Supplement: Quadratic Forms and the Principal Axes Theorem

A quadratic form is a *homogeneous* polynomial of degree two with n variables (homogeneous: same degree for each monomial). In formula, it is just an algebraic expression of the form:

$$Q(x_1, x_2, \ldots, x_n) = \sum_{i,j=1}^{n} a_{ij} x_i x_j.$$

The study of quadratic forms has two origins. The first one is in number theory, like the study of Pythagorean triple (x, y, z) of integers such that $x^2 + y^2 = z^2$, or the "sum of four squares" problem: express every positive integer into a sum of four integer squares $x^2 + y^2 + z^2 + w^2$ (prototype of quaternions). The second one is in calculus. In the Taylor's expansion (with remainder) of a multi-variable, twice continuously differentiable function f about a point $\mathbf{a} = (a_1, \ldots, a_n)$:

$$f(\mathbf{x}) = f(\mathbf{a}) + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}(\mathbf{a})(x_i - a_i) + \frac{1}{2!} \sum_{i,j=1}^{n} \frac{\partial^2 f}{\partial x_j \partial x_i}(\mathbf{a} + \theta(\mathbf{x} - \mathbf{a}))(x_i - a_i)(x_j - a_j), \quad 0 < \theta < 1.$$

The second-order term appears as a quadratic form. So at those critical points where the gradient vector vanishes: $(\frac{\partial f}{\partial x_1}(\mathbf{a}), \ldots, \frac{\partial f}{\partial x_n}(\mathbf{a})) = (0, \ldots, 0)$, the local behavior of f near the point $\mathbf{a}$ will be determined by the second-order term. If the quadratic form is always "positive", f should have a local minimum there.

Matrix Representation of a Quadratic Form:

We note that by introducing an $n \times n$ matrix $A = (a_{ij})$, we can rewrite a quadratic form into a matrix-vector product:

$$Q(x_1, \ldots, x_n) = \sum_{i,j=1}^{n} a_{ij} x_i x_j = \mathbf{x}^T A \mathbf{x}.$$

(identify an 1×1 matrix as a number.) Moreover, we can make A to be a symmetric matrix A' by choosing $a'_{ij} = \frac{1}{2}(a_{ij} + a_{ji})$ [thus we have $a_{ij} x_i x_j + a_{ji} x_j x_i = a'_{ij} x_i x_j + a'_{ji} x_j x_i$]. So from now on we can always assume that A *is a symmetric matrix* in the matrix representation of a quadratic form.

"Extremal Values" of a Quadratic Form:

The extremal points (local maxima, local minima, saddle points) are important pieces of information when studying a multivariable function. As a quadratic form $Q(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}$ will satisfy:

$$Q(c\mathbf{x}) = (c\mathbf{x})^T A (c\mathbf{x}) = c^2 \mathbf{x}^T A \mathbf{x} = c^2 Q(\mathbf{x}) \quad \text{for any } c \in \mathbb{R},$$

it will not have extremal points in the usual sense. But we can study the extremal points of $Q(\mathbf{x})$ when $\mathbf{x}$ is restricted to the unit sphere $||\mathbf{x}|| = 1$ instead. And it turns out that the eigenvectors of A will give all these extremal "directions".

Theorem 6 (P.441): Let $Q(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}$ be the quadratic form given by an $n \times n$ symmetric matrix A. Then an extremal point of the restriction of $Q(\mathbf{x})$ on the unit sphere $||\mathbf{x}|| = 1$ in $\mathbb{R}^n$ is an eigenvector of A.

Proof: As we are finding the extremal points of a function in n-variables subject to a constraint $||\mathbf{x}||^2 = 1$, the method of Lagrange multipliers applies here. So we solve:

$$(*) \qquad \begin{cases} \dfrac{\partial}{\partial x_k}\Big[Q(\mathbf{x}) - \lambda(||\mathbf{x}||^2 - 1)\Big] = 0, \quad 1 \le k \le n; \\ ||\mathbf{x}||^2 - 1 = 0. \end{cases}$$

Note that the first set of equations can be re-written as:

$$(**) \qquad \frac{\partial}{\partial x_k}\Big\{\sum_{i,j=1}^{n} a_{ij}x_ix_j - \lambda(\sum_{i=1}^{n} x_i^2 - 1)\Big\} = 2\sum_{i=1}^{n} a_{ki}x_i - \lambda(2x_k), \quad 1 \le k \le n.$$

To verify the above claim, let us first fix an index i and consider the differentiation of the partial sum $\sum_{j=1}^{n} a_{ij}x_ix_j$ withrespect to x_k.

(i) When $i = k$, we have:

$$\frac{\partial}{\partial x_k}\sum_{j=1}^{n} a_{kj}x_kx_j = \frac{\partial}{\partial x_k}\Big(a_{kk}x_k^2 + \sum_{j\neq k} a_{kj}x_kx_j\Big) = 2a_{kk}x_k + \sum_{j\neq k} a_{kj}x_j = a_{kk}x_k + \sum_{j=1}^{n} a_{kj}x_j.$$

(ii) When $i \neq k$ (there are $n-1$ such i's), we have:

$$\frac{\partial}{\partial x_k}\sum_{j=1}^{n} a_{ij}x_ix_j = \frac{\partial}{\partial x_k}\Big(a_{ik}x_ix_k + \sum_{j\neq k} a_{ij}x_ix_j\Big) = a_{ik}x_i + 0 = a_{ki}x_i,$$

since $A^T = A$, i.e. $a_{ik} = a_{ki}$.

So, when summing up the terms in (i) and (ii), we get:

$$\frac{\partial}{\partial x_k}\Big\{\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}x_ix_j\Big\} = \underbrace{a_{kk}x_k + \sum_{j=1}^{n} a_{kj}x_j}_{\text{(i)}} + \underbrace{\sum_{i\neq k} a_{ki}x_i}_{\text{(ii)}} = \sum_{j=1}^{n} a_{kj}x_j + \sum_{i=1}^{n} a_{ki}x_i = 2\sum_{i=1}^{n} a_{ki}x_i,$$

and this verifies $(**)$. Note that $\sum_{i=1}^{n} a_{ki}x_i$ is exactly the k-th component of the matrix-vector product $A\mathbf{x}$. Hence the first vector equation of $(*)$ exactly says that $A\mathbf{x} = \lambda\mathbf{x}$, and the second vector equation of $(*)$ says $\mathbf{x} \neq \mathbf{0}$.

Hence an extremal point of $Q(\mathbf{x})$ restricted to $||\mathbf{x}|| = 1$ should be an eigenvector of A.

□

Corollary: An extremal value of the restriction of $Q(\mathbf{x})$ on the unit sphere $||\mathbf{x}|| = 1$ is an eigenvalue of A.

Proof: By Theorem 6, an extremal value of $Q(\mathbf{x})$ on $||\mathbf{x}|| = 1$ should be attained at an eigenvector $\mathbf{v}$ (with $||\mathbf{v}|| = 1$) of A. Let λ be the corresponding eigenvalue. Then:

$$Q(\mathbf{v}) = \mathbf{v}^TA\mathbf{v} = \mathbf{v}^T(\lambda\mathbf{v}) = \lambda\mathbf{v}^T\mathbf{v} = \lambda||\mathbf{v}||^2 = \lambda.$$

So the corresponding extremal value is simply the eigenvalue λ. □

Positive-Definite Quadratic Forms

Definition (P.437): A quadratic form Q is called:

a. *positive definite* if $Q(\mathbf{x}) > 0$ for all $\mathbf{x} \neq \mathbf{0}$,

b. *negative definite* if $Q(\mathbf{x}) < 0$ for all $\mathbf{x} \neq \mathbf{0}$,

c. *indefinite* if $Q(\mathbf{x})$ assumes both positive and negative values.

An $n \times n$ symmetric matrix A is called positive-definite (negative-definite or indefinite) if the associated quadratic form $\mathbf{x}^T A\mathbf{x}$ is a positive-definite (negative-definite or indefinite) quadratic form.

Remark: Sometimes we will say that a quadratic form Q is *positive semi-definite* if $Q(\mathbf{x}) \geq 0$ for every $\mathbf{x}$. Similarly, Q is said to be *negative semi-definite* if $Q(\mathbf{x}) \leq 0$ for every $\mathbf{x}$.

Intuitively speaking, when all the extremal values are positive (thus the minimal one is also positive), a multivariable function should remain positive over its domain. The following theorem verifies this claim.

Theorem 5 (P.437): Let A be an $n \times n$ symmetric matrix. Then a quadratic form $\mathbf{x}^T A\mathbf{x}$ is:

a. positive definite if and only if the eigenvalues of A are *all positive*,

b. negative definite if and only if the eigenvalues of A are *all negative*,

c. indefinite if and only if A has *both* positive and negative eigenvalues.

Proof: As A is a symmetric matrix, we have an orthogonal diagonalization $A = PDP^T$, i.e. $D = P^T AP$. Let $\mathbf{y} = P^T\mathbf{x}$, thus $\mathbf{x} = P\mathbf{y}$. Then the quadratic form $Q(\mathbf{x}) = \mathbf{x}^T A\mathbf{x}$ can be expressed as:

$$\begin{aligned} Q(\mathbf{x}) &= \mathbf{x}^T A\mathbf{x} = (P\mathbf{y})^T A(P\mathbf{y}) = \mathbf{y}^T(P^T AP)\mathbf{y} = \mathbf{y}^T D\mathbf{y} \\ &= \lambda_1 y_1^2 + \ldots + \lambda_n y_n^2. \end{aligned}$$

Now, since P is invertible, $\mathbf{x} \neq \mathbf{0}$ if and only if $\mathbf{y} \neq \mathbf{0}$, so the results of the theorem can be concluded easily by the simple expression of $Q(\mathbf{x})$ in terms of the coordinates of $\mathbf{y}$. $\square$

The same proof will also shows that:

Corollary: Let A be an $n \times n$ symmetric matrix. Then a quadratic form $\mathbf{x}^T A\mathbf{x}$ is:

a. positive semi-definite if and only if the eigenvalues of A are *all non-negative*,

b. negative semi-definite if and only if the eigenvalues of A are *all non-positive*.

The above change of variable $\mathbf{x} = P\mathbf{y}$ actually proves the following result:

Theorem 4 (Principal Axes Theorem, P.435): Let A be an $n \times n$ symmetric matrix. Then there is an orthogonal change of variable, $\mathbf{x} = P\mathbf{y}$, that transforms the quadratic form $\mathbf{x}^T A\mathbf{x}$ into a quadratic form $\mathbf{y}^T D\mathbf{y}$ with no cross-product term.

Example: Let $f(x,y) = x^3 + 3xy^2 - y^3 - 75x$. By direct computations, we have:

$$\frac{\partial f}{\partial x} = 3x^2 + 3y^2 - 75, \quad \frac{\partial f}{\partial y} = 6xy - 3y^2,$$
$$\frac{\partial^2 f}{\partial x^2} = 6x, \quad \frac{\partial^2 f}{\partial x \partial y} = 6y, \quad \frac{\partial^2 f}{\partial y^2} = 6x - 6y.$$

So the critical points of f are $(-\sqrt{5}, -2\sqrt{5})$, $(\sqrt{5}, 2\sqrt{5})$, $(-5, 0)$ and $(5, 0)$. At these critical points, the corresponding matrices $\left(\frac{\partial^2 f}{\partial x_j \partial x_i}\right)$ are:

$$\begin{bmatrix} -6\sqrt{5} & -12\sqrt{5} \\ -12\sqrt{5} & 6\sqrt{5} \end{bmatrix}, \quad \begin{bmatrix} 6\sqrt{5} & 12\sqrt{5} \\ 12\sqrt{5} & -6\sqrt{5} \end{bmatrix}, \quad \begin{bmatrix} -30 & 0 \\ 0 & -30 \end{bmatrix}, \quad \begin{bmatrix} 30 & 0 \\ 0 & 30 \end{bmatrix},$$

which have eigenvalues $(-30, 30)$, $(-30, 30)$, $(-30, -30)$ and $(30, 30)$ respectively.

The corresponding quadratic forms will be indefinite, indefinite, negative-definite, and positive-definite respectively. Using continuity argument, we can show that the behavior of quadratic forms will be the same in nearby points. So f has saddle points at $(-\sqrt{5}, -2\sqrt{5})$ and $(\sqrt{5}, 2\sqrt{5})$, a local maximum point at $(-5, 0)$, and a local minimum point at $(5, 0)$.