation 3.1. Define the T space on equality constraint as

$$T_{x_0} := \{ x \in \mathbb{R}^n : \langle x_0, \nabla h_i(x_0) \rangle = 0 \ \forall i \in [k] \} \tag{3.40}$$

Example 3.3 (Counter example)**.** Define

$$\mathcal{M} := \left\{ (x, y) \in \mathbb{R}^2 : h(x, y) = xy = 0 \right\} \tag{3.41}$$

Then it is easy to verify that $(0, 0)$ is not a regular point. And

$$T_{0,0} = \{ (x, y) \in \mathbb{R}^2 : (x, y) \cdot (0, 0) = 0 \} = \mathbb{R}^2 \tag{3.42}$$

$$\neq T_{0,0}\mathcal{M} = \{ (x, y) \in \mathbb{R}^2 : x = 0 \vee y = 0 \} \tag{3.43}$$

Theorem 3.7. Suppose x_0 is a *regular point* of $\mathcal{M} := \{ h_i(x) = 0, i = 1, \cdots, k \}$, then $T_{x_0} = T_{x_0}\mathcal{M}$.

Proof. Show $T_{x_0}\mathcal{M} \subseteq T_{x_0}$.
Suppose x_0 is a regular point of $\mathcal{M}$. Let $v \in T_{x_0}\mathcal{M}$, then there exists some differentiable curve $x(\cdot) : V_\varepsilon(0) \to \mathcal{M}$ such that $x(0) = x_0$, such that

$$v = \frac{d}{ds}\bigg|_{s=0} x(s) \tag{3.44}$$

Note that $h_i(x(s)) = 0$ is constant for every $i \in [k]$, therefore

$$\left.\frac{d}{ds}\right|_{s=0} h_i(x(s)) \tag{3.45}$$

By the chain rule,

$$\nabla h_i(x_0) \cdot v = 0 \ \forall i \tag{3.46}$$

Therefore $v \in T_{x_0}$.
Show $T_{x_0} \subseteq T_{x_0}\mathcal{M}$.

(i) x_0 is regular $\implies T_{x_0}\mathcal{M}$ is a vector space;

(ii) $T_{x_0} = \text{span}\{\nabla h_1(x_0), \cdots, \nabla h_k(x_0)\}^\perp$.

Show $T_{x_0} \subseteq \text{span}\{\nabla h_1(x_0), \cdots, \nabla h_k(x_0)\}^\perp$:
Let $v \in T_{x_0}$, then $v \perp \nabla h_i(x_0)$ for every i. Therefore v is orthogonal to every linear combination of $\nabla h_i(x_0)$, and therefore orthogonal to the span.
Show $\text{span}\{\nabla h_1(x_0), \cdots, \nabla h_k(x_0)\}^\perp \subseteq T_{x_0}$:
Let v in the perp of the span, then v is orthogonal to every basis of the span, so $v \in T_{x_0}$. ■

Lemma 3.2. Let $f, h_1, \cdots, h_k \in C^1$ defined on open subset $\Omega \subseteq \mathbb{R}^n$. Define $\mathcal{M} := \{x \in \mathbb{R}^n : h_i(x) = 0 \ \forall i\}$. Suppose $x_0 \in \mathcal{M}$ is a local minimum of f on $\mathcal{M}$, then

$$\nabla f(x_0) \perp T_{x_0}\mathcal{M} \tag{3.47}$$

Proof. WLOG $\Omega = \mathbb{R}^n$, take $v \in T_{x_0}\mathcal{M}$. Then there exists some differentiable curve x on $\mathcal{M}$ satisfying $v = x'(0)$. Because x_0 is a local minimum of f on Ω, $s = 0$ is a local minimum of $f(x(s))$, moreover, it is an interior minimum. By chain rule and the necessary condition of local minimum,

$$Df(x(0)) = \nabla f(x(0)) \cdot x'(0) = 0 \tag{3.48}$$

$$\implies \nabla f(x_0) \cdot v = 0 \tag{3.49}$$

Therefore $\nabla f(x_0) \perp T_{x_0}\mathcal{M}$. ■

Theorem 3.8 (Lagrange Multipliers: First Order Necessary Condition)**.** Let $f, h_1, \cdots, h_k \in C^1$ defined on open subset $\Omega \subseteq \mathbb{R}^n$. Let x_0 be a regular point of the constraint set $\mathcal{M} := \bigcap_{i=1}^k h_i^{-1}(0)$. Suppose x_0 is a local minimum of $\mathcal{M}$, then there exists $\lambda_1, \cdots, \lambda_k \in \mathbb{R}$ such that

$$\nabla f(x_0) + \sum_{i=1}^k \lambda_i \nabla h_i(x_0) = 0 \tag{3.50}$$

Remark: if we define Lagrangian $\mathcal{L}(x, \lambda_i) := f(x) + \sum_{i=1}^k h_i(x)$, then the theorem says the local minimum is a critical point of $\mathcal{L}$.

Proof. Because x_0 is a regular point, then by previous lemma, $\nabla f(x_0) \perp T_{x_0}\mathcal{M}$. Moreover,

$$T_{x_0}\mathcal{M} = T_{x_0} = (\text{span}\{\nabla h_1(x_0), \cdots, \nabla h_k(x_0)\})^\perp \tag{3.51}$$

Also, because x_0 is a local minimum,

$$\nabla f(x_0) \perp T_{x_0}\mathcal{M} \tag{3.52}$$

Therefore, $\nabla f(x_0) \in (T_{x_0}\mathcal{M})^{\perp} = (\text{span}\{\nabla h_1(x_0), \cdots, \nabla h_k(x_0)\})^{\perp\perp} = \text{span}\{\nabla h_1(x_0), \cdots, \nabla h_k(x_0)\}$, where the last equality holds in finite dimensional cases. Hence, it is obvious that we can write $\nabla f(x_0)$ as a linear combination of $\{\nabla h_i(x_0)\}$. ■

Theorem 3.9 (Second Order Necessary Condition)**.** Let $f, h_i \in C^2$, if x_0 is a local minimum on previously defined surface $\mathcal{M}$, then there exists Lagrangian multipliers $\{\lambda_i\}$ such that

(i) $\nabla f(x_0) + \sum_{i=1}^{k} \lambda_i \nabla h_i(x_0) = 0$ ($\nabla_x \mathcal{L} = 0$);

(ii) And $\nabla^2 f(x_0) + \sum_{i=1}^{k} \lambda_i \nabla^2 h_i(x_0) \succcurlyeq 0$ on $T_{x_0}\mathcal{M}$ ($\nabla_x^2 \mathcal{L} \succcurlyeq 0$).

Remark: whenever x_0 is a local minimum, it must be a critical point of $\mathcal{L}$, and $\mathcal{L}$ is positive semidefinite on the tangent space at x_0.

Proof. The first result is exactly the same as the first order condition proven above.
To show the second result, let $x(s) \in \mathcal{M}$ be an arbitrary differentiable curve on $\mathcal{M}$ such that $x(0) = x_0$. Then,

$$\frac{d}{ds} f(x(s)) = \nabla f(x(s)) \cdot x'(s) \tag{3.53}$$

$$\frac{d^2}{ds^2} f(x(s)) = x'(s)^T \nabla^2 f(x(s)) x'(s) + \nabla f(x(s)) x''(s) \tag{3.54}$$

By the second order Taylor theorem, for every s such that $x(s) \in \mathcal{M}$,

$$f(x(s)) - f(x_0) = s\nabla f(x_0) \cdot x'(0) + \frac{s^2}{2}\left[x'(0)^T \nabla^2 f(x(0)) x'(s) + \nabla f(x(0)) x''(0)\right] + o(s^2) \tag{3.55}$$

Note that by definition, $x'(0)$ is in the tangent space at x_0. Also, we've shown previously that $\nabla f(x_0)$ is orthogonal to the tangent space at x_0, therefore,

$$f(x(s)) - f(x_0) = \frac{s^2}{2}\left[x'(0)^T \nabla^2 f(x(0)) x'(s) + \nabla f(x(0)) x''(0)\right] + o(s^2) \tag{3.56}$$

Also, by the definition of $\mathcal{M}$, all constraints hold with equality:

$$f(x_0) = f(x_0) + \sum_{i=1}^{k} \lambda_i h_i(x_0) \tag{3.57}$$

where λ_i's are from the first result. Hence,

$$f(x(s)) - f(x_0) = \frac{s^2}{2}\left[x'(0)^T \left(\nabla^2 f(x_0) + \sum_{i=1}^{k} \lambda_i \nabla^2 h_i(x_0)\right) x'(0) + \left(\nabla f(x_0) + \sum_{i=1}^{k} \lambda_i \nabla h_i(x_0)\right) x''(0)\right] + o(s^2) \tag{3.58}$$

$$= \frac{s^2}{2} x'(0)^T \left(\nabla^2 f(x_0) + \sum_{i=1}^{k} \lambda_i \nabla^2 h_i(x_0)\right) x'(0) + o(s^2) \tag{3.59}$$

And above expression is greater or equal to zero because x_0 is a local minimum,

$$\frac{s^2}{2}x'(0)^T\left(\nabla^2 f(x_0)+\sum_{i=1}^{k}\lambda_i\nabla^2 h_i(x_0)\right)x'(0)+o(s^2)\geq 0 \tag{3.60}$$

$$\implies x'(0)^T\left(\nabla^2 f(x_0)+\sum_{i=1}^{k}\lambda_i\nabla^2 h_i(x_0)\right)x'(0)+\frac{o(s^2)}{s^2}\geq 0 \tag{3.61}$$

$$\overset{s\to 0}{\implies} x'(0)^T\left(\nabla^2 f(x_0)+\sum_{i=1}^{k}\lambda_i\nabla^2 h_i(x_0)\right)x'(0)\geq 0 \tag{3.62}$$

Where $x'(0)$ is a vector in the tangent space at x_0 by definition. Moreover, the curve $x(s)$ was chosen arbitrarily, so the argument works for every curve and therefore every tangent vector, and what's desired is shown. ■

Example 3.4.

$$\min f(x,y)=x^2-y^2 \tag{3.63}$$

$$s.t.\ h(x,y)=y=0 \tag{3.64}$$

First order condition suggests $(x_0,y_0)=(0,0)$ Note that the tangent space at (x_0,y_0) is $\text{span}\{\nabla h_i\}^{\perp}$:

$$T_{x_0}\mathcal{M}=\{(u,0):u\in\mathbb{R}\} \tag{3.65}$$

and

$$\nabla_x^2\mathcal{L}=\begin{pmatrix}2 & 0\\ 0 & -2\end{pmatrix} \tag{3.66}$$

is obviously positive semidefinite (actually positive definition) on the tangent space.

Theorem 3.10 (Second Order Sufficient Conditions)**.** Let $f, h_i\in C^2$ on open $\Omega\subseteq\mathbb{R}^n$, and $x_0\in\mathcal{M}$ is a regular point, if there exists $\lambda_i\in\mathbb{R}$ such that

(i) $\nabla_x\mathcal{L}(x_0,\lambda_i)=0$;

(ii) $\nabla_x^2\mathcal{L}(x_0,\lambda_i)\succ 0$ on $T_{x_0}\mathcal{M}$,

then x_0 is a *strict* local minimum.

Proof. Recall that $\nabla^2 f(x_0)+\sum\lambda_i\nabla^2 h_i(x_0)$ positive definite on $T_{x_0}\mathcal{M}$ implies there exists $a>0$ (a is taken to be equal to the least eigenvalue of $\nabla_x^2\mathcal{L}$) such that

$$v^T[\nabla^2 f(x_0)+\sum\lambda_i\nabla^2 h_i(x_0)]v\geq a||v||^2 \quad \forall v\in T_{x_0}\mathcal{M} \tag{3.67}$$

Let $x(s)\in\mathcal{M}$ be a curve such that $x(0)=x_0$ and $v=x'(0)$. WLOG, $||x'(0)||=1$. By the second order

Taylor expansion,

$$
\begin{aligned}
f(x(s)) - f(x(0)) &= s\left.\frac{d}{ds}\right|_{s=0} f(x(s)) + \frac{s^2}{2}\left.\frac{d^2}{ds^2}\right|_{s=0} f(x(s)) + o(s^2) && (3.68)\\
&= s\left.\frac{d}{ds}\right|_{s=0}\left[f(x(s)) + \sum \lambda_i h_i(x(s))\right] + \frac{s^2}{2}\left.\frac{d^2}{ds^2}\right|_{s=0}\left[f(x(s)) + \sum \lambda_i h_i(x(s))\right] + o(s^2) && (3.69)\\
&= s\nabla_x \mathcal{L}(x_0,\lambda_i)\cdot x'(0) + \frac{s^2}{2}\left[x'(0)^T\nabla_x^2\mathcal{L}(x_0,\lambda_i)x'(0) + \nabla_x\mathcal{L}(x_0,\lambda_i)x''(0)\right] + o(s^2) && (3.70)\\
&= \frac{s^2}{2}x'(0)^T\nabla_x^2\mathcal{L}(x_0,\lambda_i)x'(0) + o(s^2) && (3.71)\\
&\geq \frac{s^2}{2}a||x'(0)||^2 + o(s^2) \quad \text{where } a > 0 && (3.72)\\
&= s^2\left(\frac{a}{2} + \frac{o(s^2)}{s^2}\right) && (3.73)\\
&\overset{s\to 0}{>} 0 && (3.74)
\end{aligned}
$$

Therefore, for sufficiently small s, $f(x(s)) - f(x(0)) > 0$. And this is true for every curve x on $\mathcal{M}$. So $x(0)$ is a strict local minimum. ■

3.3 Remark on the Connection Between Constrained and Unconstrained Optimizations

Example 3.5. Consider

$$
\begin{aligned}
&\min f(x,y,z) && (3.75)\\
&s.t. g(x,y,z) = z - h(x,y) = 0 && (3.76)
\end{aligned}
$$

where $\mathcal{M}$ is the graph of h. Using Lagrangian multiplier provides necessary condition: $\nabla f + \lambda\nabla g = 0$,

$$
\begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix} + \lambda\begin{pmatrix} -h_x \\ -h_y \\ 1 \end{pmatrix} = 0 \tag{3.77}
$$

Convert the constrained optimization into an unconstrained optimization as

$$
\min_{(x,y)\in\mathbb{R}^2} F(x,y) = f(x,y,h(x,y)) \tag{3.78}
$$

The necessary condition for unconstrained optimization is

$$
\begin{aligned}
\nabla F(x,y) &= \begin{pmatrix} f_x + f_z h_x \\ f_y + f_z h_y \end{pmatrix} && (3.79)\\
&= \begin{pmatrix} f_x \\ f_y \end{pmatrix} - f_z\begin{pmatrix} -h_x \\ -h_y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} && (3.80)
\end{aligned}
$$

Define $\lambda := -f_z$.

$$\nabla F(x, y) = \begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix} + \lambda \begin{pmatrix} -h_x \\ -h_y \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{3.81}$$

3.4 Inequality Constraints

Definition 3.9. Let x_0 satisfy the set of constraints

$$(\dagger) \begin{cases} h_i(x) & = 0 \quad i \in \{1, \cdots, k\} \\ g_j(x) & \leq 0 \quad j \in \{1, \cdots, \ell\} \end{cases} \tag{3.82}$$

we say that the constraint g_i is **active** at x_0 if $g_i(x_0) = 0$, and is **inactive** at x_0 if $g_i(x_0) < 0$.

Definition 3.10. Split the collection of inequality constraints into active and inactive constraints, let $\Theta(x_0)$ denote the collection of active indices, that's:

$$g_j(x_0) = 0 \ \forall j \in \Theta(x_0) \tag{3.83}$$

$$g_j(x_0) < 0 \ \forall j \notin \Theta(x_0) \tag{3.84}$$

Then x_0 is said to be a **regular point** of the constraint if

$$\{\nabla h_i(x_0) \ \forall i \in \{1, \cdots, k\}; \underbrace{\nabla g_j(x_0) \ \forall j \in \Theta(x_0)}_{\text{Active Constraints}}\} \tag{3.85}$$

is linearly independent.

Theorem 3.11 (The First Order Necessary Condition for Local Minimum: Kuhn-Tucker Conditions)**.** Let Ω be an open subset of $\mathbb{R}^n$ with constraints h_i and g_i to be C^1 on Ω. Suppose $x_0 \in \Omega$ is a regular point with respect to constraints, further suppose x_0 is a local minimum, then there exists some $\lambda_i \in \mathbb{R}$ and $\mu_j \in \mathbb{R}_+$ such that

(i) $\nabla f(x_0) + \sum_{i=1}^k \lambda_i \nabla h_i(x_0) + \sum_{j=1}^\ell \mu_j \nabla g_j(x_0) = 0$ (i.e. $\nabla_x \mathcal{L}(x, \lambda, \mu) = 0$);

(ii) $\mu_j g_j(x_0) = 0$ (*Complementary slackness*).

Remark 1: by complementary slackness, all μ_j corresponding to inactive inequality constraints are zero.
Remark 2: it is possible for an active constraint to have zero multiplier.

Proof. Let x_0 be a local minimum for f satisfying constraints, equivalently, it is a local minimum for equality constraints and active inequality constraints.
By the first order necessary condition for local minimum with equality constraints, there exists $\lambda_i, \mu_j \in \mathbb{R}$ such that

$$\nabla f(x_0) + \sum_{i=1}^k \lambda_i \nabla h_i(x_0) + \sum_{j \in \Theta(x_0)} \mu_j \nabla g_j(x_0) = 0 \tag{3.86}$$

Then by setting $\mu_j = 0$ for all $j \notin \Theta(x_0)$ one have

$$\nabla f(x_0) + \sum_{i=1}^k \lambda_i \nabla h_i(x_0) + \sum_{j=1}^\ell \mu_j \nabla g_j(x_0) = 0 \tag{3.87}$$

By construction, the complementary slackness is satisfied. At this stage, we have construct $\lambda_i \in \mathbb{R}$ and $\mu_j \in \mathbb{R}$ satisfying both conditions, we still need to argue that $\mu_j \geq 0$ for every j. ∎

Theorem 3.12 (The Second Order Necessary Conditions)**.** Let Ω be an open subset of $\mathbb{R}^n$, and $f, h_1, \cdots, h_k, g_1, \cdots, g_\ell \in C^2(\mathbb{R}^n, \mathbb{R})$. Let x_0 be a regular point of the constraints (†). Suppose x_0 is a local minimum of f subject to constraint (†), then there exists $\lambda_i \in \mathbb{R}$ and $\mu_j \geq 0$ such that

(i) $\nabla f(x_0) + \sum_{i=1}^k \lambda_i \nabla h_i(x_0) + \sum_{j=1}^\ell \mu_j \nabla g_j(x_0) = 0$;

(ii) $\mu_j g_j(x_0) = 0$;

(iii) $\nabla^2 f(x_0) + \sum_{i=1}^k \lambda_i \nabla^2 h_i(x_0) + \sum_{j=1}^\ell \mu_j \nabla^2 g_j(x_0)$ is positive semidefinite on the tangent space to activate constraints at x_0.

Proof. (i) and (ii) are immediate result from the first order necessary condition.
Suppose x_0 is a local minimum for (†), then x_0 is a local minimum for active constraints at x_0.
Therefore, $\nabla^2 \hat{\mathcal{L}} = \nabla^2 f(x_0) + \sum_{i=1}^k \lambda_i \nabla^2 h_i(x_0) + \sum_{j \in I(x_0)} \mu_j \nabla^2 g_j(x_0)$ is positive semidefinite on the tangent space to active constraints. Note that because $\mu_j = 0$ for inactive constraints, therefore $\nabla^2 \hat{\mathcal{L}} = \nabla^2 \mathcal{L}$ at x_0, and both of them are positive semidefinite on the tangent space corresponding to active constraints. ∎

Theorem 3.13 (The Second Order Sufficient Conditions)**.** Let Ω be an open subset of $\mathbb{R}^n$, let $f, h_i, q_j \in C^2(\Omega)$. Consider minimizing $f(x)$ with the constraint

$$(\dagger) \begin{cases} h_i(x) = 0 & \forall i \\ g_j(x) \leq 0 & \forall j \\ x \in \Omega \end{cases} \tag{3.88}$$

Suppose there exists a feasible x_0 satisfying (†) and $\lambda_i \in \mathbb{R}$ and $\mu_j \in \mathbb{R}_+$ such that

(i) $\nabla f(x_0) + \sum_{i=1}^k \lambda_i \nabla h_i(x_0) + \sum_{j=1}^\ell \mu_j \nabla g_j(x_0) = 0$;

(ii) $\mu_j g_j(x_0) = 0$ (*Complementary slackness*).

If the Hessian matrix for Lagrangian $\nabla_x^2 \mathcal{L}(x_0)$ is positive definite on $\tilde{\tilde{T}}_{x_0}$, the space of **strongly active** constraints at x_0, then x_0 is a strict local minimum.

Definition 3.11. A constraint g_j is **strongly active** at x_0 if $g_j(x_0) = 0$ (so it is active) and $\mu_j > 0$.

Notation 3.2. For convenience, we can rearrange the collection of constraints such that, among the ℓ constrains in total, the first ℓ' constraints are *active* at x_0 and the first ℓ'' constraints are *strongly active.* Note that $\ell'' \leq \ell' \leq \ell$.
Define

$$\tilde{T}_{x_0} := \{v \cdot \nabla h_i(x_0) = 0 \ \forall i \wedge v \cdot \nabla g_j(x_0) \text{ for all } g_j \text{ active.}\} \tag{3.89}$$

$$\tilde{\tilde{T}}_{x_0} := \{v \cdot \nabla h_i(x_0) = 0 \ \forall i \wedge v \cdot \nabla g_j(x_0) \text{ for all } g_j \text{ strongly active.}\} \tag{3.90}$$

Clearly, $\tilde{T}_{x_0} \subseteq \tilde{\tilde{T}}_{x_0}$ because there are (weakly) more active constraints than strongly active constraints.

Proof of the Sufficient Condition. Suppose, for contradiction, x_0 is not a strict local minimum.
Claim 1: There exists unit vector $v \in \mathbb{R}^n$ such that

(a) $\nabla f(x_0) \cdot v \leq 0$;

(b) $\nabla h_i(x_0) \cdot v = 0$ for every i;

(c) $\nabla g_j(x_0) \cdot v \le 0$ for all $j \le \ell'$ (active constraints).

Proof of Claim 1. Because x_0 is not a strictly local minimum, one can construct a sequence of feasible points $(x_k) \to x_0$ by setting $\varepsilon = \frac{1}{k}$ for every $k \in \mathbb{N}$ such that $f(x_k) \le f(x_0)$.
Let $v_k := \frac{x_k - x_0}{||x_k - x_0||}$, $s_k := ||x_k - x_0||$. Note that every v_k is in unit sphere, which is compact. Therefore, there exists a subsequence of (v_k) converges to some unit vector v.

$$0 \ge f(x_k) - f(x_0) = f(x_0 + s_k v_k) - f(x_0) \ \forall k \in \mathbb{N} \tag{3.91}$$

The first order Taylor series suggests the following holds for every $k \in \mathbb{N}$:

$$0 \ge f(x_0 + s_k v_k) - f(x_0) \tag{3.92}$$
$$= s_k \nabla f(x_0) \cdot v_k + o(s_k) \tag{3.93}$$
$$0 = h_i(x_0 + s_k v_k) - h_i(x_0) = s_k \nabla h_i(x_0) \cdot v_k + o(s_k) \tag{3.94}$$
$$0 \ge g_j(x_0 + s_k v_k) - g_j(x_0) = s_k \nabla g_j(x_0) \cdot v_k + o(s_k) \quad \forall j \le \ell' \tag{3.95}$$

Above inequalities are preserved by limit operation, therefore,

$$\nabla f(x_0) \cdot v_k + \frac{o(s_k)}{s_k} \to \nabla f(x_0) \cdot v \le 0 \tag{3.96}$$
$$\nabla h_i(x_0) \cdot v_k + \frac{o(s_k)}{s_k} \to \nabla h_i(x_0) \cdot v = 0 \tag{3.97}$$
$$\nabla g_j(x_0) \cdot v_k + \frac{o(s_k)}{s_k} \to \nabla g_j(x_0) \cdot v \le 0 \quad \forall j \le \ell' \tag{3.98}$$

■

Claim 2: $\nabla g_j(x_0) \cdot v = 0$ for $j = 1, \cdots, \ell''$.

Proof of Claim 2. Suppose not, there exists $j \in \{1, \cdots, \ell''\}$ such that $\nabla g_j(x_0) \cdot v < 0$. Then by (i),

$$0 \ge \nabla f(x_0) \cdot v = -\sum_{i=1}^{k} \lambda_i \nabla h_i(x_0) \cdot v - \sum_{j=1}^{\ell} \mu_j \nabla g_j(x_0) \cdot v \tag{3.99}$$
$$= -\sum_{j=1}^{\ell} \mu_j \nabla g_j(x_0) \cdot v > 0 \tag{3.100}$$

the last inequality is from the fact that $\mu_j \nabla g_j(x_0) \cdot v \le 0$ for all active constraints and $\mu_j = 0$ for all inactive constraints.

■

(b) and claim 2 suggests $v \in \tilde{\tilde{T}}_{x_0}$.
By the second order Taylor approximation,

$$0 \ge f(x_k) - f(x_0) = s_k \nabla f(x_0) \cdot v_k + \frac{s_k^2}{2} v_k \cdot \nabla^2 f(x_0) \cdot v_k + o(s_k^2) \tag{3.101}$$
$$0 = h_i(x_k) - h_i(x_0) = s_k \nabla h_i(x_0) \cdot v_k + \frac{s_k^2}{2} v_k \cdot \nabla^2 h_i(x_0) \cdot v_k + o(s_k^2) \quad \forall i \tag{3.102}$$
$$0 \ge g(x_k) - g(x_0) = s_k \nabla g_j(x_0) \cdot v_k + \frac{s_k^2}{2} v_k \cdot \nabla^2 g_j(x_0) \cdot v_k + o(s_k^2) \quad \forall j \le \ell' \tag{3.103}$$

Multiply the second equation by λ_i and third equation by μ_j, and use the fact that $\mu_j = 0$ for every $j > \ell'$. Also, given $\nabla \mathcal{L} = 0$ in (i):

$$0 \geq \frac{s_k^2}{2} v_k \cdot \nabla^2 \mathcal{L} \cdot v_k + o(s_k^2) \tag{3.104}$$

Divide by s_k^2 and take the limit $(v_k) \to v$:

$$v \cdot \nabla^2 \mathcal{L} \cdot v \leq 0 \tag{3.105}$$

which contradicts the assumption that $\nabla^2 \mathcal{L}$ is positive definite in $\tilde{\tilde{T}}_{x_0}$ because we've shown that $v \in \tilde{\tilde{T}}_{x_0}$. ■

4 Iterative Algorithms for Optimization

4.1 Newton's Method

Example 4.1 (Motivation: a second order iterative algorithm)**.** Let $f : I \subseteq \mathbb{R} \to \mathbb{R}$ where I is an open interval. Let $x_i \in I$ be a starting point, consider the second order linear approximation of f at x_0:

$$g(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2 \tag{4.1}$$

By construction, the second order Taylor polynomial, $g(x)$, is the best second order approximation to f at x_0 in the following sense:

$$g(x_0) = f(x_0) \tag{4.2}$$
$$g'(x_0) = f'(x_0) \tag{4.3}$$
$$g''(x_0) = f''(x_0) \tag{4.4}$$

The Newton's method aims to solve the critical point of $g(x)$ and define x_1 to be the critical point found:

$$g'(x_1) = f'(x_0) + f''(x_0)(x_1 - x_0) = 0 \tag{4.5}$$
$$\implies x_1 \leftarrow x_0 - \frac{f'(x_0)}{f''(x_0)} \tag{4.6}$$

Algorithm 4.1 (Newton's Method in $\mathbb{R}$)**.** Given initial point $x_0 \in I$, while not terminated:

$$x_{n+1} \leftarrow x_n - \frac{f'(x_n)}{f''(x_n)} \tag{4.7}$$

Theorem 4.1. Let $f \in C^3$ on open interval $I \subseteq \mathbb{R}$. Suppose $x_* \in I$ satisfies $f'(x_*) = 0$ and $f''(x_*) \neq 0$, then the sequence of points (x_n) generated by Newton's method converges to x_* if x_0 *is sufficiently close to* x_*.

Example 4.2. Let $f(x) = x^2$, then $\frac{f'(x)}{f''(x)} = \frac{2x}{2}$. For any starting point x_0, $x_1 = x_0 - \frac{2x_0}{x_0} = 0$. That is, the algorithm converges to the global minimum in one iteration.

Proof. Let $g(x) = f'(x)$ so that $x_{n+1} = x_n - \frac{g(x_n)}{g'(x_n)}$.
Because $f \in C^3$, then $g \in C^2$.
Note that by $g \in C^2$, $g' = f''$ is bounded away from zero near x_*.
And by continuity again, $g'' = f^{(3)}$ is bounded near the bounded region $V_\varepsilon(x_*)$.

That is, within small region near x_*, $V_\delta(x_*)$, there exists a sufficiently small $\alpha > 0$ such that

$$\begin{cases} |g'(x_1)| > \alpha \ \forall x_1 \in V_\delta(x_*) \\ |g''(x_2)| < \frac{1}{\alpha} \ \forall x_2 \in V_\delta(x_*) \end{cases} \tag{4.8}$$

Further, note that $g(x_*) = f'(x_*) = 0$.
WLOG, let $n \in \mathbb{N}$, suppose $x_n > x_*$:

$$\begin{align} x_{n+1} - x_* &= x_n - \frac{g(x_n)}{g'(x_n)} - x_* \tag{4.9} \\ &= x_n - x_* - \frac{g(x_n) - g(x_*)}{g'(x_n)} \tag{4.10} \\ &= -\frac{g(x_n) - g(x_*) - g'(x_n)(x_n - x_*)}{g'(x_n)} \tag{4.11} \\ &= -\frac{1}{2}\frac{g''(\xi)}{g'(x_n)}(x_n - x_*)^2 \quad \text{for some } \xi \in (x_*, x_n) \tag{4.12} \end{align}$$

By taking the absolute values on both sides:

$$\begin{align} |x_{n+1} - x_*| &= \frac{1}{2}\frac{|g''(\xi)|}{|g'(x_n)|}|x_n - x_*|^2 \tag{4.13} \\ &< \frac{1}{2\alpha^2}|x_n - x_*|^2 \tag{4.14} \end{align}$$

Let $\rho := \frac{1}{\alpha^2}|x_0 - x_*|^2$, choose x_0 sufficiently close to x_* such that $\rho < 1$.
Remark: we are showing the iterative algorithm induces a contraction map.
Then,

$$\begin{align} |x_1 - x_*| &< \frac{1}{2\alpha^2}|x_0 - x_*|^2 \tag{4.15} \\ &= \frac{1}{2\alpha^2}|x_0 - x_*|\,|x_0 - x_*| \tag{4.16} \\ &= \rho\,|x_0 - x_*| \tag{4.17} \end{align}$$

Inductively,

$$\begin{align} |x_2 - x_*| &< \frac{1}{2\alpha^2}|x_1 - x_*|^2 \tag{4.18} \\ &< \frac{1}{2\alpha^2}\rho^2|x_0 - x_*|^2 \tag{4.19} \\ &= \rho^3|x_0 - x_*| \tag{4.20} \\ &< \rho^2|x_0 - x_*| \tag{4.21} \end{align}$$

By induction,

$$|x_n - x_*| < \rho^2|x_0 - x_*| \tag{4.22}$$

Therefore, as $n \to \infty$, $(x_n) \to x_*$. ■

Theorem 4.2 (2nd Order MVT)**.**

$$g(x) = g(y) + g'(y)(x-y) + \frac{1}{2}g''(\xi)(x-y)^2 \quad \xi \in (x,y) \tag{4.23}$$

Algorithm 4.2 (Newton's Method in $\mathbb{R}^n$)**.** Let $f : \Omega \subseteq \mathbb{R}^n \to \mathbb{R}$ where Ω is open, let initial point $x_0 \in \Omega$. Suppose $\nabla^2 f(x_n)$ is invertible for every generated n, and $\nabla f(x_*) = 0$ so that algorithm stops at minimum. The iterative algorithm is defined as following:

$$x_{n+1} \leftarrow x_n - [\nabla^2 f(x_n)]^{-1} \nabla f(x_n) \tag{4.24}$$

Theorem 4.3 (Generalization)**.** Suppose $x_* \in \Omega$ and $f \in C^3(\Omega, \mathbb{R})$ such that $\nabla f(x_*) = 0$ and $\nabla^2 f(x_*)$ is invertible.TODO: *check this* Then if initial point x_0 is sufficiently closed to x_*, then Newton's method converges to x_*.

Proof. The basic idea is the same as the $\mathbb{R}$ case: prove the iterative algorithm induces a contraction mapping. ■

Example 4.3 (Newton's Method Fails to Converge)**.** Even if f has an unique global minimum x_*, and x_0 is arbitrarily close to the x_*, Newton's method could fail to converge.
Consider

$$f(x) = \frac{2}{3} |x|^{\frac{3}{2}} \tag{4.25}$$

Note that

$$f(x) = \begin{cases} \frac{2}{3}x^{\frac{3}{2}} & x \geq 0 \\ -\frac{2}{3}x^{\frac{3}{2}} & x < 0 \end{cases} \tag{4.26}$$

$$f'(x) = \begin{cases} x^{\frac{1}{2}} & x \geq 0 \\ -x^{\frac{1}{2}} & x < 0 \end{cases} \tag{4.27}$$

$$f''(x) = \begin{cases} \frac{1}{2}x^{-\frac{1}{2}} & x > 0 \\ -\frac{1}{2}x^{-\frac{1}{2}} & x < 0 \\ \text{DNE} & x = 0 \end{cases} \tag{4.28}$$

Therefore $f \notin C^2$.
Let $\delta > 0$ arbitrarily small, take initial point $x_0 \in V_\delta(0)$. WLOG, $x_0 = \varepsilon \in V_\delta(0)$ with $\varepsilon > 0$. The algorithm will oscillate between $\pm\varepsilon$ and never converge.

Remark 4.1. Newton's method does not necessarily converge to a global minimum, it may converge to local minimum or local maximum or even saddle point.

Example 4.4 (Newton's Method Converges to a Saddle Point)**.** Consider $f(x) = x^3$, $x_{n+1} \to \frac{x_n}{2}$, which converges to 0 (a saddle point).

Example 4.5 (Newton's Method on Quadratic Function)**.** Let Q be a symmetric $n \times n$ invertible matrix. Define quadratic form $f(x) := \frac{1}{2}x^T Q x : \mathbb{R}^n \to \mathbb{R}$. The optimal is $x = 0$.
Let $x_0 \in \mathbb{R}^n$, then $x_1 := x_0 - H_f(x_0)^{-1} \nabla f(x_0) = x_0 - Q^{-1}Qx_0 = 0$. *Therefore, Newton's method converges in one iteration.*

4.2 Steepest/Gradient Descent

Algorithm 4.3 (Steepest Descent)**.** Let $f : \Omega \to \mathbb{R}$ where Ω is an open subset of $\mathbb{R}^n$. Let initial point $x_0 \in \Omega$.
To minimize f on Ω, iteratively update x follows at each step k:

$$x_{k+1} \leftarrow x_k - \alpha_k \nabla f(x_k) \tag{4.29}$$

where $\alpha_k = \operatorname{argmin}_{\alpha \geq 0} f(x_k - \alpha \nabla f(x_k))$.
Remark: There might be multiple minimizing α, in real world implementations, we take the least minimizer found.

Theorem 4.4 (Gradient Descending is Descending)**.** At every step k, if $\nabla f(x_k) = 0$, the algorithm terminates. Otherwise,

$$f(x_{k+1}) < f(x_k) \tag{4.30}$$

Proof. Suppose $\nabla f(x_k) \neq 0$.
Note that for the first minimizing α_k found:

$$f(x_{k+1}) = f(x_k - \alpha_k \nabla f(x_k)) \tag{4.31}$$
$$\leq f(x_k - \alpha \nabla f(x_k)) \quad \forall 0 \leq \alpha \leq \alpha_k \tag{4.32}$$

Recall that

$$\left.\frac{d}{ds}\right|_{s=0} f(x_k - s\nabla f(x_k)) = -\nabla f(x_k) \cdot \nabla f(x_k) = -||\nabla f(x_k)||_2^2 < 0 \tag{4.33}$$

Therefore,

$$f(x_{k+1}) \leq f(x_k - \alpha \nabla f(x_k)) < f(x_k) \text{ for small } \alpha \tag{4.34}$$

■

Theorem 4.5 (Gradient Descending Induces Perpendicular Steps)**.** The consecutive steps induced by gradient descending are perpendicular. That is

$$(x_{k+2} - x_{k+1}) \cdot (x_{k+1} - x_k) = 0 \tag{4.35}$$

Proof. Note that

$$(x_{k+2} - x_{k+1}) \cdot (x_{k+1} - x_k) = (-\alpha_{k+1} \nabla f(x_{k+1})) \cdot (-\alpha_k \nabla f(x_k)) \tag{4.36}$$
$$= \alpha_k \alpha_{k+1} \nabla f(x_k) \cdot \nabla f(x_{k+1}) \tag{4.37}$$

If $\alpha_k = 0$, done.

If $\alpha_k > 0$,

$$
\begin{aligned}
f(x_{k+1}) &= f(x_k) - \alpha_k \nabla f(x_k) && (4.38)\\
&= \min_{\alpha \geq 0} \{ f(x_k - \alpha \nabla f(x_k)) \} && (4.39)\\
&= \min_{\alpha > 0} \{ f(x_k - \alpha \nabla f(x_k)) \} && (4.40)\\
&\implies \left. \frac{\partial}{\partial \alpha} \right|_{\alpha = \alpha_k} f(x_k - \alpha \nabla f(x_k)) = 0 && (4.41)\\
&\implies -\nabla f(x_k - \alpha_k \nabla f(x_k)) \cdot \nabla f(x_k) = 0 && (4.42)\\
&\implies -\nabla f(x_{k+1}) \cdot \nabla f(x_k) = 0 && (4.43)
\end{aligned}
$$

■

Theorem 4.6 (Sufficient Condition for Gradient Descent to Converge)**.** Let $f \in C^1$ on open $\Omega \subseteq \mathbb{R}^n$.
Let $\{x_k\}$ be the sequence generated by gradient descent: $x_{k+1} \leftarrow x_k - \alpha_k \nabla f(x_k)$.
If (x_k) is bounded in Ω, that is, there exists a compact set $K \subseteq \Omega$ such that $(x_k) \subseteq K$,
then every convergent subsequence of (x_k) converges to a critical point $x_* \in \Omega$ of f.

Proof. TODO: *Need to fix this proof.* Let $x_k \in K$ compact.
Then there exists subsequence $x_{k_i} \to x_* \in K$.
Show: $\nabla f(x_*) = 0$.
Note that $f(x_k) \geq f(x_{k+1})$ for every $k \in \mathbb{N}$, therefore $f(x_{k_i}) \searrow f(x_*)$. Therefore, $f(x_k) \searrow f(x_*)$. TODO: *Show this.* Suppose, for contradiction, $\nabla f(x_*) \neq 0$.
By continuity of ∇f, $(\nabla f(x_{k_i})) \to \nabla f(x_*)$.
Let $y_{k_i} := x_{k_i} - \alpha_{k_i} \nabla f(x_{k_i}) = x_{k_{i+1}}$.
Note that y_{k_i} has a convergent subsequence converging to y_*.
WLOG, $(y_{k_i}) \to y_*$.
Observe

$$
\begin{aligned}
\alpha_{k_i} &= \frac{|y_{k_i} - x_{k_i}|}{||\nabla f(x_{k_i})||} && (4.44)\\
\implies \lim_{k_i \to \infty} a_{k_i} &= \frac{|y_* - x_*|}{||\nabla f(x_*)||} =: \alpha_* && (4.45)
\end{aligned}
$$

Put back: $y_* = x_* - \alpha_* \nabla f(x_*)$.
Now $f(y_{k_i}) = f(x_{k_{i+1}}) = \min_{\alpha \geq 0} f(x_{k_i} - \alpha \nabla f(x_{k_i}))$, which implies

$$
\begin{aligned}
f(y_{k_i}) &\leq f(x_{k_i} - \alpha f(x_{k_i}))\ \forall \alpha \geq 0 && (4.46)\\
\forall \alpha \geq 0 \ \ \lim_{i \to \infty} f(y_{k_i}) = f(y_*) &\leq \lim_{i \to \infty} f(x_{k_i} - \alpha f(x_{k_i})) = f(x_* - \alpha \nabla f(x_*)) && (4.47)\\
\implies f(y_*) &\leq \min_{\alpha \geq 0} f(x_* - \alpha \nabla f(x_*)) < f(x_*) && (4.48)
\end{aligned}
$$

Further note that

$$
f(y_*) = \lim_{i \to \infty} f(y_{k_i}) = \lim_{i \to \infty} f(x_{k_{i+1}}) = f(x_*) \tag{4.49}
$$

Contradiction. ■