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Generalized Global Sensitivity and Correlation Analysis

KEN-ICHI KANATANI

Department of Computer Science, Gunma University, Kiryu, Gunma 376, Japan

Quantities measuring sensitivities and correlations of parameters involved in an engineering system are systematically defined by means of lattice theory. Consideration of lattice duality leads to recognition of polymatroid structure of the sensitivity and correlation measures. Analogous algebraic structures are shown to exist in the formulation of mutual information in information theory and multivariate analysis in statistics. Then, the sensitivity and correlation measures thus obtained are transformed into more tractable analytic expressions by means of expansion in series of orthogonal functions. Finally, a scheme of the so-called number-theoretic or quasi-Monte Carlo method is given for numerical evaluation of these expressions. This formulation generalizes the existing method of nonlinear sensitivity analysis.

1. INTRODUCTION

In many physical, engineering and economical systems, the output is influenced by a large number of parameters involved in the system. If the governing equations are given in the form of differential, integral or difference equations, the numerical output values corresponding to a particular prescription of parameter values are easily calculated by the use of a computer. In many cases, however, it is difficult to understand the way each parameter is related to the output. Let f be the output of the system under consideration, and let $a_1,..., a_n$ be the parameters of the system. Then, a function $f(a_1,..., a_n)$ is algorithmically well defined via the numerical solution of the governing equations. Throughout this paper, the output $f(a_1,..., a_n)$ is assumed to be a real continuous function of parameters $a_1,..., a_n$. Suppose the explicit function form of f is not known. The traditional sensitivity analysis is to evaluate partial derivatives $\partial f/\partial a_1,...,$ $\partial f/\partial a_n$ at a representative point $(a_1,..., a_n)$ in the n-dimensional parameter space and to regard them as quantities measuring influence of each of the parameters exerted on the output f. However, this analysis is of practical value only if function f is approximately linear over the physically significant region in the parameter space.

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Recently, a new type of sensitivity analysis applicable to large variations of parameters has been developed by Shuler *et al.* (Cukier *et al.*, 1973, 1975, 1978; Schaibly *et al.*, 1973). Their method is referred to as the *Fourier amplitude senstivity test* (FAST) or the *nonlinear sensitivity analysis*, and is applied to chemical kinetic reaction systems (e.g., Cukier *et al.*, 1973, 1975, 1978; Schaibly *et al.*, 1973; Boni and Penner, 1977; Koda *et al.*, 1979a, 1979b). They originally based their formulation on a heuristic approach: They considered one-dimensional variation of parameters $a_1,..., a_n$, i.e., they defined a one-parameter curve, which they called the *search curve*, in the n-dimensional parameter space in the form

$$a_i(t) = h_i(\cos 2\pi\omega_i t, \sin 2\pi\omega_i t), \qquad i = 1,..., n, \tag{1.1}$$

where $\omega_1,..., \omega_n$ are approximately incommensurate integers. Then, they applied the harmonic analysis to the corresponding output and calculated the Fourier coefficients corresponding to the frequencies $\omega_1,..., \omega_n$ of the output function, hence the name "FAST." Later, they interpreted their sensitivity measure as the "variance"

$$S(i) = \int (f_i(a_i) - \bar{f})^2 \rho_i(a_i)\, \mathrm{d}a_i, \tag{1.2}$$

where $\rho_i(a_i)$ is the weight function which describes "physical significance," in a sense, of a particular prescription of the value of a_i. Here, $f_i(a_i)$ is a function of a_i obtained by "averaging" f with respect to parameters other than a_i, and $\bar{f}$ is the "total average," i.e.,

$$f_i(a_i) = \int \cdots \int f(a_1,..., a_n) \prod_{j\neq i} \rho_j(a_j)\, \mathrm{d}a_j, \tag{1.3}$$

$$\bar{f} = \int \cdots \int f(a_1,..., a_n) \prod_{j=1}^{n} \rho_j(a_j)\, \mathrm{d}a_j. \tag{1.4}$$

They also suggested the possibility of formulating the couplings of sensitivities among the parameters by the same principle. A full development of their suggestion is one of the main purposes of this paper.

In this paper, we shall present a systematic way of deriving quantities that measure not only sensitivity of each parameter but also the amount of mutual coupling or correlation of the parameters by means of the lattice-theoretic formulation which Han (1975, 1977, 1978, 1980, 1981) applied to the formulation of mutual information in information theory and multivariate analysis in statistics. We shall further show that consideration of lattice duality leads to recognition of polymatroid structure found in information theory (Fujishige, 1978; Han, 1979) and in other engineering problems (cf.

Iri, 1979). This observation enables us to understand the inherent underlying algebraic structure and to treat many seemingly unrelated problems in the same mathematical discipline. Then, the sensitivity and correlation measures thus obtained are transformed into more tractable analytic expressions by means of expansion in series of orthogonal functions. Finally, we shall give a scheme of the so-called number-theoretic or quasi-Monte Carlo method (Haselgrove, 1961; Korobov, 1963, Hlawka, 1964a, 1964b; Zarembe, 1966, 1968; Conroy, 1967; Haber, 1970; Stroud, 1971; Chang *et al.*, 1973; Niederreiter, 1977) for numerical evaluation of these expressions. It will thus be shown that our scheme is a generalization of the method of Shuler *et al.*

2. Measures of Sensitivity and Correlation

In the following, we assume that the weight function $\rho(a_1,..., a_n)$ of parameters $a_1,..., a_n$ has the form

$$\rho(a_1,..., a_n) = \rho_1(a_1) \cdots \rho_n(a_n), \tag{2.1}$$

i.e., we consider the parameters to be "independent" a priori from each other. We further assume that each $\rho_i(a_i)$ is nonnegative and normalized:

$$\rho(a_i) \geqslant 0, \qquad \int \rho_i(a_i)\, \mathrm{d}a_i = 1, \qquad i = 1,..., n. \tag{2.2}$$

Henceforth, we do not specify the domain of integration, assuming that the weight function vanishes outside the physically significant region in the n-dimensional parameter space.

Now, we put $E = \{1,..., n\}$ and identify this set with the set of parameters, associating integer i with parameter a_i for $i = 1,..., n$. The parameters associated with integers contained in a subset A of E are simply referred to as parameters A. Let

$$f_A = \int \cdots \int f(a_1,..., a_n) \prod_{i \in \bar{A}} \rho_i(a_i)\, \mathrm{d}a_i, \tag{2.3}$$

where $\bar{A} = E - A$ is the complement of subset A with respect to E. In other words, f_A is a function of parameters A alone obtained from f by averaging it with respect to the remaining parameters $\bar{A}$. There exist 2^n f_A's for $A \subseteq E$, and we call them *partial averages*. In particular, f_E is identical to f itself, and f_ϕ, where ϕ is the empty set, equals the *total average* $\bar{f}$ defined by (1.4). The amount of variation of f induced by simultaneous variation of parameters A is described by

$$S(A)=\int\cdots\int (f_A-\bar{f})^2 \prod_{i\in A} \rho_i \, da_i, \tag{2.4}$$

which we call the *sensitivity* of parameters A. This generalizes the sensitivity measure (1.2) to that of multiple parameters. We say that f is *additive* with respect to A and $\bar{A}$ if f is decomposed to $f=f_1+f_2$, where f_1 and f_2 are functions of parameters A alone and parameters $\bar{A}$ alone, respectively. If this is the case, it is easy to show that $S(E)=S(A)+S(\bar{A})$. If $f=\sum_{i=1}^n f_i(a_i)$ in particular, i.e., if f is written as a sum of functions of a single argument, we say that f is *completely additive*. In this case, we obtain $S(E)=\sum_{i=1}^n S(\{i\})$. If f is not a completely additive function, quantities like $S(E)-S(A)-S(\bar{A})$ and $S(A)-\sum_{i\in A} S(\{i\})$ do not necessarily vanish. We say that these kinds of quantities, or more precisely, those linear combinations of $S(A)$'s, $A\subseteq E$ which vanish whenever f is completely additive, are *correlations* of parameters involved.

3. Vector Space of Partial Averages

Let V be the real vector space generated by the 2^n partial averages f_A's, $A\subseteq E$. We say that elements $f_1,\ldots,f_r$ of V are *linearly independent*, when $\sum_{i=1}^r c_i f_i=0$ holds identically for *any function form* of f if and only if $c_1=\cdots=c_r=0$. It is evident that all the partial averages f_A's, $A\subseteq E$ are linearly independent. Indeed, we can always define a function f such that $f_A\neq 0$ for some $A\subseteq E$ and $f_B=0$ for $B\neq A$. Thus, we obtain

Proposition 1. *The vector space V of partial averages is 2^n-dimensional, and $\{f_A \mid A\subseteq E\}$ is a basis of V.*

Next, we introduce *inner product* and *norm* into the vector space V. Define the inner product (f_1, f_2) of $f_1, f_2 \in V$ by

$$(f_1, f_2)=\int\cdots\int f_1 f_2 \prod_{i=1}^n \rho_i \, da_i, \tag{3.1}$$

and the norm $\|f_1\|$ of $f_1\in V$ by

$$\|f_1\|=\sqrt{(f_1, f_1)}. \tag{3.2}$$

If $(f_1, f_2)=0$, then we say that f_1 and f_2 are mutually *orthogonal*. We can easily verify

PROPOSITION 2.

$$(f_A, f_B) = \|f_{A\cap B}\|^2, \tag{3.3}$$

$$(f_A, f_B) = \bar{f}^2 \qquad \textit{for} \quad A \cap B = \phi. \tag{3.4}$$

Now, we define the deviation of f_A from $\bar{f}$ by

$$f'_A = f_A - \bar{f}. \tag{3.5}$$

By virtue of Proposition 2, f'_A is orthogonal to $\bar{f}$ for all $A \subseteq E$. Let V' be the orthogonal complement of $\bar{f}$ and call it the *deviatoric subspace* of V. Then, Proposition 1 and Proposition 2 are rewritten respectively as follows:

PROPOSITION 3. *The deviatoric subspace V' is $(2^n - 1)$-dimensional, and $\{f'_A \mid A \subseteq E, A \neq \phi\}$ is a basis of V'.*

PROPOSITION 4.

$$(f'_A, f'_B) = \|f'_{A\cap B}\|^2, \tag{3.6}$$

$$(f'_A, f'_B) = 0 \qquad \textit{for} \quad A \cap B = \phi. \tag{3.7}$$

The definition (2.4) of the sensitivity $S(A)$ of parameters A is now written as

$$S(A) = \|f'_A\|^2. \tag{3.8}$$

4. BOOLEAN LATTICE, THE DIFFERENCE OPERATION AND CORRELATIONS

The collection of all the subsets of E, i.e., the power set 2^E, is regarded as a Boolean lattice L with the set-inclusion relations and the union-intersection operations as the partial order relations and the basic operations. Let ξ: $2^E \to V$ be an arbitrary mapping. The *difference* $\Delta\xi$: $2^E \to V$ of ξ is defined by

$$\Delta\xi(A) = \sum_{B \subseteq A} \mu(B, A)\, \xi(B), \tag{4.1}$$

where $\mu(B, A)$ is the *Möbius function* on L, which is recurrently defined by

$$\sum_{C \subseteq B \subseteq A} \mu(C, B) = \delta_{CA} \begin{pmatrix} = 1 & \text{for} \quad C = A \\ = 0 & \text{otherwise} \end{pmatrix}, \tag{4.2}$$

(Rota, 1964). We can easily verify

$$\begin{aligned} \mu(B, A) &= (-1)^{|A|-|B|} \quad &\text{for} \quad B \subseteq A \\ &= 0 &\text{otherwise,} \end{aligned} \tag{4.3}$$

where $|A|$ is the cardinality, i.e., the number of elements, of set A. Expression (4.1) is inverted in the form

$$\xi(A) = \sum_{B \subseteq A} \Delta\xi(B), \tag{4.4}$$

hence the name "difference." Expressions (4.1) and (4.4) are also referred to as the *principle of inclusion–exclusion* (Rota, 1964).

Consider the difference of the partial averaging $f_\cdot : 2^E \to V$ and put

$$g_A = \Delta f_A. \tag{4.5}$$

Application of the principle of inclusion–exclusion yields

$$g_A = \sum_{B \subseteq A} \mu(B, A) f_B, \tag{4.6}$$

$$f_A = \sum_{B \subseteq A} g_B. \tag{4.7}$$

The following proposition is a direct consequence of (4.3).

PROPOSITION 5. *If f is completely additive, then*

$$\begin{aligned} g_A &= \bar{f} \quad &\textit{for} \quad A = \phi \\ &= f_{\{i\}} - \bar{f} &\textit{for} \quad A = \{i\} \\ &= 0 &\textit{for} \quad |A| > 1. \end{aligned} \tag{4.8}$$

Let V_0 be the set of elements of V that vanish identically whenever f is completely additive. It is evident that V_0 is a subspace of V, which we call the *correlative subspace* of V. Since $\{f_A \mid A \subseteq E\}$ is a basis of V and is mapped to $\{g_A \mid A \subseteq E\}$ by the invertible linear mapping indicated by (4.6) and (4.5), the latter is also a basis of V. Hence, we obtain from (4.8)

PROPOSITION 6. *The correlative subspace V_0 is $(2^n - (n+1))$-dimensional, and $\{g_A \mid A \subseteq E, |A| > 1\}$ is a basis of V_0.*

Then, the squared norm of g_A, which we put

$$R(A) = \| g_A \|^2, \tag{4.9}$$

is a measure of parameter correlation when $|A| > 1$. The following lemma is of fundamental importance.

LEMMA 1. *$\{g_A | A \subseteq E\}$ is an orthogonal basis of V, i.e.,*

$$(g_A, g_B) = R(A)\,\delta_{AB}. \tag{4.10}$$

Indeed, $\{g_A | A \subseteq E\}$ is nothing but the Gram–Schmidt orthogonalization of $\{f_A | A \subseteq E\}$. Since this lemma was proved by Han (1977, 1980), though in a different context, we omit the proof.

THEOREM 1.

$$S(A) = \sum_{\phi \subset B \subseteq A} R(B), \tag{4.11}$$

$$R(A) = \sum_{B \subseteq A} \mu(B, A)\, S(B) \qquad \textit{for} \quad A \neq \phi. \tag{4.12}$$

Proof. From (3.5) and (4.7), we can see that

$$f'_A = \sum_{\phi \subset B \subseteq A} g_B \qquad \text{for} \quad A \neq \phi. \tag{4.13}$$

Taking the squared norm of both sides, we obtain (4.11) from the orthogonality of g_A's. Application of the principle of inclusion–exclusion yields (4.12).

Thus, the set function $R: 2^E \to \mathbb{R}$ is the difference ΔS of the set function S: $2^E \to \mathbb{R}$. From Proposition 6, we obtain

THEOREM 2. *The necessary and sufficient condition that f be completely additive is $R(A) = 0$ for all $|A| > 1$.*

Suppose $f_A = f_1 + f_2$, where f_1 and f_2 are functions of parameters A_1 alone and parameters A_2 alone, respectively, and $A_1 \cup A_2 = A$, $A_1 \cap A_2 = \phi$. Then, it is easily confirmed that $R(A) = 0$. Hence, as long as $R(A) \neq 0$, parameters A are intimately correlated and they cannot be separated additively in any way. Thus, we are justified to call $R(A)$ the *correlation* of parameters A.

EXAMPLE 1. Let $E = \{1, 2, 3\}$. Then

$$g_{\{1\}} = f_{\{1\}} - \bar{f},$$

$$g_{\{1,2\}} = f_{\{1,2\}} - f_{\{1\}} - f_{\{2\}} + \bar{f},$$

$$g_{\{1,2,3\}} = f_{\{1,2,3\}} - f_{\{1,2\}} - f_{\{2,3\}} - f_{\{3,1\}} + f_{\{1\}} + f_{\{2\}} + f_{\{3\}} - \bar{f},$$

$$R(\{1\}) = S(\{1\}),$$

$$R(\{1, 2\}) = S(\{1, 2\}) - S(\{1\}) - S(\{2\}),$$

$$R(\{1, 2, 3\}) = S(\{1, 2, 3\}) - S(\{1, 2\}) - S(\{2, 3\}) - S(\{3, 1\}) + S(\{1\}) + S(\{2\}) + S(\{3\}).$$

If $f(a_1, a_2, a_3) = f_1(a_1, a_2) + f_2(a_2, a_3)$, then $R(\{1, 2\}) \neq 0$ and $R(\{2, 3\}) \neq 0$ in general, whereas $R(\{1, 3\}) = 0$ and $R(\{1, 2, 3\}) = 0$. If $f(a_1, a_2, a_3) = f_1(a_1, a_2) + f_2(a_2, a_3) + f_3(a_3, a_1)$ on the other hand, then $R(\{1, 2\}) \neq 0$, $R(\{2, 3\}) \neq 0$ and $R(\{3, 1\}) \neq 0$ in general, whereas $R(\{1, 2, 3\}) = 0$.

5. Lattice Duality and Polymatroid

Theorem 3.

$$(1) \quad S(A) \geqslant 0, \tag{5.1}$$

$$(2) \quad S(\phi) = 0, \tag{5.2}$$

$$(3) \quad S(A) \leqslant S(B) \qquad \textit{for} \quad A \subseteq B, \tag{5.3}$$

$$(4) \quad S(A) + S(B) \leqslant S(A \cup B) + S(A \cap B). \tag{5.4}$$

This theorem states that the set function $S: 2^E \to \mathbb{R}$ is (1) nonnegative, (2) normalized, (3) monotone nondecreasing and (4) *supermodular*. If we put $A \cap B = \phi$ in (5.4), then this supermodularity reduces to the condition of *superadditivity*, which in turn implies monotone nondecrease.

Proof of the theorem. Conditions (5.1) and (5.2) follow from definition (3.8). Let $A_1 \cap A_2 = \phi$. From Proposition 2, we obtain superadditivity

$$\begin{aligned} S(A_1 \cup A_2) - S(A_1) - S(A_2) &= \|f_{A_1 \cup A_2} - \bar{f}\|^2 - \|f_{A_1} - \bar{f}\|^2 - \|f_{A_2} - \bar{f}\|^2 \\ &= \|f_{A_1 \cup A_2} - f_{A_1} - f_{A_2} + \bar{f}\|^2 \geqslant 0. \end{aligned} \tag{5.5}$$

Hence, we have

$$S(A_1 \cup A_2) - S(A_1) \geqslant S(A_2) \geqslant 0, \tag{5.6}$$

which coincides with (5.3) if we put $A_1 = A$ and $A_2 = B - A$. Next, let A_1, A_2 and A_3 be mutually disjoint subsets of E. From Proposition 2, we obtain

$$\begin{aligned} &S(A_1 \cup A_2 \cup A_3) - S(A_1 \cup A_2) - S(A_2 \cup A_3) - S(A_3 \cup A_1) \\ &\qquad + S(A_1) + S(A_2) + S(A_3) \\ &\quad = \|f_{A_1 \cup A_2 \cup A_3} - f_{A_1 \cup A_2} - f_{A_2 \cup A_3} - f_{A_3 \cup A_1} + f_{A_1} + f_{A_2} + f_{A_3} - \bar{f}\|^2 \geqslant 0. \end{aligned}$$

Combination of this and (5.5) yields

$$\begin{aligned} &S(A_1 \cup A_2 \cup A_3) + S(A_2) - (S(A_1 \cup A_2) + S(A_2 \cup A_3)) \\ &\qquad \geqslant S(A_3 \cup A_1) - S(A_3) - S(A_1) \geqslant 0, \end{aligned}$$

which coincides with (5.4) if we put $A_1 = A - B$, $A_2 = A \cap B$ and $A_3 = B - A$.

Consider the following function f_A^* "dual" to f_A for $A \subseteq E$.

$$f_A^* = f - f_{\bar{A}}, \qquad f_A = f - f_{\bar{A}}^*. \tag{5.7}$$

It follows from Proposition 2 that $\bar{f}$ is orthogonal to all f_A^*'s, $A \subseteq E$. Since f_A's and f_A^*'s are related by the invertible linear mapping (5.7), we obtain

PROPOSITION 7. *$\{f_A^*, f \mid A \subseteq E, A \neq \phi\}$ is a basis of the vector space V of partial averages.*

PROPOSITION 8, *$\{f_A^* \mid A \subseteq E, A \neq \phi\}$ is a bais of the deviatoric subspace V' of V.*

Let the squared norm of f_A^* be

$$S^*(A) = \|f_A^*\|^2. \tag{5.8}$$

LEMMA 2.

$$S^*(E) = S(E), \tag{5.9}$$

$$S^*(A) = S(E) - S(\bar{A}), \qquad S(A) = S^*(E) - S^*(\bar{A}), \tag{5.10}$$

$$S^*(A) \geqslant S(A). \tag{5.11}$$

Proof. Equality (5.9) is obvious from the defining equations (3.8), (5.7) and (5.8). To see (5.10), note that from Proposition 2 we have

$$\begin{aligned} S^*(A) &= \|f_E - f_{\bar{A}}\|^2 = \|f_E\|^2 - 2(f_E, f_{\bar{A}}) + \|f_{\bar{A}}\|^2 = \|f_E\|^2 - \|f_{\bar{A}}\|^2 \\ &= \|f_E - \bar{f}\|^2 - \|f_{\bar{A}} - \bar{f}\|^2 = S(E) - S(\bar{A}). \end{aligned}$$

To see (5.11), note that from the superadditivity (5.5) we have

$$S^*(A) - S(A) = S(E) - S(A) - S(\bar{A}) \geqslant 0. \tag{5.12}$$

From (5.10), we can see that $S^*(A)$ is the amount of variation of f induced by simultaneous variation of all the parameters minus that induced by parameters other than A. Hence, $S^*(A)$ is regarded as a measure of "significance" or "predominance," in a sense, of parameters A. From (5.12), we can see the equality in (5.11) holds when f is additive with respect to A and $\bar{A}$.

THEOREM 4.

(1) $S^*(A) \geqslant 0,$ (5.13)

(2) $S^*(\phi) = 0,$ (5.14)

(3) $S^*(A) \leqslant S^*(B) \quad \textit{for} \quad A \subseteq B,$ (5.15)

(4) $S^*(A) + S^*(B) \geqslant S^*(A \cup B) + S^*(A \cap B).$ (5.16)

This theorem states that the set function $S^*: 2^E \to \mathbb{R}$ is (1) nonnegative, (2) normalized, (3) monotone nondecreasing and (4) *submodular*. If we put $A \cap B = \phi$ in (5.16), this condition reduces to that of *subadditivity*. Conditions (5.13)–(5.16) imply that the pair (E, S^*) of the set E of parameters and the set function S^* on it constitutes a *polymatroid* (cf. Welsh, 1976; Fujishige, 1978; Iri, 1979).

Proof of the theorem. Conditions (5.13) and (5.14) follow from definition (5.8). Let $A \subseteq B$. Since $\bar{B} \subseteq \bar{A}$, we obtain from (5.3)

$$S^*(A) = S(E) - S(\bar{A}) \leqslant S(E) - S(\bar{B}) = S^*(B),$$

which proves (5.15). Next, since $\overline{A \cup B} = \bar{A} \cap \bar{B}$ and $\overline{A \cap B} = \bar{A} \cup \bar{B}$, we obtain from (5.4)

$$\begin{aligned} S^*(A \cup B) + S^*(A \cap B) &= (S(E) - S(\overline{A \cup B})) + (S(E) - S(\overline{A \cap B})) \\ &= 2S(E) - S(\bar{A} \cap \bar{B}) - S(\bar{A} \cap \bar{B}) \\ &\leqslant 2S(E) - S(\bar{A}) - S(\bar{B}) \\ &= (S(E) - S(\bar{A})) + (S(E) - S(\bar{B})) \\ &= S^*(A) + S^*(B), \end{aligned}$$

which proves (5.16).

Now, we consider the difference of f_A^*, which is dual, in a sense, to the difference $g_A = \Delta f_A$ of f_A. Put

$$g_A^* = (-1)^{|A|-1} \Delta f_A^*. \tag{5.17}$$

Physical meaning of this function is made clear if we consider the dual lattice L^* obtained from L by inverting the set-inclusion relations and the union-intersection operations. Since the Möbius function $\mu^*(A, B)$ of lattice L^* is obtained by

$$\mu^*(A, B) = \mu(B, A), \tag{5.18}$$

the *dual difference*, i.e., the difference on the dual lattice L^*, is defined by

$$\Delta^*\xi(A) = \sum_{B \supseteq A} \mu(A, B)\, \xi(B), \tag{5.19}$$

where $\xi\colon 2^E \to V$ is an arbitrary mapping (Rota, 1964). The following lemma shows the relation between the dual difference operation Δ^* and the (primal) difference operation Δ.

LEMMA 3 (Han, 1975).

$$\Delta^*\xi(A) = (-1)^{|\bar{A}|} \sum_{B \supseteq \bar{A}} \Delta\xi(B), \tag{5.20}$$

$$\Delta\xi(A) = (-1)^{|A|} \sum_{B \subseteq \bar{A}} \Delta^*\xi(B). \tag{5.21}$$

If we define the dual mapping ξ^* of mapping ξ by

$$\xi^*(A) = \xi(E) - \xi(\bar{A}), \qquad \xi(A) = \xi^*(E) - \xi^*(\bar{A}), \tag{5.22}$$

then we obtain

LEMMA 4.

$$\Delta\xi^*(A) = -\Delta^*\xi(\bar{A}) \qquad \textit{for} \quad A \neq \phi, \tag{5.23}$$

$$\Delta^*\xi(A) = -\Delta\xi^*(\bar{A}) \qquad \textit{for} \quad A \neq E. \tag{5.24}$$

Proof.

$$\begin{aligned}
\Delta\xi^*(A) &= \sum_{B \subseteq A} \mu(B, A)(\xi(E) - \xi(\bar{B})) = \xi(E) \sum_{B \subseteq A} \mu(B, A) - \sum_{B \subseteq A} \mu(B, A)\, \xi(\bar{B}) \\
&= \xi(E)\, \delta_{\phi A} - \sum_{\bar{B} \subseteq A} \mu(\bar{B}, A)\, \xi(B) = \xi(E)\, \delta_{\phi A} - \sum_{B \supseteq \bar{A}} \mu(\bar{B}, A)\, \xi(B) \\
&= \xi(E)\, \delta_{\phi A} - \sum_{B \supseteq \bar{A}} \mu(\bar{A}, B)\, \xi(B) = \xi(E)\, \delta_{\phi A} - \Delta^*\xi(\bar{A}),
\end{aligned}$$

where we have made use of identities

$$\sum_{C \subseteq B \subseteq A} \mu(B, A) = \delta_{CA},$$

$$\mu(A, B) = \mu(\bar{B}, \bar{A}) = (-1)^{|B| - |A|} \qquad \text{for} \quad A \subseteq B.$$

Hence, (5.23) follows when $A \neq \phi$, and (5.24) follows by replacing A by $\bar{A}$.

Combination of Lemmas 3 and 4 yields the following two lemmas.

LEMMA 5.

$$g_A^* = (-1)^{|E|} \sum_{B \supseteq \bar{A}} (-1)^{|B|} f_B \qquad \textit{for} \quad A \neq \phi. \tag{5.25}$$

LEMMA 6.

$$g_A^* = \sum_{B \supseteq A} g_B \qquad \textit{for} \quad A \neq \phi, \tag{5.26}$$

$$g_A = \sum_{B \supseteq A} \mu(A, B)\, g_B^* \qquad \textit{for} \quad A \neq \phi. \tag{5.27}$$

Lemma 6 expresses nothing but the principle of inclusion–exclusion in the dual form. We can see from this lemma that $\{ g_A^* | A \subseteq E, A \neq \phi \}$ is mapped to $\{ g_A | A \subseteq E, A \neq \phi \}$ by an invertible linear mapping. Hence, the former is a basis of the deviatoric subspace V' of V. In particular, $\{ g_A^* \,|\, A \subseteq E, |A| > 1 \}$ is mapped to $\{ g_A \,|\, A \subseteq E, |A| > 1 \}$ by the same mapping. Hence, we obtain

PROPOSITION 9. *$\{ g_A^* \,|\, A \subseteq E, \; |A| > 1 \}$ is a basis of the correlative subspace V_0 of V.*

EXAMPLE 2. Let $E = \{1, 2, 3\}$. Then, form (5.25) and (5.26),

$$g_{\{1,2\}}^* = f_{\{1,2,3\}} - f_{\{2,3\}} - f_{\{1,3\}} + f_{\{3\}} = g_{\{1,2\}} + g_{\{1,2,3\}}.$$
$$g_{\{1,2,3\}}^* = g_{\{1,2,3\}}.$$

If we let the squared norm of g_A^* be

$$R^*(A) = \| g_A^* \|^2, \tag{5.28}$$

it is a measure of parameter correlations for $|A| > 1$ according to Proposition 9. Indeed, we obtain the following theorem.

THEOREM 5.

$$R^*(A) = \sum_{B \supseteq A} R(B) \qquad \textit{for} \quad A \neq \phi, \tag{5.29}$$

$$R(A) = \sum_{B \supseteq A} \mu(A, B)\, R^*(B) \qquad \textit{for} \quad A \neq \phi. \tag{5.30}$$

Proof. According to Lemma 1, all g_A's are mutually orthogonal. Hence, we obtain (5.29) by taking the squared norm of both sides of (5.26). Then

(5.30) follows by applying to (5.29) the principle of inclusion–exclusion in the dual form.

Since $R(A)$'s and $R^*(A)$'s are nonnegative quantities by definition, we can observe that if $R^*(A)=0$, then not only $R(A)=0$ but also $R(B)=0$ for $B \supseteq A$. This implies that if $R^*(A)=0$, then parameters A have no close correlations with all sets of parameters which include A. Hence, it may be justifiable to call $R^*(A)$ the *external correlation*, whereas $R(A)$ the *internal correlation*.

THEOREM 6.

$$R^*(A)=(-1)^{|A|-1}\Delta S^*(A)=(-1)^{|E|}\sum_{B\supseteq \bar{A}}(-1)^{|B|}S(B) \quad \textit{for } A\neq\phi. \tag{5.31}$$

Proof. Comparing Theorem 5 with Lemma 6, we can observe that $R(A)$'s and $R^*(A)$'s, $A\neq\phi$, are related to each other in the same way that g_A's and g_A^*'s, $A\neq\phi$, are. Comparing Theorem 1 with (4.6) and (4.7), we can also observe that, due to the orthogonality of g_A's, $S(A)$'s and $R(A)$'s, $A\neq\phi$, are related to each other just in the same way that f_A's and g_A's, $A\neq\phi$, are. Hence, $R^*(A)$'s and $S(A)$'s, $A\neq\phi$, must necessarily be related to each other by (5.31) just as g_A^*'s and f_A's, $A\neq\phi$, are by (5.17) and (5.25).

EXAMPLE 3. Let $E=\{1,2,3\}$. Then, from (5.29) and (5.31),

$$\begin{aligned} R^*(\{1,2\}) &= S(\{1,2,3\})-S(\{2,3\})-S(\{1,3\})+S(\{3\}) \\ &= R(\{1,2\})+R(\{1,2,3\}), \\ R^*(\{1,2,3\}) &= R(\{1,2,3\}). \end{aligned}$$

6. ANALOGIES IN STATISTICS AND INFORMATION THEORY

We have so far shown the algebraic background and the physical implication of the four basic quantities $S(A)$, $S^*(A)$, $R(A)$ and $R^*(A)$, which are all nonnegative. In particular, we have shown that (E, S^*) is a polymatroid, which has been recognized to exist in a variety of engineering problems (cf. Iri, 1979). This observation enables us to utilize various results of the theory of polymatroid and submodular functions. Fujishige (1978), for example, showed a way of decomposing mutually correlated random variables appearing in information theory into several groups, applying the so-called *principal partition of polymatroid*. His procedure is applicable to the present subject without any modification. Nemhauser *et al.* (Nemhauser *et al.*, 1978; Fisher *et al.*, 1978) studied heuristic algorithms choosing the set of variables with fixed cardinality that maximizes a given submodular function. Their algorihtms are also applicable here to choose the "most significant," say k, parameters of the system.

Meanwhile, the algebraic structure observed here has many analogies in other engineering problems. For example, if all the parameters $a_1,\ldots,a_n$ take only on a finite number of discrete values, and if all the integrations carried out to obtain partial averages are replaced by corresponding summations, then the whole analysis is interpreted in terms of the analysis of variance in statistics (see the lattice-theoretic formulation of Han (1977)). In statistical terminologies, the parameters $a_1,\ldots,a_n$ are called *factors*, and the discrete values they assume are called *levels* of corresponding factors. Quantities like $S(A)$, $S^*(A)$, $R(A)$ and $R^*(A)$ are *statistics* called *quadratic forms*. In particular, statistic $R(A)$ is the quadratic form of *multifactor interaction*. If on the observed values of the output f are superposed random errors which are subject to normal distributions identical but independent for each specification of factors and levels, then $R(A)$ obeys a noncentral χ^2-distribution due to the orthogonality of g_A's (Lemma 1) and Cochran's theorem known in statistics. Hence, one can resort to the F-test to test the hypothesis that the multifactor interaction does not exist. On the other hand, Han (1980) showed that the analysis of contingency tables, or frequency data, has the same lattice-theoretic structure if the entropy function is used instead of the simple averaging. However, the polymatroid structure, which is a natural consequence of the latice-theoretic formulation, has not yet be fully recognized in statistics.

In information theory, Han (1975) presented a lattice-theoretic formulation of multivariate correlations of random variables by the use of the entropy function. Since the underlying algebraic structure is identical to ours, various notions introduced there have sense in our context as well. For example, what is called *McGill's multiple mutual information* and its dual correspond to $R(A)$ and $R^*(A)$. The quantity called *Watanabe's cohesion measure* and its dual correspond to

$$S(A)-\sum_{i\in A} S(\{i\}) \left(=\sum_{B\subseteq A,|B|\neq 1} R(B)\right), \tag{6.1}$$

$$\sum_{i\in A} S^*(\{i\})-S^*(A) \left(=\sum_{B\subseteq A,|B|\neq 1} (-1)^{|B|} R^*(B)\right). \tag{6.2}$$

It is easily observed that to specify all the cohesion measures, or its duals, for $A\subseteq E$, $|A|>1$ is equivalent to specify all $R(A)$'s, or $R^*(A)$'s, for $A\subseteq E$, $|A|>1$. Thus, they are also fundamental quantities, which are nonnegative due to Theorems 3 and 4, describing mutual correlations. Han (1978) also studied the algebraic structure of symmetric quantities. After translation to our notations, the fundamental nonnegative quantities are

$$s_k = \sum_{|A|=k} S(A) \Big/ \binom{n}{k}, \qquad s_k^* = \sum_{|A|=k} S^*(A) \Big/ \binom{n}{k}, \tag{6.3}$$

$$r_k = \sum_{|A|=k} R(A) \Big/ \binom{n}{k}, \qquad r_k^* = \sum_{|A|=k} R^*(A) \Big/ \binom{n}{k}. \tag{6.4}$$

Various identities and inequalities satisfied by these quantities are listed in Han (1978). Fujishige (1978) introduced another set of nonnegative quantities, which are, after translation to our notations,

$$f_k = \frac{k}{n} s_n - s_k, \qquad f_k^* = s_k^* - \frac{k}{n} s_n^*, \qquad k = 1,..., n-2, \tag{6.5}$$

and showed that

$$f_k^* = f_{n-k}, \qquad f_k = f_{n-k}^*, \qquad k = 1,..., n-1, \tag{6.6}$$

$$\frac{k}{k+1} f_{k+1} \leqslant f_k \leqslant \frac{n-k}{n-k-1} f_{k+1}, \qquad k = 1,..., n-2, \tag{6.7}$$

$$\frac{k}{k+1} f_{k+1} \leqslant f_k^* \leqslant \frac{n-k}{n-k-1} f_{k+1}^*, \qquad k = 1,..., n-2. \tag{6.8}$$

Hence, if f_k or f_k^* vanishes for some k, then so do f_k's and f_k^*'s for all k. This fact is easily understood in our case by noting that f_k and f_k^* are linear combinations of nonnegative $R(A)$'s, or $R^*(A)$'s, for all $A \subseteq E$, $|A| > 1$ with positive coefficients.

EXAMPLE 4. Let $E = \{1, 2, 3\}$. Then

$$\begin{aligned} f_1 &= (S(\{1, 2, 3\}) - S(\{1\}) - S(\{2\}) - S(\{3\}))/3 \\ &= (R(\{1, 2, 3\}) + R(\{1, 2\}) + R(\{2, 3\}) + R(\{3, 1\})/3, \\ f_2 &= (2S(\{1, 2, 3\}) - S(\{1, 2\}) - S(\{2, 3\}) - S(\{3, 1\}))/3 \\ &= (2R(\{1, 2, 3\}) + R(\{1, 2\}) + R(\{2, 3\}) + R(\{3, 1\}))/3. \end{aligned}$$

7. EXPANSION IN SERIES OF ORTHOGONAL FUNCTIONS

We now consider a practical way for evaluation of $S(A)$ and $R(A)$. The defining expressions for them involve multiple integrations in a complicated order, so that direct evaluation of them is difficult and impractical. However, they can be transformed into more tractable analytic expressions by means of expansion in series of orthogonal functions. Let $\{\varphi_i^{(k)}(x) \mid k=0, 1, 2,...\}$ be a set of normalized complete orthogonal functions with respect to weight function $\rho_i(x)$ and expand $f(a_1,..., a_n)$ in series of them. We obtain

$$f(a_1,..., a_n) = \sum_{k_1,...,k_n} C(k_1,..., k_n) \prod_{j=1}^{n} \varphi_j^{(k_j)}(a_j), \tag{7.1}$$

$$C(k_1,..., k_n) = \int \cdots \int f(a_1,..., a_n) \prod_{j=1}^{n} \bar{\varphi}_j^{(k_j)}(a_j)\, \rho_j(a_j)\, \mathrm{d}a_j, \tag{7.2}$$

where the bar designates the complex conjugate. Assume $\varphi_i^{(0)}(x) = 1$, $i = 1,..., n$. Then, we can observe that $C(0,..., 0)$ equals the total average $\bar{f}$. Denote by $C_A(k)$ the coefficient $C(k_1,..., k_n)$ with k_i, $i \in \bar{A}$ replaced by 0. We can easily confirm that

$$f'_A = \sum_{k_i, i \in A}{}' C_A(k) \prod_{j \in A} \varphi_j^{(k_j)}(a_j), \tag{7.3}$$

where $\sum'$ denotes summation which excludes the term corresponding to $k_i = 0$ for all $i \in A$. If we take the squared norm of both sides of (7.3), and recalling the Parseval identity of orthogonal expansion, we obtain

THEOREM 7.

$$S(A) = \sum_{k_i, i \in A}{}' |C_A(k)|^2. \tag{7.4}$$

Now, observe that (7.4) is rewritten as

$$S(A) = \sum_{B \subseteq A} \sum_{k_i \neq 0, i \in B} |C_B(k)|^2. \tag{7.5}$$

Then, the principle of inclusion–exclusion and the uniqueness of the difference operation yield the following theorem.

THEOREM 8.

$$R(A) = \sum_{k_i \neq 0, i \in A} |C_A(k)|^2. \tag{7.6}$$

EXAMPLE 5. Let $E = \{1, 2, 3\}$. Then

$$S(\{1\}) = \sum_{k_1}' |C(k_1, 0, 0)|^2 = \sum_{k_1 \neq 0} |C(k_1, 0, 0)|^2,$$

$$\begin{aligned} S(\{1, 2\}) &= \sum_{k_1, k_2}' |C(k_1, k_2, 0)|^2 \\ &= \sum_{k_1 \neq 0, k_2 \neq 0} |C(k_1, k_2, 0)|^2 \\ &\quad + \sum_{k_1 \neq 0} |C(k_1, 0, 0)|^2 + \sum_{k_2 \neq 0} |C(0, k_2, 0)|^2, \end{aligned}$$

$$\begin{aligned} S(\{1, 2, 3\}) &= \sum_{k_1, k_2, k_3}' |C(k_1, k_2, k_3)|^2 \\ &= \sum_{k_1 \neq 0, k_2 \neq 0, k_3 \neq 0} |C(k_1, k_2, k_3)|^2 \\ &\quad + \sum_{k_1 \neq 0, k_2 \neq 0} |C(k_1, k_2, 0)|^2 + \sum_{k_2 \neq 0, k_3 \neq 0} |C(0, k_2, k_3)|2 \\ &\quad + \sum_{k_3 \neq 0, k_1 \neq 0} |C(k_1, 0, k_3)|^2 + \sum_{k_1 \neq 0} |C(k_1, 0, 0)|^2 \\ &\quad + \sum_{k_2 \neq 0} |C(0, k_2, 0)|^2 + \sum_{k_3 \neq 0} |C(0, 0, k_3)|^2, \end{aligned}$$

$$R(\{1\}) = \sum_{k_1 \neq 0} |C(k_1, 0, 0)|^2 = \sum_{k_1}' |C(k_1, 0, 0)|^2,$$

$$\begin{aligned} R(\{1, 2\}) &= \sum_{k_1 \neq 0, k_2 \neq 0} |C(k_1, k_2, 0)|^2 \\ &= \sum_{k_1, k_2}' |C(k_1, k_2, 0)|^2 \\ &\quad - \sum_{k_1} |C(k_1, 0, 0)|^2 - \sum_{k_2} |C(0, k_2, 0)|^2, \end{aligned}$$

$$\begin{aligned} R(\{1, 2, 3\}) &= \sum_{k_1 \neq 0, k_2 \neq 0, k_3 \neq 0} |C(k_1, k_2, k_3)|^2 \\ &= \sum_{k_1, k_2, k_3}' |C(k_1, k_2, k_3)|^2 \\ &\quad - \sum_{k_1, k_2}' |C(k_1, k_2, 0)|^2 - \sum_{k_2, k_3}' |C(0, k_2, k_3)|^2 \\ &\quad - \sum_{k_3, k_1}' |C(k_1, 0, k_3)|^2 + \sum_{k_1}' |C(k_1, 0, 0)|^2 \\ &\quad + \sum_{k_2}' |C(0, k_2, 0)|^2 + \sum_{k_3}' |C(0, 0, k_3)|^2. \end{aligned}$$

EXAMPLE 6. Normal distribution: $x \in (-\infty, \infty)$,

$$\rho_i(x) = e^{-x^2/2}/\sqrt{2\pi}, \qquad \varphi_i^{(k)}(x) = H_k(x/\sqrt{2})/\sqrt{2^k k!},$$

where $H_k(x)$ is the kth Hermite polynomial.

EXAMPLE 7. Exponential distribution: $x \in [0, \infty)$,

$$\rho_i(x) = e^{-x}, \qquad \varphi_i^{(k)}(x) = L_k(x)/k!,$$

where $L_k(x)$ is the kth Laguerre polynomial.

EXAMPLE 8. Uniform distribution: $x \in [-1, 1]$,

$$\rho_i(x) = 1/2, \qquad \varphi_i^{(k)}(x) = \sqrt{2k+1}\, P_k(x),$$

where $P_k(x)$ is the kth Legendre polynomial.

8. NUMERICAL INTEGRATION ON A TORUS

A convenient way for numerical evaluation of $S(A)$ and $R(A)$ is given by the use of Fourier coefficients. Suppose that for each i we can choose a suitable function $h_i(x, y)$ such that the transformation of parameters from $a_1, \ldots, a_n$ to $\theta_1, \ldots, \theta_n$ by

$$a_i = h_i(\cos 2\pi\theta_i, \sin 2\pi\theta_i), \qquad i = 1, \ldots, n, \tag{8.1}$$

reduces the weight function to unity. (The choice of $h_i(x, y)$ will be discussed later.) The output is now looked on as a function $f(\theta_1, \ldots, \theta_n)$ over the n-dimensional torus, i.e., a function periodic in each θ_i with period 1. Hence, $f(\theta_1, \ldots, \theta_n)$ is expanded in the multiple Fourier series in the form

$$f(\theta_1, \ldots, \theta_n) = \sum_{k_1, \ldots, k_n} C(k_1, \ldots, k_n)\, e^{2\pi i(k_1\theta_1 + \cdots + k_n\theta_n)}, \tag{8.2}$$

$$C(k_1, \ldots, k_n) = \int_0^1 \cdots \int_0^1 f(\theta_1, \ldots, \theta_n) \times e^{-2\pi i(k_1\theta_1 + \cdots + k_n\theta_n)}\, d\theta_1 \cdots d\theta_n. \tag{8.3}$$

If a practical method of evaluating the Fourier coefficient $C(k_1, \ldots, k_n)$ is available, one can compute $S(A)$ and $R(A)$ by (7.4) and (7.6), respectively, appropriately truncating the coefficients of high harmonics. Here, we consider the so-called *number-theoretic*, or *quasi-Monte Carlo* method of numerical integration (Haselgrove, 1961; Korobov, 1963; Hlawka, 1964a, 1964b; Zaremba, 1966, 1968; Conroy, 1967; Haber, 1970; Stroud, 1971; Cheng *et al.*, 1973; Niederreiter, 1977). We obtain an identity

$$C(k_1,\dots,k_n)=\frac{1}{N}\sum_{j=0}^{N-1} f\left(\frac{\omega_1 j}{N},\dots,\frac{\omega_n j}{N}\right) e^{-2\pi i(k_1\omega_1+\cdots+k_n\omega_n)j/N}$$
$$-\sum_{k_1'\neq k_1,\dots,k_n'\neq k_n} C(k_1',\dots,k_n')$$
$$\times\,\delta_N((k_1'-k_1)\,\omega_1+\cdots+(k_n'-k_n)\,\omega_n), \tag{8.4}$$

where $\omega_1,\dots,\omega_n$ are integers and we have adopted the notation

$$\begin{aligned}\delta_N(m)&=1 \quad \text{for} \quad m\equiv 0 \pmod N\\ &=0 \quad \text{for} \quad m\not\equiv 0 \pmod N\end{aligned}, \tag{8.5}$$

according to Korobov (1963). If f has the αth continuous partial derivative for each θ_i, there exists a constant C such that

$$|C(k_1,\dots,k_n)|\leqslant\frac{C}{(\bar{k}_1\bar{k}_2\cdots\bar{k}_n)^\alpha}, \tag{8.6}$$

where we have used the notation

$$\begin{aligned}\bar{m}&=|m| \quad \text{for} \quad m\neq 0\\ &=1 \quad \text{for} \quad m=0\end{aligned} \tag{8.7}$$

(Korobov, 1963). Hence, if we choose as $\omega_1,\dots,\omega_n$ the *optimal coefficients* in the sense of Korobov, we obtain

$$C(k_1,\dots,k_n)=\frac{1}{N}\sum_{j=0}^{N-1} f\left(\frac{\omega_1 j}{N},\dots,\frac{\omega_n j}{N}\right)$$
$$\times\, e^{-2\pi i(k_1\omega_1+\cdots+k_n\omega_n)j/N}+\varepsilon, \tag{8.8}$$

$$|\varepsilon|\leqslant CC'\frac{\log^{\alpha\beta}N}{N^\alpha}, \tag{8.9}$$

where C' is a constant and β is the *index* of the optimal coefficients (Korobov, 1963). The first term on the right-hand side of (8.8) has a form easily computed by a simple algorithm of computer programming. However, the choice of optimal coefficients depends on the choice of the indices $k_1,\dots,k_n$ and hence in general one must choose distinct sets of optimal coefficients for distinct Fourier coefficients. For practical purposes, therefore, it is more preferable to use a fixed set of optimal coefficients determined for

$k_1 = \cdots = k_n = 0$ at the cost of less accuracy. Indeed, we are not iterested in the values of $S(A)$ and $R(A)$ themselves but in the comparison of their magnitude.

There still remains one problem to be remarked; namely, the choice of the transformation function $h_i(x, y)$. Given an arbitrary weight function in the form of (2.1), one can determine the transformation of the form (8.1) that reduces the weight function to unity on the torus in principle, as is indicated in Cukier *et al.* (1978). However, this process often introduces singularities at $x, y = \pm 1$, which drastically increases the error term ε in (8.8) as can be seen from the estimate (8.9). One way to circumvent this difficulty is to reverse the process and first to consider a family of candidate functions for $h_i(x, y)$ which are smooth enough to have a fairly large value of α to assure small ε. Next, examine what kind of weight is introduced in the original parameter space. Then, we can choose one that gives an appropriate weight function in the parameter space, because essentially the weight function of the parameters is determined not by the system under consideration itself but rather by our choice. A list of such possible choices is found in Koda *et al.* (1979b).

Finally, we should note that our scheme is identical to the method of Shuler *et al.* (Cukier *et al.*, 1973, 1975, 1978; Schaibly *et al.*, 1973). Indeed, the discrete Fourier transform of f along their search curve (1.1) coincides with the first term in the right-hand side of (8.8). Thus, our formulation of the sensitivity and correlation analysis generalizes the sensitivity analysis of Shuler *et al.* and gives an algebraic and analytical foundation to it.

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