Note on extrema

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Definition. (Hermitian matrix) A Hermitian matrix is a complex square matrix that is equal to its own conjugate transpose, or self-adjoint matrix.

Definition. (Hessian matrix) A Hessian matrix is a matrix whose (i,j) component is $\frac{\partial^2}{\partial x_i \partial x_j} f(x)$.

If $f \in C^2$, then the Hessian matrix is a Hermitian matrix.

Definition. (Quadratic form) Over a field $F \in \{\mathbb{R}, \mathbb{C}\}$, a *quadratic form* over F^n is the function defined by

$$Q(\mathbf{x}) = A[\mathbf{x}] = \sum_{i,j} a_{ij} x_i x_j,$$

where $A \in M(n, F)$ is called the *coefficient matrix.*

We denote the set of quadratic forms over F^n by $\mathcal{Q}_n(F)$.

Note. Over a field $F \in \{\mathbb{R}, \mathbb{C}\}$, the set of quadratic forms $\mathcal{Q}_n(F)$ corresponds one-to-one to the set of n-dimensional symmetric matrices if $F \neq \mathbb{C}$, otherwise to the set of n-dimensional Hermitian matrices, both of which are denoted by $\mathrm{Sym}(n, F)$ in this article.

This can be shown as follows.

1. The transform $M(n, F) \xrightarrow{\frac{X+X^*}{2}} \mathrm{Sym}(n, F)$ invariates the quadratic form: the coefficient of $x_i x_j$ amounts to $2^{-\delta_{ij}}(a_{ij} + a_{ji})$, having the same form by applying the transformation;
2. If $A \neq B$ for $A, B \in \mathrm{Sym(n, F)}$, then $A[\mathbf{x}] \neq B[\mathbf{x}]$: obvious when we think of the form of i, j coefficient, $2^{-\delta_{ij}}(a_{ij} + a_{ji})$.

Example. For the case $A = \begin{pmatrix} 1 & 2 \\ 1 & 1 \end{pmatrix}$, the transformed version is $B = \begin{pmatrix} 1 & 3/2 \\ 3/2 & 1 \end{pmatrix}$.

These matrices admit the equivalent quadratic forms $Q_2(x) = x^2 + y^2 + 3xy$.

Definition. (m-th differential) Let $f \in C^k(U, \mathbb{R})$ be a function of class C^k for $k \geq 1$ and an open set $U \subset \mathbb{R}^n$.

For $m \leq k$, the function defined by

$$(d^m f)_x : U \to \mathcal{H}_m(\mathbb{R}); \quad (d^m f)_x(a) = \sum_{1 \leq i_1;\ldots,i_m \leq n} \frac{\partial^m f}{\partial x_{i_1} \cdots \partial x_{i_m}}(x)\, a_{i_1} \cdots a_{i_m},$$

is called *m-th differential at x*, where $\mathcal{H}_m(\mathbb{R})$ is a set of homogeneous polynomial of degree m [**II-7 (7.2)**, 2].

Note. When $m = 2 \leq k$, we can speak of the definiteness of the quadratic form $(d^2 f)_x$.

Fact 1. (signature) For n-dimensional Hermitian matrix $A = (a_{ij})$, let $A^{(k)}$ denote the submatrix

$$A^{(k)} = \begin{pmatrix} a_{11} & \ldots & a_{1k} \\ & \ddots & \\ a_{k1} & \ldots & a_{kk} \end{pmatrix}, \quad 1 \leq k \leq n,$$

whose determinant is the principal k-minor. Then the following holds [**IV-4 Theorem 6**, 1].

$$A > 0 \iff \det A^{(k)} > 0, \quad \forall k \leq n$$

Corollary 1. If $A > 0$, then $-A < 0$.

This is because by assumption, we have $T \in U(n)$ such that

$$TAT^* = \begin{pmatrix} \alpha_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \alpha_n \end{pmatrix},$$

with $\alpha_j > 0$, hence that

$$-A = T^* \begin{pmatrix} -\alpha_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & -\alpha_n \end{pmatrix} T.$$

Since signature represents the multiplicity of sign of eigenvalues, and the eigenvalues are $GL(n, F)$ invariance, we see that $-A$ is indeed negative-definite. The opposite is also true.

Corollary 2. Applying Fact 1 to the statement $-A > 0$, we have

$$A < 0 \iff \begin{cases} \det A^{(k)} < 0, & \text{if } k = 1 \mod 2 \\ \det A^{(k)} > 0, & \text{if } k = 0 \mod 2 \end{cases}$$

or equivalently

$$(-1)^k A^{(k)} > 0.$$

Fact 2. (connection between extrema of a real-valued function and the 2nd differential, [**II-8**, **Theorem 8.4**, 2])

Let $f \in C^2(U, \mathbb{R})$ be a real-valued function of class C^2 at an open set $U \subset \mathbb{R}^n$. Suppose that $(df)_a = 0$ for $a \in U$, then the followings hold.

1. The quadratic form $(d^2f)_a$ is positive-definite $\iff$ f attains a strict local minimum at a;
2. The quadratic form $(d^2f)_a$ is negative-definite $\iff$ f attains a strict local maximum at a;
3. The quadratic form $(d^2f)_a$ is indefinite $\iff$ a is a saddle point of f;

Proof. (1) Choosing $\epsilon > 0$ such that $U(a, \epsilon) \subset U$, by Taylor we have

$$f(a + x) - f(a) = \frac{1}{2}(d^2f)_{a+\theta x}(x),$$

for any $x \in \mathbb{R}^n$ such that $|x| < \epsilon$ and some $\theta \in (0, 1)$. Since $(d^2f)_a > 0$, the principal k-minor $D^{(k)}(a)$ of quadratic form $(d^2f)_a$ stays positive for all $1 \leq k \leq n$, which is still true within sufficiently small neighbourhood of a; hence $(d^2f)_{a+\theta x} > 0$ holds when we choose $\epsilon > 0$ sufficiently small, which implies that f attains a strictly local minimum at a □

(2) By applying the result 1 to $g = -f$, the statement follows □

(3) $(d^2f)_a$ being indefinite implies that we have $x, y \in \mathbb{R}^n$ such that

$$(d^2f)_a(y) < 0 < (d^2f)_a(x).$$

Without loss of generality, we can assume $|x|, |y| < \epsilon$ for any $\epsilon > 0$ since the inequality does not depend on the norm of variables (i.e. replacing x, y with cx, cy for any $c \in \mathbb{R}^*$ does not change the inequality).

Again by choosing $\epsilon > 0$ so that $U(a, \epsilon) \subset U$, the line segments $L(a, a + x), L(a, a + y)$ are contained in U.

With a real variable $t \in (-1, 1)$, directional k-th derivatives of f yields the equations

$$\begin{aligned} g^{(k)}(0) =& \frac{d^k}{dt^k} f(a + tx)\Big|_{t=0} = (d^kf)_a(x), \\ h^{(k)}(0) =& \frac{d^k}{dt^k} f(a + ty)\Big|_{t=0} = (d^kf)_a(y). \end{aligned} \tag{1}$$

By assumption, $g'(0) = h'(0) = 0$ and $h^{(2)}(0) < 0 < g^{(2)}(0)$, implying that $t = 0$ is a strictly local minimum for h and strictly local maximum for g, equivalently a is a saddle point for f (i.e. neither a point of local minimum nor local maximum). $\square$

References

[1] Ichiro Satake. *Senkei Daisu Gaku*. ja. June 2015.

[2] Mitsuo Sugiura. *Kaiseki Nhumon I*. ja. 1980.