4 Optimality conditions for unconstrained problems

The definitions of global and local solutions of optimization problems are intuitive, but usually impossible to check directly. Hence, we will derive easily verifiable conditions that are either necessary for a point to be a local minimizer (thus helping us to identify candidates for minimizers), or sufficient (thus allowing us to confirm that the point being considered is a local minimizer), or, sometimes, both.

\[ \text{(P)} \quad \min \quad f(x) \]
\[ \text{s.t.} \quad x \in X, \]

where \( x = (x_1, \ldots, x_n)^T \in \mathbb{R}^n \), \( f : \mathbb{R}^n \to \mathbb{R} \), and \( X \) — an open set.

4.1 Optimality conditions: the necessary and the sufficient

**Necessary** condition for local optimality: “if \( \bar{x} \) is a local minimizer of (P), then \( \bar{x} \) must satisfy...” Such conditions help us identify all candidates for local optimizers.

**Theorem 4.1** Suppose that \( f \) is differentiable at \( \bar{x} \in X \). If there is a vector \( d \) such that \( \nabla f(\bar{x})^T d < 0 \), then for all \( \lambda > 0 \) sufficiently small, \( f(\bar{x} + \lambda d) < f(\bar{x}) \) (\( d \) is called a descent direction if it satisfies the latter condition).

**Proof:** Note that since \( X \) is an open set, \( \bar{x} + \lambda d \in X \) for sufficiently small \( \lambda > 0 \). We have:

\[ f(\bar{x} + \lambda d) = f(\bar{x}) + \lambda \nabla f(\bar{x})^T d + \lambda \|d\| \alpha_x(\lambda d), \]

where \( \alpha_x(\lambda d) \to 0 \) as \( \lambda \to 0 \). Rearranging,

\[ \frac{f(\bar{x} + \lambda d) - f(\bar{x})}{\lambda} = \nabla f(\bar{x})^T d + \|d\| \alpha_x(\lambda d). \]

Since \( \nabla f(\bar{x})^T d < 0 \) and \( \alpha_x(\lambda d) \to 0 \) as \( \lambda \to 0 \), \( f(\bar{x} + \lambda d) - f(\bar{x}) < 0 \) for all \( \lambda > 0 \) sufficiently small. \( \blacksquare \)

**Corollary 4.2** Suppose \( f \) is differentiable at \( \bar{x} \). If \( \bar{x} \) is a local minimizer, then \( \nabla f(\bar{x}) = 0 \) (such a point is called a stationary point).

**Proof:** If \( \nabla f(\bar{x}) \neq 0 \), then \( d = -\nabla f(\bar{x}) \) is a descent direction, whereby \( \bar{x} \) cannot be a local minimizer. \( \blacksquare \)

The above corollary is a **first order necessary optimality condition** for an unconstrained minimization problem. However, a stationary point can be a local minimizer, a local maximizer, or neither. The following theorem will provide a **second order necessary optimality condition**. First, a definition:

**Definition 4.3** An \( n \times n \) matrix \( M \) is called symmetric if \( M_{ij} = M_{ji} \ \forall i, j \). A symmetric \( n \times n \) matrix \( M \) is called

- positive definite if \( d^T M d > 0 \ \forall d \in \mathbb{R}^n, \ d \neq 0 \)
- positive semidefinite if \( d^T M d \geq 0 \ \forall d \in \mathbb{R}^n \)
- negative definite if \( d^T M d < 0 \ \forall d \in \mathbb{R}^n, \ d \neq 0 \)
- negative semidefinite if \( d^T M d \leq 0 \ \forall d \in \mathbb{R}^n \)
• indefinite if \( \exists d, p \in \mathbb{R}^n : d^T Md > 0, \ p^T Mp < 0 \).

**Example 1**

\[
M = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix}
\]

is positive definite.

**Example 2**

\[
M = \begin{pmatrix} 8 & -1 \\ -1 & 1 \end{pmatrix}
\]

is positive definite. To see this, note that for \( d \neq 0 \),

\[
d^T Md = 8d_1^2 - 2d_1d_2 + d_2^2 = 7d_1^2 + (d_1 - d_2)^2 > 0.
\]

Since \( M \) is a symmetric matrix, all its eigenvalues are real numbers. It can be shown that \( M \) is positive semidefinite if and only if all of its eigenvalues are nonnegative, positive definite if all of its eigenvalues are positive, etc.

**Theorem 4.4** Suppose that \( f \) is twice continuously differentiable at \( \bar{x} \in X \). If \( \bar{x} \) is a local minimizer, then \( \nabla f(\bar{x}) = 0 \) and \( H(\bar{x}) \) (the Hessian at \( \bar{x} \)) is positive semidefinite.

**Proof:** From the first order necessary condition, \( \nabla f(\bar{x}) = 0 \). Suppose \( H(\bar{x}) \) is not positive semidefinite. Then \( \exists d \) such that \( d^T H(\bar{x})d < 0 \). We have:

\[
f(\bar{x} + \lambda d) = f(\bar{x}) + \lambda \nabla f(\bar{x})^T d + \frac{1}{2} \lambda^2 d^T H(\bar{x})d + \lambda^2 \|d\|^2 \alpha_2(\lambda d)
\]

where \( \alpha_2(\lambda d) \to 0 \) as \( \lambda \to 0 \). Rearranging,

\[
\frac{f(\bar{x} + \lambda d) - f(\bar{x})}{\lambda^2} = \frac{1}{2} d^T H(\bar{x})d + \|d\|^2 \alpha_2(\lambda d).
\]

Since \( d^T H(\bar{x})d < 0 \) and \( \alpha_2(\lambda d) \to 0 \) as \( \lambda \to 0 \), \( f(\bar{x} + \lambda d) - f(\bar{x}) < 0 \) for all \( \lambda > 0 \) sufficiently small — contradiction.

**Example 3** Let

\[
f(x) = \frac{1}{2} x_1^2 + x_1x_2 + 2x_2^2 - 4x_1 - 4x_2 - x_3^2.
\]

Then

\[
\nabla f(x) = (x_1 + x_2 - 4, x_1 + 4x_2 - 4 - 3x_3^2)^T,
\]

and

\[
H(x) = \begin{pmatrix} 1 & 1 \\ 1 & 4 - 6x_2 \end{pmatrix}.
\]

\( \nabla f(x) = 0 \) has exactly two solutions: \( \bar{x} = (4, 0) \) and \( \tilde{x} = (3, 1) \). But

\[
H(\tilde{x}) = \begin{pmatrix} 1 & 1 \\ 1 & -2 \end{pmatrix}
\]

is indefinite, therefore, the only possible candidate for a local minimizer is \( \bar{x} = (4, 0) \).
Necessary conditions only allow us to come up with a list of candidate points for minimizers. 
**Sufficient** condition for local optimality: “if \( \bar{x} \) satisfies ..., then \( \bar{x} \) is a local minimizer of (P).”

**Theorem 4.5** Suppose that \( f \) is twice differentiable at \( \bar{x} \). If \( \nabla f(\bar{x}) = 0 \) and \( H(\bar{x}) \) is positive definite, then \( \bar{x} \) is a (strict) local minimizer.

**Proof:**
\[
f(x) = f(\bar{x}) + \frac{1}{2}(x - \bar{x})^T H(\bar{x})(x - \bar{x}) + \|x - \bar{x}\|^2 \alpha_2(x - \bar{x}).
\]

Suppose that \( \bar{x} \) is not a strict local minimizer. Then there exists a sequence \( x_k \to \bar{x} \) such that \( x_k \neq \bar{x} \) and \( f(x_k) \leq f(\bar{x}) \) for all \( k \). Define \( d_k = \frac{x_k - \bar{x}}{\|x_k - \bar{x}\|} \). Then
\[
f(x_k) = f(\bar{x}) + \|x_k - \bar{x}\|^2 \left( \frac{1}{2} d_k^T H(\bar{x}) d_k + \alpha_2(x_k - \bar{x}) \right),
\]
so
\[
\frac{1}{2} d_k^T H(\bar{x}) d_k + \alpha_2(x_k - \bar{x}) = \frac{f(x_k) - f(\bar{x})}{\|x_k - \bar{x}\|^2} \leq 0.
\]
Since \( \|d_k\| = 1 \) for any \( k \), there exists a subsequence of \( \{d_k\} \) converging to some point \( d \) such that \( \|d\| = 1 \) (by Theorem 3.9). Assume wolog that \( d_k \to d \). Then
\[
0 \geq \lim_{k \to \infty} \frac{1}{2} d_k^T H(\bar{x}) d_k + \alpha_2(x_k - \bar{x}) = \frac{1}{2} d^T H(\bar{x}) d,
\]
which is a contradiction with positive definiteness of \( H(\bar{x}) \). \( \blacksquare \)

**Note:**
- If \( \nabla f(\bar{x}) = 0 \) and \( H(\bar{x}) \) is negative definite, then \( \bar{x} \) is a local maximizer.
- If \( \nabla f(\bar{x}) = 0 \) and \( H(\bar{x}) \) is positive semidefinite, we cannot be sure if \( \bar{x} \) is a local minimizer.

**Example 4** Consider the function
\[
f(x) = \frac{1}{3} x_1^3 + \frac{1}{2} x_1^2 + 2x_1x_2 + \frac{1}{2} x_2^2 - x_2 + 9.
\]

Stationary points are candidates for optimality; to find them we solve
\[
\nabla f(x) = \left( \begin{array}{c} x_1^2 + x_1 + 2x_2 \\ 2x_1 + x_2 - 1 \end{array} \right) = 0.
\]

Solving the above system of equations results in two stationary points: \( x_a = (1, -1)^T \) and \( x_b = (2, -3) \). The Hessian is
\[
H(x) = \left( \begin{array}{cc} 2x_1 + 1 & 2 \\ 2 & 1 \end{array} \right).
\]

In particular,
\[
H(x_a) = \left( \begin{array}{cc} 3 & 2 \\ 2 & 1 \end{array} \right), \quad \text{and} \quad H(x_b) = \left( \begin{array}{cc} 5 & 2 \\ 2 & 1 \end{array} \right).
\]

Here, \( H(x_a) \) is indefinite, hence \( x_a \) is neither a local minimizer or maximizer. \( H(x_b) \) is positive definite, hence \( x_b \) is a local minimizer. Therefore, the function has only one local minimizer — does this mean that it is also a global minimizer?
4.2 Convexity and minimization

Definitions:

• Let \( x, y \in \mathbb{R}^n \). Points of the form \( \lambda x + (1 - \lambda)y \) are called convex combinations of \( x \) and \( y \) for \( \lambda \in [0, 1] \). More generally, point \( y \) is a convex combination of points \( x_1, \ldots, x_k \) if \( y = \sum_{i=1}^{k} \alpha_i x_i \) where \( \alpha_i \geq 0 \) \( \forall i \), and \( \sum_{i=1}^{k} \alpha_i = 1 \).

• A set \( S \subseteq \mathbb{R}^n \) is called convex if \( \forall x, y \in S \) and \( \forall \lambda \in [0, 1], \lambda x + (1 - \lambda)y \in S \).

• A function \( f : S \to \mathbb{R} \), where \( S \) is a nonempty convex set is a convex function if

\[
f(\lambda x + (1 - \lambda)y) \leq \lambda f(x) + (1 - \lambda)f(y) \quad \forall x, y \in S, \forall \lambda \in [0, 1].
\]

• A function \( f \) as above is called a strictly convex function if the inequality above is strict for all \( x \neq y \) and \( \lambda \in (0, 1) \).

• A function \( f : S \to \mathbb{R} \) is called concave (strictly concave) if \( -f \) is convex (strictly convex).

Consider the problem:

\[
(CP) \quad \min_x \quad f(x) \\
\text{s.t.} \quad x \in S.
\]

**Theorem 4.6** Suppose \( S \) is a nonempty convex set, \( f : S \to \mathbb{R} \) is a convex function, and \( \bar{x} \) is a local minimizer of \((CP)\). Then \( \bar{x} \) is a global minimizer of \( f \) over \( S \).

**Proof:** Suppose \( \bar{x} \) is not a global minimizer, i.e., \( \exists y \in S: f(y) < f(\bar{x}) \). Let \( y(\lambda) = \lambda \bar{x} + (1 - \lambda)y \), which is a convex combination of \( \bar{x} \) and \( y \) for \( \lambda \in [0, 1] \) (and therefore, \( y(\lambda) \in S \) for \( \lambda \in [0, 1] \)). Note that \( y(\lambda) \to \bar{x} \) as \( \lambda \to 1 \).

From the convexity of \( f \),

\[
f(y(\lambda)) = f(\lambda \bar{x} + (1 - \lambda)y) \leq \lambda f(\bar{x}) + (1 - \lambda)f(y) \leq \lambda f(\bar{x}) + (1 - \lambda)f(\bar{x}) = f(\bar{x})
\]

for all \( \lambda \in (0, 1) \). Therefore, \( f(y(\lambda)) < f(\bar{x}) \) for all \( \lambda \in (0, 1) \), and so \( \bar{x} \) is not a local minimizer, resulting in a contradiction. \( \blacksquare \)

**Note:**

• A problem of minimizing a convex function over a convex feasible region (such as we considered in the theorem) is a convex programming problem.

• If \( f \) is strictly convex, a local minimizer is the unique global minimizer.

• If \( f \) is (strictly) concave, a local maximizer is a (unique) global maximizer.

The following results help us to determine when a function is convex.

**Theorem 4.7** Suppose \( X \subseteq \mathbb{R}^n \) is a non-empty open convex set, and \( f : X \to \mathbb{R} \) is differentiable. Then \( f \) is convex iff ("if and only if") it satisfies the gradient inequality:

\[
f(y) \geq f(x) + \nabla f(x)^T(y - x) \quad \forall x, y \in X.
\]

**Proof:** Suppose \( f \) is convex. Then, for any \( \lambda \in (0, 1) \),

\[
f(\lambda y + (1 - \lambda)x) \leq \lambda f(y) + (1 - \lambda)f(x) \Rightarrow \frac{f(x + \lambda(y - x)) - f(x)}{\lambda} \leq f(y) - f(x).
\]
Letting $\lambda \to 0$, we obtain: $\nabla f(x)^T(y-x) \leq f(y) - f(x)$, establishing the “only if” part.

Now, suppose that the gradient inequality holds $\forall x, y \in X$. Let $w$ and $z$ be any two points in $X$. Let $\lambda \in [0, 1]$, and set $x = \lambda w + (1 - \lambda)z$. Then

$$f(w) \geq f(x) + \nabla f(x)^T (w-x) \quad \text{and} \quad f(z) \geq f(x) + \nabla f(x)^T (z-x).$$

Taking a convex combination of the above inequalities,

$$\lambda f(w) + (1 - \lambda) f(z) \geq f(x) + \nabla f(x)^T (\lambda(w-x) + (1 - \lambda)(z-x)) = f(x) + \nabla f(x)^T 0 = f(\lambda w + (1 - \lambda)z),$$

so that $f(x)$ is convex. $\blacksquare$

In one dimension, the gradient inequality has the form $f(y) \geq f(x) + f'(x)(y-x) \forall x, y \in X$.

The following theorem provides another necessary and sufficient condition, for the case when $f$ is twice continuously differentiable.

**Theorem 4.8** Suppose $X$ is a non-empty open convex set, and $f : X \to \mathbb{R}$ is twice continuously differentiable. Then $f$ is convex iff the Hessian of $f$, $H(x)$, is positive semidefinite $\forall x \in X$.

**Proof:** Suppose $f$ is convex. Let $\bar{x} \in X$ and $d$ be any direction. Then for $\lambda > 0$ sufficiently small, $\bar{x} + \lambda d \in X$. We have:

$$f(\bar{x} + \lambda d) = f(\bar{x}) + \nabla f(\bar{x})^T (\lambda d) + \frac{1}{2}(\lambda d)^T H(\bar{x}) (\lambda d) + \|\lambda d\|^2 \alpha_{\bar{x}}(\lambda d),$$

where $\alpha_{\bar{x}}(y) \to 0$ as $y \to 0$. Using the gradient inequality, we obtain

$$\lambda^2 \left( \frac{1}{2} d^T H(\bar{x}) d + \|d\|^2 \alpha_{\bar{x}}(\lambda d) \right) \geq 0.$$

Dividing by $\lambda^2 > 0$ and letting $\lambda \to 0$, we obtain $d^T H(\bar{x}) d \geq 0$, proving the “only if” part.

Conversely, suppose that $H(z)$ is positive semidefinite for all $z \in X$. Let $x, y \in S$ be arbitrary. Invoking the second-order version of the Taylor’s theorem, we have:

$$f(y) = f(x) + \nabla f(x)^T (y-x) + \frac{1}{2}(y-x)^T H(z)(y-x)$$

for some $z$ which is a convex combination of $x$ and $y$ (and hence $z \in S$). Since $H(z)$ is positive semidefinite, the gradient inequality holds, and hence $f$ is convex. $\blacksquare$

In one dimension, the Hessian is the second derivative of the function, the positive semidefiniteness condition can be stated as $f'' \geq 0 \ \forall x \in X$.

One can also show the following sufficient (but not necessary!) condition:

**Theorem 4.9** Suppose $X$ is a non-empty open convex set, and $f : X \to \mathbb{R}$ is twice continuously differentiable. Then $f$ is strictly convex if the Hessian of $f$, $H(x)$, is positive definite $\forall x \in X$.

For convex (unconstrained) optimization problems, the optimality conditions of the previous subsection can be simplified significantly, providing a single necessary and sufficient condition for global optimality:
**Theorem 4.10** Suppose $f : X \to \mathbb{R}$ is convex and differentiable on $X$. Then $\bar{x} \in X$ is a global minimizer iff $\nabla f(\bar{x}) = 0$.

**Proof:** The necessity of the condition $\nabla f(\bar{x}) = 0$ was established regardless of convexity of the function.

Suppose $\nabla f(\bar{x}) = 0$. Then, by gradient inequality, $f(y) \geq f(\bar{x}) + \nabla f(\bar{x})^T(y - \bar{x}) = f(\bar{x})$ for all $y \in X$, and so $\bar{x}$ is a global minimizer. 

**Example 5** Let

$$f(x) = -\ln(1 - x_1 - x_2) - \ln x_1 - \ln x_2.$$ 

Then

$$\nabla f(x) = \left( \frac{1}{1 - x_1 - x_2} - \frac{1}{x_1} , \frac{1}{1 - x_1 - x_2} - \frac{1}{x_2} \right),$$

and

$$H(x) = \begin{pmatrix} \left( \frac{1}{1 - x_1 - x_2} \right)^2 + \left( \frac{1}{x_1} \right)^2 & \left( \frac{1}{1 - x_1 - x_2} \right)^2 \\ \left( \frac{1}{1 - x_1 - x_2} \right)^2 & \left( \frac{1}{x_2} \right)^2 \end{pmatrix}.$$ 

It is actually easy to prove that $f(x)$ is a strictly convex function, and hence that $H(x)$ is positive definite on its domain $X = \{(x_1, x_2) : x_1 > 0, x_2 > 0, x_1 + x_2 < 1\}$. At $\bar{x} = (\frac{1}{3}, \frac{1}{3})$ we have $\nabla f(\bar{x}) = 0$, and so $\bar{x}$ is the unique global minimizer of $f(x)$. 
