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Title	多変量統計解析の感度分析
Author(s)	垂水, 共之
Citation	大阪大学, 1986, 博士論文
Version Type	VoR
URL	https://hdl.handle.net/11094/1755
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Osaka University

Sensitivity Analysis
in
Multivariate Statistical Methods

1986

Tomoyuki Tarumi

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Abstract

The present thesis discusses the sensitivity analysis in multivariate statistical methods. The main objective is to evaluate the influence of a small change of the input data on the result of analysis, find influential observations and judge whether the result is stable or not.

In Chapter 2, we show three lemmas concerning the perturbation theory of eigenvalue problems assuming simple and multiple eigenvalues. The formulation of the perturbation methods is different, depending on whether the eigenvalues of interest are all simple or not.

In Chapter 3, we consider a method of sensitivity analysis in Hayashi's second method of quantification. To develop sensitivity analysis we introduce weights for individuals and evaluate the changes of eigenvalues and the scores of categories due to a small change of the weights for a single or multiple individuals. Then in Chapter 4 we try to apply the idea shown in Chapter 2 to other statistical methods and propose a unified method of sensitivity analysis in descriptive multivariate methods, which are formulated by the generalized singular value decomposition. The unified method can treat principal component analysis, the third method of quantification, and canonical

correlation analysis among others.

Finally in Chapter 5 we discuss a computational aspect. We perform numerical experiments and make some recommendations on the problem of whether to choose the method based on simple eigenvalues or that based on multiple eigenvalues and also on the problem of whether to use the first order approximation or the second order approximation.

Contents

1 Introduction 1

2 Perturbation Theory of Eigenvalue Problems 5

3 Sensitivity Analysis in Hayashi's Second Method of Quantification 15

3.1 Hayashi's second method of quantification 15

3.2 Sensitivity analysis 20

3.3 Summarized measures of the influence on the scores 25

3.4 Numerical example 25

3.5 Discussion 29

4 Sensitivity Analysis in Descriptive Multivariate Methods 35

4.1 Unified formulation of multivariate methods by the generalized singular value decomposition 36

4.2 Sensitivity analysis 39

4.3 Measures of the amount of influence 51

4.4 Numerical examples 52

4.5 Discussion and summary 60

5 Computational Aspect of Sensitivity Analysis 64

5.1 Computational methods 65

5.2 Discussion and summary 74

Acknowledgment 76

References 77

1 Introduction

In recent years, mainly in regression analysis many methods have been proposed for the evaluation of the influence of a single or multiple observations on the result of analysis (Belsley, Kuh and Welsch(1980), Cook and Weisberg(1982)). There are two aspects in these studies. One is to detect influential observations and the other is to evaluate the stability of the result. If the result depends heavily upon a few observations we must be very careful to form a conclusion, though we cannot prescribe what to do with influential observations without the use of additional information.

The problem of influential observations is not special to regression analysis, but common to other multivariate statistical methods. Thus, from a similar viewpoint to the case of regression analysis we propose some methods of sensitivity analysis in multivariate methods in a more general perspective.

We may consider that a statistical method is a system, a set of data is an input and the result of analysis is an output. We are interested in the sensitivity of this system, that is, how a small change of data (input) affects the result of analysis

(output). Here we use the term "sensitivity analysis" instead of "detecting influential observations", because various types of data different from those which appear in regression analysis are treated and not only the influence of individuals but also other types of influence are discussed in multivariate methods.

As statistical methods we consider Hayashi's second method of quantification and other descriptive multivariate methods, which are formulated as eigenvalue problems. The methods of quantification were developed and investigated for the purpose to analyze qualitative data by Hayashi(1952) and his colleagues in the Institute of Statistical Mathematics and are widely used in many fields such as social survey, behavioral science, medicine and quality control in Japan. On the other hand, multivariate statistical methods such as principal component analysis (Hotelling(1933)), biplot (Gabriel(1971)), canonical correlation analysis (Hotelling(1936)) and correspondence analysis (Benzécri et al.(1973)) are effectively used for looking into multivariate data. However, in applying these methods we sometimes feel uncertain over how reliable or stable the result is. To evaluate the reliability some authors introduced probabilistic models and developed methods of statistical inference. See, for example with respect to quantification methods, Okamoto and Endo(1974), Endo(1978), Tanaka(1978,1979), etc. From a different point of view Tanaka (1983,1984a,1984b) and Tanaka and Tarumi(1986a,1986b) tried to apply the idea of regression diagnostics and proposed methods of sensitivity analysis in quantification methods. The present paper consider also the sensitivity analysis in other

multivariate methods.

As small changes of input data we can treat various types. Among them we discuss mainly the influence of the changes of weights for a single or multiple individuals.

The basic idea of our sensitivity analysis can be summarized as follows: 1)Introduce small changes of weights for a single or multiple individuals. 2)Calculate the corresponding changes of eigenvalues, eigenvectors and the associated quantities by using the perturbation theory of eigenvalue problems. 3)Evaluate the amount of influence and detect influential observations. 4)Show their influence graphically for the convenience to make a decision based on it.

In the above procedure of sensitivity analysis we must solve many eigenvalue problems derived from the original one by changing the weight for each individual. Therefore it is important to use a computing method which is as efficient as possible. It is the reason why we apply the perturbation methods.

As preparations we give some lemmas concerning the perturbation theory of eigenvalue problems in Chapter 2 (Tanaka and Tarumi(1986b)). They are used as mathematical tools in the following chapters. The formulation of the perturbation theory is different, depending on whether the eigenvalues of interest are all simple or not.

In Chapter 3 we propose a method of sensitivity analysis in Hayashi's second method of quantification (Tanaka and Tarumi (1986a)). Here we discuss precisely the basic idea and

formulation of sensitivity analysis.

In Chapter 4 we intend to treat other multivariate methods, and consider the general multivariate procedure formulated by the generalized singular value decomposition (GSVD) (Tarumi(1986)). As shown in Greenacre(1984) and Greenacre and Underhill(1982), a number of descriptive multivariate methods such as principal component analysis, biplot, Hayashi's third method of quantification and canonical correlation analysis can be formulated by using the GSVD. Since the GSVD leads to an eigenvalue problem, we can construct a unified method of sensitivity analysis by using the perturbation theory of eigenvalue problems. This unified method can treat different kinds of multivariate analysis by changing the symmetric matrix of the eigenvalue problem. As individual multivariate methods we consider principal component analysis, the third method of quantification and canonical correlation analysis.

Finally in Chapter 5 we discuss the computational aspect of sensitivity analysis (Tanaka and Tarumi(1986b)). In actual data analysis the eigenvalues of interest are usually all simple in the strict sense. However, if there are close eigenvalues we should better apply the perturbation method under the assumption of multiple eigenvalues to get the result with high accuracy, because the method under the assumption of simple eigenvalues may not work well in such cases. The problem whether we should use the first order approximation or second order approximation is another problem. To investigate such problems we perform numerical experiments and make some recommendations based on them.

2 Perturbation Theory of Eigenvalue Problems

We consider the eigenvalue problem of a K×K symmetric matrix H, such that

$$(2.1) \qquad (H - \theta_s I)\mathbf{v}_s = \mathbf{0}, \quad s=1,2,\ldots,K,$$

and investigate how the eigenvalues and eigenvectors change when the matrix H varies to

$$(2.2) \qquad H(\varepsilon) = H + \varepsilon H^{(1)} + \varepsilon^2 H^{(2)} + \varepsilon^3 H^{(3)} + \cdots ,$$

for small ε.

Generally it is well known from perturbation theory of eigenvalue problems that, when the matrix H is expanded in a convergent power series, all the eigenvalues θ's and eigenvectors $\mathbf{v}$'s can also be expanded in convergent power series (Kato(1980), Rellich(1969)).

Let us express the eigenvalues and eigenvectors of $H(\varepsilon)$ as

$$(2.3) \qquad \theta_s(\varepsilon) = \theta_s + \varepsilon\theta_s^{(1)} + \varepsilon^2\theta_s^{(2)} + O(\varepsilon^3), \quad s=1,\ldots,K,$$

$$(2.4) \qquad \mathbf{v}_s(\varepsilon) = \mathbf{v}_s + \varepsilon\mathbf{v}_s^{(1)} + \varepsilon^2\mathbf{v}_s^{(2)} + O(\varepsilon^3), \quad s=1,\ldots,K,$$

then the coefficients of the above two equations are given by the following lemmas. The proof of Lemma 1 is given in Tanaka(1984a).

Lemma 1. Assume that the eigenvalue of interest is simple. Then

the coefficients of the 1st and 2nd orders of (2.3)-(2.4) are given by the following.

1st order:

$$(2.5)\quad \begin{cases} \theta_s^{(1)} = \mathbf{v}_s^T H^{(1)} \mathbf{v}_s, \\ z_{rs}^{(1)} = \mathbf{v}_r^T H^{(1)} \mathbf{v}_s / (\theta_s - \theta_r), \qquad r \neq s, \\ z_{ss}^{(1)} = 0, \\ v_{js}^{(1)} = \sum_r v_{jr} z_{rs}^{(1)}. \end{cases}$$

2nd order:

$$(2.6)\quad \begin{cases} \theta_s^{(2)} = \mathbf{v}_s^T H^{(2)} \mathbf{v}_s + \mathbf{v}_s^T H^{(1)} \mathbf{v}_s^{(1)}, \\ z_{rs}^{(2)} = (\mathbf{v}_r^T H^{(2)} \mathbf{v}_s + \mathbf{v}_r^T H^{(1)} \mathbf{v}_s^{(1)} - \theta_s^{(1)} \mathbf{v}_r^T \mathbf{v}_s^{(1)}) / (\theta_s - \theta_r), \quad r \neq s, \\ z_{ss}^{(2)} = -(\mathbf{v}_s^{(1)})^T \mathbf{v}_s^{(1)} / 2, \\ v_{js}^{(2)} = \sum_r v_{jr} z_{rs}^{(2)}. \end{cases}$$

Lemma 2-1. Assume that the matrix H is diagonalized as

$$(2.7)\quad X^T H X = \mathrm{diag}(\theta_1, \ \ldots \ , \theta_K),$$

by using an orthogonal matrix $X=(\mathbf{x}_1, \ \ldots \ , \mathbf{x}_K)$ and that the eigenvalue of interest is multiple, i.e. without loss of generality

$$(2.8)\quad \theta_1 = \ \ldots \ = \theta_k \ (=\theta) \neq \theta_{k+1}, \ \ldots \ , \theta_K \ .$$

Let

$$(2.9)\quad c_{ij}^{(l)} = \mathbf{x}_i^T H^{(l)} \mathbf{x}_j, \quad i,j=1,\ldots,K, \quad l=1,2,$$

and denote the $k \times k$ matrix of $\{c_{ij}^{(l)}, i,j=1,\ldots,k\}$ by $C_{11}^{(l)}$. Then the coefficients $\theta_s^{(1)}, s=1,..,k$ of the 1st order terms of the eigenvalues are given as the eigenvalues of $C_{11}^{(1)}$. If we denote the eigenvector associated with $\theta_s^{(1)}$ as $\mathbf{g}_s=(g_{is})$, the linear

combination such that

$$(2.10)\quad \mathbf{v}_s = \sum_{i=1}^{k} g_{is}\mathbf{x}_i$$

is the limit of eigenvector $\mathbf{v}_s(\varepsilon)$ associated with $\theta_s(\varepsilon)$ as $\varepsilon \to 0$.

(Proof) The eigenvalue problems of $H(\varepsilon)$ can be expressed as follows for the s-th eigenvalue $\theta_s(\varepsilon)$ and the associated eigenvectors $\mathbf{v}_s(\varepsilon)$.

$$(2.11)\quad \begin{aligned}&(H+\varepsilon H^{(1)}+\varepsilon^2 H^{(2)}+\varepsilon^3 H^{(3)}+\ldots)(\mathbf{v}_s+\varepsilon \mathbf{v}_s^{(1)}+\varepsilon^2 \mathbf{v}_s^{(2)}+\varepsilon^3 \mathbf{v}_s^{(3)}+\ldots)\\ &=(\theta_s+\varepsilon\theta_s^{(1)}+\varepsilon^2\theta_s^{(2)}+\varepsilon^3\theta_s^{(3)}+\ldots)(\mathbf{v}_s+\varepsilon\mathbf{v}_s^{(1)}+\varepsilon^2\mathbf{v}_s^{(2)}+\varepsilon^3\mathbf{v}_s^{(3)}+\ldots)\end{aligned}$$

Comparing the coefficients of ε in the both side of (2.11), we see that

$$(2.12)\quad H^{(1)}\mathbf{v}_s+H\mathbf{v}_s^{(1)} = \theta_s^{(1)}\mathbf{v}_s+\theta_s\mathbf{v}_s^{(1)}.$$

From (2.7) and (2.9) the matrices can be expanded as

$$(2.13)\quad H = \sum_{i=1}^{k} \theta\mathbf{x}_i\mathbf{x}_i^T + \sum_{i=k+1}^{K} \theta_i\mathbf{x}_i\mathbf{x}_i^T,$$

$$(2.14)\quad H^{(1)} = \sum_{i=1}^{K}\sum_{j=1}^{K} c_{ij}^{(1)}\mathbf{x}_i\mathbf{x}_j^T,$$

where $c_{ij}^{(1)}$ is defined in (2.9). Since the vectors $\mathbf{x}_1,\ldots,\mathbf{x}_K$ construct an orthonormal basis of the K-dimensional vector space, the vector $\mathbf{v}_s^{(1)}$ is expressed as

$$(2.15)\quad \mathbf{v}_s^{(1)} = \sum_{i=1}^{K} d_{is}\mathbf{x}_i.$$

Substituting (2.13)-(2.15) and (2.10) into (2.12) we obtain the following relation from the coefficients of $\mathbf{x}_i, i \leq k$.

$$(2.16)\quad \sum_{j=1}^{k} c_{ij}^{(1)} g_{js} = \theta_s^{(1)} g_{is}, \quad i=1,\ldots,k.$$

This indicates that $\theta_s^{(1)}$ and $g_s=(g_{is})$ are the eigenvalue and the associated eigenvector of the matrix $C_{11}^{(1)}$. Q.E.D.

Lemma 2-2. Assume the same conditions as in Lemma 2-1. Consider an orthonormal basis of K-dimensional vector space such that

$$(2.17)\quad v_s = \begin{cases} \sum_{i=1}^{k} g_{is}x_i, & s=1,\ldots,k, \\ x_s, & s=k+1,\ldots,K. \end{cases}$$

Define

$$(2.18)\quad \tilde{c}_{ij}^{(1)} = v_i^T H^{(1)} v_j, \quad i,j=1,\ldots,K,$$

denote the k×k submatrix of $\{\tilde{c}_{ij}^{(1)}, i,j=1,\ldots,K\}$ by $\tilde{C}_{11}^{(1)}$ and let

$$(2.19)\quad v_s^{(1)} = \sum_{i=1}^{K} d_{is}^{(1)} v_i, \quad l=1,2.$$

Then the 1st order terms of the eigenvectors and the 2nd order terms of the eigenvalues and eigenvectors can be calculated as follows.

1st order terms of the eigenvectors :

$$(2.20)\quad d_{is}^{(1)} = \begin{cases} \tilde{c}_{is}^{(1)}/(\theta-\theta_i), & s=1,\ldots,k,\ i=k+1,\ldots,K, \\ \{\tilde{c}_{is}^{(2)} + \sum_{j=k+1}^{K} \tilde{c}_{is}^{(1)} d_{js}^{(1)}\}/(\theta_s^{(1)}-\theta_i^{(1)}), & i,s=1,\ldots,k,\ i\neq s, \\ 0, & i=1,\ldots,k,\ i=s. \end{cases}$$

2nd order terms of the eigenvalues and eigenvectors :

$$(2.21)\quad \theta_s^{(2)} = \tilde{c}_{ss}^{(2)} + \sum_{i=k+1}^{K} \tilde{c}_{is}^{(1)} d_{is}^{(1)}$$

$$= \tilde{c}_{ss}^{(2)} + \sum_{i=k+1}^{K} (\tilde{c}_{is}^{(1)})^2/(\theta-\theta_i), \quad s=1,\ldots,k.$$

$$
(2.22)\quad d_{is}^{(2)} = \begin{cases} \{\tilde{c}_{is}^{(2)} + \sum_{j=1}^{K} \tilde{c}_{ij}^{(1)} d_{js}^{(1)} - \theta_s^{(1)} d_{is}^{(1)}\}/(\theta-\theta_i), \\ \qquad\qquad s=1,\ldots,k, \quad i=k+1,\ldots,K, \\ \{\tilde{c}_{is}^{(3)} + \sum_{j=1}^{K} \tilde{c}_{ij}^{(2)} d_{js}^{(1)} \\ \qquad + \sum_{j=k+1}^{K} \tilde{c}_{ij}^{(1)} d_{js}^{(2)} - \theta_s^{(2)} d_{is}^{(1)}\}/(\theta_s^{(1)}-\theta_i^{(1)}), \\ \qquad\qquad i,s=1,\ldots,k, \quad i\neq s, \\ -\sum_{j=1}^{K} (d_{js}^{(1)})^2/2, \qquad i=1,\ldots,k, \quad s=i. \end{cases}
$$

From (2.9),(2.17) and (2.18) the following relations hold between $\tilde{c}_{ij}^{(1)}$ and $c_{ij}^{(1)}$.

$$
(2.23)\quad \tilde{c}_{ij}^{(1)} = \begin{cases} \sum_{t=1}^{k} \sum_{m=1}^{k} g_{ti} g_{mj} c_{tm}^{(1)}, & \text{for } i\leq k, \quad j\leq k, \\ \sum_{t=1}^{k} g_{ti} c_{tj}^{(1)}, & \text{for } i\leq k, \quad j>k, \\ c_{ij}^{(1)}, & \text{for } i>k, \quad j>k. \end{cases}
$$

(Proof) The vectors $\mathbf{v}_i, i=1,\ldots,K$ also construct an orthonormal basis of the K-dimensional vector space. Then, using $\tilde{c}_{ij}^{(1)}$ defined by (2.18) the matrices H and $H^{(1)}$ are expanded as follows.

$$
(2.13)'\quad H = \sum_{i=1}^{k} \theta \mathbf{v}_i \mathbf{v}_i^T + \sum_{i=k+1}^{K} \theta_i \mathbf{v}_i \mathbf{v}_i^T,
$$

$$
(2.14)'\quad H^{(1)} = \sum_{i=1}^{K} \sum_{j=1}^{K} \tilde{c}_{ij}^{(1)} \mathbf{v}_i \mathbf{v}_j^T,
$$

where

$$
(2.24)\quad \tilde{C}_{11}^{(1)} = (\tilde{c}_{ij}^{(1)}), \quad 1\leq i,j\leq k.
$$

Now we shall express $\mathbf{v}_s^{(1)}$ as

$$(2.15)' \quad v_s^{(1)} = \sum_{i=1}^{K} d_{is}^{(1)} v_i, \quad s=1,\ldots,k.$$

by using the new basis $(v_1,\ldots,v_K)$. Then, substituting (2.13)'-(2.15)' into (2.12) we obtain the following relation from the coefficients of v_i for $i>k$.

$$\tilde{c}_{is}^{(1)} + \theta_i d_{is}^{(1)} = \theta d_{is}^{(1)}.$$

Thus

$$(2.25) \quad d_{is}^{(1)} = \tilde{c}_{is}^{(1)}/(\theta-\theta_i), \quad s=1,\ldots,k, \ i=k+1,\ldots,K.$$

Next let us consider the order of ε^2. Comparing the coefficients of ε^2 in the both sides of (2.11) we have

$$(2.26) \quad H^{(2)}v_s + H^{(1)}v_s^{(1)} + Hv_s^{(2)} = \theta_s^{(2)}v_s + \theta_s^{(1)}v_s^{(1)} + \theta_s v_s^{(2)}.$$

Substituting (2.13)'-(2.15)' into (2.26) we obtain the following relation from the coefficients of v_i for $i\leq k$, $i\neq s$.

$$\tilde{c}_{is}^{(2)} + \theta_i^{(1)} d_{is}^{(1)} + \sum_{j=k+1}^{K} \tilde{c}_{ij}^{(1)} d_{js}^{(1)} = \theta_s^{(1)} d_{is}^{(1)}.$$

Hence

$$(2.27) \quad d_{is}^{(1)} = \{\tilde{c}_{is}^{(2)} + \sum_{j=k+1}^{K} \tilde{c}_{ij}^{(1)} d_{js}^{(1)}\}/(\theta_s^{(1)}-\theta_i^{(1)}), \quad i,s=1,\ldots,k, \ i\neq s.$$

From the normalizing condition such that

$$(2.28) \quad (v_s+\varepsilon v_s^{(1)}+\varepsilon^2 v_s^{(2)}+\ldots)^T(v_s+\varepsilon v_s^{(1)}+\varepsilon^2 v_s^{(2)}+\ldots) = 1,$$

the coefficient of ε must satisfy the following.

$$(2.29) \quad (v_s^{(1)})^T v_s + v_s^T v_s^{(1)} = 0.$$

Substituting (2.15)' into (2.29) we have

$$(2.30) \quad d_{ss}^{(1)} = 0, \quad s=1,\ldots,k.$$

Thus the equation (2.20) is proved.

If we substitute (2.13)'-(2.15)' into (2.26) and compare the coefficients of v_s we easily have the second order term $\theta_s^{(2)}$ as

(2.21). If we compare the coefficients of v_i for $i>k$, we have

$$\tilde{c}_{is}^{(2)} + \theta_i d_{is}^{(2)} + \sum_{j=1}^{K} \tilde{c}_{ij}^{(1)} d_{js}^{(1)} = \theta_s^{(1)} d_{is}^{(1)} + \theta_s d_{is}^{(2)}.$$

Hence

$$(2.31) \quad d_{is}^{(2)} = \{\tilde{c}_{is}^{(2)} + \sum_{j=1}^{K} \tilde{c}_{ij}^{(1)} d_{js}^{(1)} - \theta_s^{(1)} d_{is}^{(1)}\}/(\theta-\theta_i), \qquad s=1,\ldots,k, \quad i=k+1,\ldots,K.$$

Now we shall consider the order of ε^3. From the coefficients of ε^3,

$$(2.32) \quad H^{(3)}v_s + H^{(2)}v_s^{(1)} + H^{(1)}v_s^{(2)} + Hv_s^{(3)} = \theta_s^{(3)}v_s + \theta_s^{(2)}v_s^{(1)} + \theta_s^{(1)}v_s^{(2)} + \theta_s v_s^{(3)}.$$

Substituting (2.13)'-(2.15)' into (2.32) we obtain the following relation from the coefficients of v_i for $i \leq k$, $i \neq s$.

$$\tilde{c}_{is}^{(3)} + \sum_{j=1}^{K} \tilde{c}_{ij}^{(2)} d_{js}^{(1)} + \theta_i^{(1)} d_{is}^{(2)} + \sum_{j=k+1}^{K} \tilde{c}_{ij}^{(1)} d_{js}^{(2)} + \theta d_{is}^{(3)} = \theta_s^{(2)} d_{is}^{(1)} + \theta_s^{(1)} d_{is}^{(2)} + \theta d_{is}^{(3)}.$$

Therefore

$$(2.33) \quad d_{is}^{(2)} = \{\tilde{c}_{is}^{(3)} + \sum_{j=1}^{K} \tilde{c}_{ij}^{(2)} d_{js}^{(1)} + \sum_{j=k+1}^{K} \tilde{c}_{ij}^{(1)} d_{js}^{(2)} - \theta_s^{(2)} d_{is}^{(1)}\}/(\theta_s^{(1)}-\theta_i^{(1)}), \qquad i,s=1,\ldots,k, \quad i \neq s.$$

From the order of ε^2 in the normalizing condition (2.28),

$$(2.34) \quad (v_s^{(2)})^T v_s + (v_s^{(1)})^T v_s^{(1)} + v_s^T v_s^{(2)} = 0 .$$

Substituting (2.15)' into (2.34) we easily obtain the following equation.

$$(2.35) \quad d_{is}^{(2)} = -\sum_{j=1}^{K} (d_{js}^{(1)})^2/2 , \qquad i=1,\ldots,k, \quad s=i.$$

Q.E.D.

Lemma 3. Assume the same conditions as in Lemma 2-1. Then the approximate eigenvalues up to the 2nd order are given as the eigenvalues of

$$\theta I + \varepsilon C_{11}^{(1)} + \varepsilon^2 (C_{11}^{(2)} + Q), \tag{2.36}$$

where

$$\begin{cases} Q = (q_{ii'}), \\ q_{ii'} = \sum_{j=k+1}^{K} c_{ij}^{(1)} c_{i'j}^{(1)} / (\theta - \theta_j) . \end{cases} \tag{2.37}$$

(Proof) We shall show that the second order perturbation to the s-th eigenvalue of the matrix (2.36) is given by $\{\theta + \varepsilon\theta_s^{(1)} + \varepsilon^2\theta_s^{(2)}\}$, where $\theta_s^{(1)}$ and $\theta_s^{(2)}$ are defined in Lemma 2-1 and 2-2. It is sufficient to show that the first order perturbation to the s-th eigenvalue of $C_{11}^{(1)} + \varepsilon(C_{11}^{(2)} + Q)$ is given by $\{\theta_s^{(1)} + \varepsilon\theta_s^{(2)}\}$. Since the eigenvalues are invariant for an orthogonal transformation, we may consider the eigenvalue problem of the matrix

$$(\theta_i^{(1)}\delta_{ii'}) + \varepsilon\{\tilde{c}_{ii'}^{(2)} + \sum_{j=k+1}^{K} \tilde{c}_{ij}^{(1)} \tilde{c}_{i'j}^{(1)} / (\theta - \theta_j)\}, \tag{2.38}$$

which is made by multiplying $G=(g_1,\ldots,g_k)$ and its transpose from right and left. $\theta_s^{(1)}$ and g_s are the eigenvalue and the associated eigenvector of $C_{11}^{(1)}$ as defined in Lemma 1. With probability one we can assume $\{\theta_s^{(1)},\ s=1,\ldots,k\}$ are all distinct. Then, by applying Lemma 1 we may easily show that the first order perturbation to the s-th eigenvalue of (2.38) is given by $\{\theta_s^{(1)} + \varepsilon\theta_s^{(2)}\}$ where $\theta_s^{(2)}$ is defined in (2.21). Q.E.D.

In the above we derived up to the second order perturbation of the eigenvalues $\{\theta_s(\varepsilon)\}$ and the eigenvectors $\{\mathbf{v}_s(\varepsilon)\}$ when the unperturbed eigenvalue of interest is multiple. Concerning the perturbation of a symmetric matrix with multiple eigenvalues several authors such as Anderson(1963), Fujikoshi(1977), Konishi(1975), vom Scheidt and Purkert(1983) among others have already studied. Our formulation is different from the first three among the above papers in the sense that we derive expressions of the power series expansions of multiple eigenvalues and the associated eigenvectors explicitly, numbering the multiple eigenvalues by the order of the eigenvalues $\theta^{(1)}$'s of $C_{11}^{(1)}$. The last one discussed the case $H(\varepsilon)=H+\varepsilon H^{(1)}$ and its results coincide with ours when $H^{(2)}=H^{(3)}=0$. But the technique used is quite different from us.

Actually we often meet with the case when the eigenvalues of interest are not exactly multiple but very close, i.e.

$$\theta_1 \tilde{=} \theta_2 \tilde{=} \cdots \tilde{=} \theta_k \neq \theta_{k+1}, \cdots, \theta_K . \tag{2.39}$$

In that case the matrix H is expressed as

$$H = \sum_{i=1}^{K} \theta_i \mathbf{v}_i \mathbf{v}_i^T = \bar{H} + \varepsilon \bar{E} , \tag{2.40}$$

where

$$
(2.41)\quad \begin{cases} \bar{H} = \sum_{i=1}^{k} \theta v_i v_i^T + \sum_{i=k+1}^{K} \theta_i v_i v_i^T, \\ \bar{E} = \sum_{i=1}^{k} (\theta_i - \theta) v_i v_i^T / \varepsilon \ , \\ \theta = \sum_{i=1}^{k} \theta_i / k \ . \end{cases}
$$

If the magnitudes of $|\theta_i - \theta|$'s are of the order of ε, the perturbed matrix $H(\varepsilon)$ is expanded as

$$
(2.42)\quad H(\varepsilon) = H + \varepsilon H^{(1)} + \varepsilon^2 H^{(2)} + \varepsilon^3 H^{(3)} + \ldots
$$

$$
= \bar{H} + \varepsilon (H^{(1)} + \bar{E}) + \varepsilon^2 H^{(2)} + \varepsilon^3 H^{(3)} + \ldots \ .
$$

Thus, applying Lemma 2-1, 2-2 and/or 3 we can obtain the asymptotic approximations to the eigenvalues and eigenvectors of $H(\varepsilon)$.

3 Sensitivity Analysis in Hayashi's Second Method of Quantification

Among various quantification methods we investigate the so-called second method of quantification, which is used for discrimination of qualitative data.

In section 3.1 we briefly formulate Hayashi's second method of quantification in a generalized way for the convenience to develop the sensitivity analysis. Then in 3.2 we propose a method of sensitivity analysis to evaluate the influence of a single or multiple individuals on the result of analysis, in 3.3 propose summarized measures of the influence on the score, and show a numerical example in 3.4. Finally in 3.5 we discuss some problems such as the accuracy of the numerical computation and the reason why we sometimes observe rotations of the configurations of the scores assigned to the categories.

3.1 Hayashi's second method of quantification

Suppose that we have response patterns of n individuals to

I+1 items as in Table 3.1, where every individual responds to one and only one category of the outside variable and also of each factor item.

Table 3.1 Observations for Hayashi's second method of quantification.

Individual No.	Outside variable				Item 1					Item I				
	1	2	.....	r	1	2	...	c(1)	....	1	2	...	c(I)	
1	✓						✓							✓
2		✓					✓					✓		
⋮														
α			✓					✓				✓		
⋮														
n		✓					✓							✓

To represent such qualitative observations we introduce the following dummy variables.

$$(3.1)\qquad z_\alpha(i) = \begin{cases} 1, & \text{if the individual } \alpha \text{ responds to the i-th} \\ & \text{category of the outside variable.} \\ 0, & \text{otherwise.} \end{cases}$$

$$(3.2)\qquad x_\alpha(kl) = \begin{cases} 1, & \text{if the individual } \alpha \text{ responds to the l-th} \\ & \text{category of the k-th factor item.} \\ 0, & \text{otherwise.} \end{cases}$$

In the second method of quantification the matter of concern is to analyze the relationship between the outside variable and

the factor items and discriminate the categories of the outside variable from the information concerning the factor items. For that purpose numerical scores $\mathbf{s}=(s_{11},\ldots,s_{1c(1)},\ldots,s_{I1},\ldots,s_{Ic(I)})'$ for the categories of I factor items are introduced so that the categories of the outside variable can be discriminated as well as possible by using these scores. The problem is formulated as the canonical discriminant analysis of the dummy variables $\{x_\alpha(kl)\}$. By introducing the scores $\mathbf{t}=(t_1,\ldots,t_r)'$ for the categories of the outside variables it can also be formulated as the canonical correlation analysis between $\{z_\alpha(i)\}$ and $\{x_\alpha(kl)\}$ (cf. Aoyama(1965), Tanaka(1983), Niki(1981)).

Then the optimal scores $\mathbf{t}$ and $\mathbf{s}$ are obtained as the solution to the optimization problem:

Maximize

(3.3) $\quad \mathbf{t}'Z'WX\mathbf{s},$

subject to the constraints

(3.4) $\quad \mathbf{1}_n'WZ\mathbf{t} = \mathbf{1}_n'WXE_j\mathbf{s} = \mathbf{0}, \quad j=1,\ldots,I,$

(3.5) $\quad (1/N)\mathbf{t}'Z'WZ\mathbf{t} = (1/N)\mathbf{s}'X'WX\mathbf{s} = 1,$

where Z and X are defined as n×r and n×c matrices ($c=\Sigma_j c(j)$), such as

(3.6) $\quad Z = (z_\alpha(i)), \quad X = (x_\alpha(kl)),$

respectively. The matrices W, E_j, and $\mathbf{1}_n$ are defined as follows.

(3.7)
$$\begin{cases} W = \mathrm{diag}(w_1,w_2,\ldots,w_n) : n\times n, \\ E_j = \mathrm{diag}(\underbrace{0,\ldots,0}_{c(1)+\ldots+c(j-1)}, \underbrace{1,\ldots,1}_{c(j)}, \underbrace{0,\ldots,0}_{c(j+1)+\ldots+c(I)}) : c\times c, \quad j=1,\ldots,I, \\ \mathbf{1}_n = (1,1,\ldots,1)' : n\times 1, \end{cases}$$

where $\{w_\alpha\}$ are the weights for the individuals which we

introduced for the convenience to develop the sensitivity analysis. A scalar variable N is given by the summation of w_α's for n individuals. The two constraints (3.4) and (3.5) indicate that the scores should have zero means and unit variances.

Some calculations by using Lagrange multipliers lead to the following two eigenvalue problems.

(3.8) $\quad Z'WX(X'WX)^{-}X'WZ\mathbf{t} - \rho^2 Z'WZ\mathbf{t} = \mathbf{0}$,

(3.9) $\quad X'WZ(Z'WZ)^{-}Z'WX\mathbf{s} - \rho^2 X'WX\mathbf{s} = \mathbf{0}$.

Since the dimension of **t** is generally smaller than that of **s**, it may be better to solve the former than the latter and then calculate **s** by substituting the obtained eigenvector **t** into the equation

(3.10) $\quad \mathbf{s} = (1/\rho)(X'WX)^{-}X'WZ\mathbf{t}$.

We can easily verify that the eigenvalue problem (3.8) has a trivial eigenvalue $\rho^2=1$ and the associated eigenvector $\mathbf{t}=\mathbf{1}_r$, and then each eigenvector associated with $\rho^2\neq 1$ satisfies the first equation of (3.4) from the orthogonality of eigenvectors. Similarly the eigenvalue problem (3.9) has also an eigenvalue $\rho^2=1$ (with multiplicity I) and the associated eigenvectors $\mathbf{s}=E_j\mathbf{1}_c$, $j=1,\ldots,I$. However, we should use (3.10) and the constraint (3.4) to get **s**'s actually.

The eigenvalue $\rho^2(\neq 1)$ is equal to the squared canonical correlation coefficient and also correlation ratio when the elements of the associated eigenvectors **s** (and **t**) are used as the scores for the categories. Therefore, we should pick up the largest q eigenvalues excepting $\rho^2=1$ and use the associated eigenvectors **t**'s and **s**'s as the q-dimensional scores for the

categories of the outside variable and the factor items, respectively, where q is the number of dimensions of interest.

Note that the matrix $W^{1/2}X(X'WX)^{-}X'W^{1/2}$ in (3.8) is uniquely determined for different definitions of g-inverse and we may use any $(X'WX)^{-}$ which is easy to calculate. Generally the rank of X'WX is c-I+1, because the sum of the columns of $W^{1/2}X$ corresponding to the categories of any specified item is equal to the constant vector $\{w_{\alpha}^{1/2}\}$. Let X* be an n×(c-I+1) matrix which is made from X by omitting every last category of each item except for the first item, then X* is, in general, of full column rank. We may use $X^*(X^{*\prime}WX^*)^{-1}X^{*\prime}$ instead of $X(X'WX)^{-}X'$ in (3.8). Let the covariance matrices of the dummy variables $\{z_{\alpha}(i)\}$ and $\{x_{\alpha}(kl)\}$ be

$$S_{11} = (1/N)Z'WZ, \tag{3.11}$$

$$S_{12} = (1/N)Z'WX, \qquad S_{12}^{*} = (1/N)Z'WX^*, \tag{3.12}$$

$$S_{21} = (1/N)X'WX, \qquad S_{22}^{*} = (1/N)X^{*\prime}WX^*, \tag{3.13}$$

then, note that S_{11} is diagonal, we obtain the following ordinary eigenvalue problem

$$\mathbf{Hu} - \theta\mathbf{u} = \mathbf{0}\ , \tag{3.14}$$

where

$$H = S_{11}^{-1/2}S_{12}^{*}S_{22}^{*-1}S_{21}^{*}S_{11}^{-1/2}, \tag{3.15}$$

$$\mathbf{u} = S_{11}^{1/2}\mathbf{t}, \tag{3.16}$$

$$\theta = \rho^2. \tag{3.17}$$

The matrix $S_{11}^{1/2}$ indicates a diagonal matrix, each element of which is given by the square root of the corresponding element of S_{11}, and $S_{11}^{-1/2}$ is its inverse. If an eigenvector **u** is normalized to satisfy **u'u**=1, the corresponding score vector satisfies $\mathbf{t}'S_{11}\mathbf{t}$

=1, i.e. the variance of $\{t'z_\alpha\}$ is equal to 1. Throughout this chapter we use the symbol (*) to express the omission of every last category of each item except for the first item as in the case of X*.

3.2 Sensitivity analysis

3.2.1 Basic idea of sensitivity analysis

In order to evaluate the influence of a single or multiple individuals we change the weights for individuals slightly and investigate how the result of analysis changes.

First consider the influence of a single individual α.

Let the weight for the individuals be

$$(3.18) \qquad w_{\alpha'} = \begin{cases} 1-\varepsilon, & \alpha'=\alpha \ , \\ 1 \ , & \alpha'\neq\alpha \ . \end{cases}$$

Then the covariance matrices of the dummy variables $\{S_{jk}(\varepsilon), j,k=1,2\}$ can be expanded as

$$(3.19) \qquad S_{jk}(\varepsilon) = S_{jk}+(\varepsilon/n)S_{jk}^{(1)}+(\varepsilon/n)^2S_{jk}^{(2)}+O((\varepsilon/n)^3), \quad j,k=1,2,$$

where the matrices S_{jk}'s indicate the values of $S_{jk}(\varepsilon)$'s calculated by putting $\varepsilon=0$, and the matrices $S_{jk}^{(1)}$'s and $S_{jk}^{(2)}$'s are given by

$$(3.20) \qquad \begin{cases} S_{11}^{(1)} = S_{11}^{(2)} = S_{11} - z_\alpha z_\alpha', \\ S_{12}^{(1)} = S_{12}^{(2)} = S_{12} - z_\alpha x_\alpha', \\ S_{22}^{(1)} = S_{22}^{(2)} = S_{22} - x_\alpha x_\alpha'. \end{cases}$$

Now, in the case when we wish to evaluate the influence of a single individual we put

$$\tilde{\varepsilon} = \varepsilon/n. \tag{3.21}$$

Then the expansion (3.19) is simply expressed as

$$S_{jk}(\tilde{\varepsilon}) = S_{jk} + \tilde{\varepsilon}S_{jk}^{(1)} + \tilde{\varepsilon}^2 S_{jk}^{(2)} + O(\tilde{\varepsilon}^3). \tag{3.22}$$

The matrix $H(\tilde{\varepsilon})$ defined by (3.15) can be expanded as

$$\begin{aligned} H(\tilde{\varepsilon}) &= S_{11}^{-1/2}(\tilde{\varepsilon})S_{12}^{*}(\tilde{\varepsilon})S_{22}^{*-1}(\tilde{\varepsilon})S_{21}^{*}(\tilde{\varepsilon})S_{11}^{-1/2}(\tilde{\varepsilon}) \\ &= H + \tilde{\varepsilon}H^{(1)} + \tilde{\varepsilon}^2 H^{(2)} + O(\tilde{\varepsilon}^3), \end{aligned} \tag{3.23}$$

where

$$\begin{cases} H = A'BA, \\ H^{(1)} = A^{(1)'}BA + A'B^{(1)}A + A'BA^{(1)}, \\ H^{(2)} = A^{(2)'}BA + A'B^{(2)}A + A'BA^{(2)}, \\ \qquad + 2A^{(1)'}B^{(1)}A + 2A^{(1)'}BA^{(1)} + 2A'B^{(1)}A^{(1)}, \end{cases} \tag{3.24}$$

$$\begin{cases} A = S_{21}^{*}S_{11}^{-1/2}, \\ A^{(1)} = S_{21}^{*(1)}S_{11}^{-1/2} - (1/2)S_{21}^{*}S_{11}^{-3/2}S_{11}^{(1)}, \\ A^{(2)} = S_{21}^{*(2)}S_{11}^{-1/2} - S_{21}^{*(1)}S_{11}^{-3/2}S_{11}^{(1)} \\ \qquad + (3/4)S_{21}^{*}S_{11}^{-5/2}(S_{11}^{(1)})^2 - (1/2)S_{21}^{*}S_{11}^{-3/2}S_{11}^{(2)}, \\ B = S_{22}^{*-1}, \\ B^{(1)} = -S_{22}^{*-1}S_{22}^{*(1)}S_{22}^{*-1}, \\ B^{(2)} = -B^{(1)}S_{22}^{*(1)}S_{22}^{*-1} - S_{22}^{*-1}S_{22}^{*(2)}S_{22}^{*-1} - S_{22}^{*-1}S_{22}^{*(1)}B^{(1)}. \end{cases} \tag{3.25}$$

In the above we showed that how the eigenvalue problem changed when the weight for a specified single individual was slightly changed from 1 to $1-\varepsilon$. Next we consider the case when we wish to evaluate the influence of multiple individuals.

Let M be a set of m individuals and let the weights for the individuals be

$$(3.26)\qquad w_\alpha = \begin{cases} 1-\varepsilon, & \alpha\in M, \\ 1, & \alpha\notin M. \end{cases}$$

Then the covariance matrices of the dummy variables $\{S_{jk}(\varepsilon),\ j,k=1,2\}$ can be expanded as

$$(3.27)\qquad S_{jk}(\varepsilon) = S_{jk} + (m\varepsilon/n)S_{jk}^{(1)} + (m\varepsilon/n)^2 S_{jk}^{(2)} + O((m\varepsilon/n)^3),$$

where S_{jk}'s indicate the values of $S_{jk}(\varepsilon)$'s calculated by putting $\varepsilon=0$, and the matrices $S_{jk}^{(1)}$'s and $S_{jk}^{(2)}$'s are given by

$$(3.28)\qquad S_{11}^{(1)} = S_{11}^{(2)} = S_{11} - (1/m)\sum_{k\in M} z_k z_k',$$

$$(3.29)\qquad S_{12}^{(1)} = S_{12}^{(2)} = S_{12} - (1/m)\sum_{k\in M} z_k x_k',$$

$$(3.30)\qquad S_{22}^{(1)} = S_{22}^{(2)} = S_{22} - (1/m)\sum_{k\in M} x_k x_k'.$$

In the case when we wish to evaluate the influence of multiple individuals we put

$$(3.31)\qquad \tilde{\varepsilon} = m\varepsilon/n\ .$$

Then the expansion (3.27) is also written as (3.22). Therefore we obtain the same form of expansion (3.23) - (3.25), though the definitions of $S_{jk}^{(1)}$'s are different from the case of a single individual.

Note that, if we consider up to the first order, the first derivatives $S_{jk}^{(1)}$'s ($S_{jk}^{*(1)}$'s) and $H^{(1)}$ for a set M of m individuals are equal to the averages of those for each single individual belonging to the set M. Utilizing such relations we can easily calculate the values which appear in the following two sections for multiple individuals from those for a single individual.

3.2.2 The influence on the product and sum of eigenvalues

The eigenvalues θ's (or ρ^2's) are equal to the squared correlation coefficients or the correlation ratios when the elements of associated eigenvectors **s**'s (and **t**'s) are used as the scores for the categories of I items (and the outside variables). Therefore we can use the product $\prod_{j=1}^{r-1} \theta_j$, the sum $\sum_{j=1}^{r-1} \theta_j$ or other functions of the eigenvalues as a measure to show the degree to which the differences among the categories of the outside variable are expressed in the r-1 dimensional space. Let us evaluate the influence of a small change of $\tilde{\varepsilon}$ by the differential coefficients as follows.

$$(3.32)\quad \frac{d}{d\varepsilon}\left(\prod_{j=1}^{r-1} \theta_j(\varepsilon)\right)\Big|_{\varepsilon=0} = \frac{d}{d\varepsilon}(|H(\varepsilon)|)\Big|_{\varepsilon=0}$$

$$= |H|\,\mathrm{tr}(H^{-1}H^{(1)}),$$

$$(3.33)\quad \frac{d}{d\varepsilon}\left(\sum_{j=1}^{r-1} \theta_j(\varepsilon)\right)\Big|_{\varepsilon=0} = \frac{d}{d\varepsilon}\mathrm{tr}(H(\varepsilon))\Big|_{\varepsilon=0}$$

$$= \mathrm{tr}(H^{(1)}).$$

3.2.3 The influence on the eigenvalues and the scores for categories

(i) The case when the eigenvalue of interest is simple

Suppose that the eigenvalue of interest θ_s of the eigenvalue problem (3.14) except for $\theta=1$ is simple.

Then we can use Lemma 1 in Chapter 2, and obtain the following power series expansion of the eigenvalue $\theta_s(\tilde{\varepsilon})$ and the associated eigenvector $\mathbf{u}_s(\tilde{\varepsilon})$ corresponding to the expansion of

$H(\varepsilon)$ in (3.23).

(3.34) $\theta_s(\tilde{\varepsilon}) = \theta_s + \tilde{\varepsilon}\theta_s^{(1)} + \tilde{\varepsilon}^2\theta_s^{(2)} + O(\tilde{\varepsilon}^3)$,

(3.35) $u_s(\tilde{\varepsilon}) = u_s + \tilde{\varepsilon}u_s^{(1)} + \tilde{\varepsilon}^2u_s^{(2)} + O(\tilde{\varepsilon}^3)$,

where $\theta_s^{(1)}$, $\theta_s^{(2)}$, $u_s^{(1)}$ and $u_s^{(2)}$ are shown in Lemma 1. From the values of $\theta_s(\tilde{\varepsilon})(=\rho_s^2(\tilde{\varepsilon}))$ and $u_s(\tilde{\varepsilon})$ we can calculate $t_s(\tilde{\varepsilon})$ and $s_s(\tilde{\varepsilon})$ by using (3.16) and (3.10), respectively.

(ii) The case when the eigenvalue of interest is multiple

Suppose that the eigenvalue of interest is not simple and that, without loss of generality, we are interested in the eigenvalue $\theta_1=\ldots=\theta_k=\theta$ with multiplicity k.

Now suppose that an unperturbed r×r symmetric matrix H is diagonalizable by multiplying an orthogonal matrix $V=(v_1,\ldots,v_r)$ and its transpose from right and left, i.e.

(3.36) $$V'HV = \begin{pmatrix} \theta_1 & & & 0 \\ & \ddots & & \\ & & \theta_k & \\ & & & \theta_{k+1} \\ 0 & & & & \ddots \\ & & & & & \theta_r \end{pmatrix}.$$

Then we can use Lemma 2-1 and 2-2, and obtain the following expansions.

For small $\tilde{\varepsilon}$ the eigenvalues $\theta_1(\tilde{\varepsilon}),\ldots,\theta_k(\tilde{\varepsilon})$ and the associated eigenvectors $u_1(\tilde{\varepsilon}),\ldots,u_k(\tilde{\varepsilon})$ of the perturbed matrix

(3.37) $H(\tilde{\varepsilon}) = H + \tilde{\varepsilon}H^{(1)} + \tilde{\varepsilon}^2H^{(2)} + \tilde{\varepsilon}^3H^{(3)} + O(\tilde{\varepsilon}^4)$

can be expanded as

(3.38) $\theta_s(\tilde{\varepsilon}) = \theta + \tilde{\varepsilon}\theta_s^{(1)} + \tilde{\varepsilon}^2\theta_s^{(2)} + O(\tilde{\varepsilon}^3)$, $s=1,\ldots,k$,

(3.39) $u_s(\tilde{\varepsilon}) = u_s + \tilde{\varepsilon}u_s^{(1)} + \tilde{\varepsilon}^2u_s^{(2)} + O(\tilde{\varepsilon}^3)$, $s=1,\ldots,k$,

where the coefficient $\theta_s^{(1)}$, $\theta_s^{(2)}$, $u_s^{(1)}$ and $u_s^{(2)}$ are determined by Lemma 2-1 and 2-2 in Chapter 2.

3.3 Summarized measures of the influence on the scores

The influence of a small change of the weights for a single or multiple individuals on the scores is expressed by the differences between the unperturbed scores S (or T) and the perturbed scores $S(\tilde{\varepsilon})$ or $T(\tilde{\varepsilon})$. Considering $q(\leq \min\{r-1, \Sigma_j(c(j)-1)\})$ dimensional scores we may summarize these differences as follows.

(i) Euclidean norm of the differences between the unperturbed and perturbed scores

$$(3.40) \qquad \|S(\tilde{\varepsilon}) - S\| \; / \; \|S\|$$

$$(3.41) \qquad \|T(\tilde{\varepsilon}) - T\| \; / \; \|T\|$$

(ii) Euclidean norm of the differences between the configurations of the unperturbed and perturbed scores

$$(3.42) \qquad \|S(\tilde{\varepsilon})S(\tilde{\varepsilon})' - SS'\| \; / \; \|SS'\|$$

$$(3.43) \qquad \|T(\tilde{\varepsilon})T(\tilde{\varepsilon})' - TT'\| \; / \; \|TT'\|$$

3.4 Numerical example

In order to show the usefulness of the proposed method we shall apply it to a set of artificial data given in Table 3.2.

Table 3.2 Artificial data.

Outside variable	Item 1	2	3	4	5
3	3	3	3	1	3
2	1	3	2	1	3
1	1	1	1	3	3
2	3	2	1	2	1
1	2	1	2	2	2
1	1	1	2	2	2
2	2	3	1	1	1
3	3	1	2	1	1
2	2	2	1	1	2
2	2	2	3	3	1
1	2	1	2	2	3
2	2	2	3	2	3
2	3	1	1	2	1
3	3	3	1	2	1
2	3	1	1	3	2
3	3	3	1	3	3
3	3	3	1	1	1
2	1	2	3	3	2
3	3	2	1	3	2
2	1	3	2	3	3
1	1	2	2	1	2
1	1	1	3	1	2
2	2	3	2	2	3
2	2	3	2	1	2
2	3	2	3	2	3
1	1	1	2	2	1
3	3	2	1	2	1
3	3	2	3	2	2
3	3	3	2	1	2
2	1	3	2	2	2

Outside variable	Item 1	2	3	4	5
2	2	1	2	1	1
3	3	3	1	2	1
2	2	2	2	1	2
1	1	3	2	1	3
3	3	2	3	2	1
2	2	2	1	2	1
3	3	2	1	1	3
3	3	3	2	3	2
3	2	3	2	1	1
1	1	1	1	3	3
1	1	3	2	3	1
1	1	2	2	2	3
3	3	2	3	2	3
2	1	2	3	3	1
3	3	1	2	2	2
2	2	3	2	2	3
3	2	3	3	2	3
2	2	2	1	1	1
3	3	2	3	3	3
3	3	3	3	1	2
3	3	3	3	3	2
3	3	3	2	3	2
1	1	1	3	1	1
1	1	2	1	1	2
1	1	2	1	2	3
2	2	1	3	2	1
2	3	1	3	1	2
3	2	2	3	3	1
3	3	1	2	1	1
1	1	2	1	3	3
1	2	2	3	3	1
3	1	1	1	3	3

These data were generated as follows. First, continuous data were made by using the models such as

Model 1. $y_i = 20x_{1i}+10x_{2i}+5x_{3i}+0x_{4i}-5x_{5i}+5e_i$, $i=1,2,..,60$,

and

Model 2. $y_i=-20x_{1i}-10x_{2i}-5x_{3i}+0x_{4i}+5x_{5i}+5e_i$, $i=61,62$,

where $\{x_{1i},..,x_{5i},e_i\}$ were NID(0,1) random numbers. And then they were transformed into categorical data by the following rules.

$$X_{ji} = \begin{cases} 1, & \text{if } x_{ji} \leq -0.5, \\ 2, & \text{if } -0.5 < x_{ji} \leq 0.5, \\ 3, & \text{if } 0.5 < x_{ji}. \end{cases} \tag{3.44}$$

$$Y_i = \begin{cases} 1, & \text{if } y_i \leq -10, \\ 2, & \text{if } -10 < y_i \leq 10, \\ 3, & \text{if } 10 < y_i. \end{cases} \tag{3.45}$$

Choosing Y as the outside variable and $X_1,..,X_5$ as the factor items we apply Hayashi's second method of quantification to these data.

Since there are 3 categories of the outside variable, we can obtain up to 2 dimensional scores. The eigenvalues (or correlation ratios) are $\rho_1^2=0.66414$ and $\rho_2^2=0.18611$ and their associated eigenvectors give the optimal scores for the categories. The eigenvectors **s** and **t** associated with ρ_1^2 are shown in Table 3.3. Looking at the elements of these eigenvectors (=category scores) we observe that the order of the scores for each item is $1<2<3$ or $1>2>3$ except for those of

Table 3.3 The result of analysis by Hayashi's second method of quantification (Axis 1).

Item NO. 1			
Freq.	Cat.score	Range	Partial cor.
1 : (19)	-1.12237	2.14161	0.31703
2 : (18)	-0.23090		
3 : (25)	1.01924		
Item NO. 2			
Freq.	Cat.score	Range	Partial cor.
1 : (17)	-0.38009	0.78168	0.54635
2 : (24)	-0.08216		
3 : (21)	0.40159		
Item NO. 3			
Freq.	Cat.score	Range	Partial cor.
1 : (21)	-0.08859	0.23675	0.16002
2 : (23)	-0.03507		
3 : (18)	0.14816		
Item NO. 4			
Freq.	Cat.score	Range	Partial cor.
1 : (21)	0.01856	0.34088	0.07997
2 : (23)	-0.15916		
3 : (18)	0.18172		
Item NO. 5			
Freq.	Cat.score	Range	Partial cor.
1 : (22)	0.09163	0.20397	0.05290
2 : (20)	-0.11235		
3 : (20)	0.01156		

Outside variable	
Freq.	Cat.score
1 : (16)	-1.14756
2 : (22)	-0.15130
3 : (24)	0.90373

Eta-squaare (Correlation ratio)

0.66412

the fourth and fifth items. This fact corresponds well to the model(Model 1) used to generate the data.

Next we apply the sensitivity analysis of the first order approximation by setting $\tilde{\varepsilon}=0.3$. Changing α from 1 to 62 we calculate the proposed measures of influence. The results are shown in Table 3.4. From the nature of our model it is obvious that the second axis is not important. It is noted that the individual No.61 and No.62 (which were generated differently from the others) look influential especially with respect to the measures such as $\Sigma_j \rho_j^2$ and ρ_1^2 for which the first axis plays important roles. Actually, if we omit the individual No.61 or 62, the largest eigenvalue becomes $\rho_1^2=0.70130$ or $\rho_1^2=0.75931$, either of which is much larger than the original value $\rho_1^2=0.66414$.

3.5 Discussion

We proposed a method to evaluate how the result of Hayashi's second method of quantification changes when the weight for a single or multiple individuals changes.

In the above example we evaluated the proposed measures of influence of each individual by applying simple differentiation and the perturbation theory of eigenvalue problems. The fact that the individuals No. 61 and No. 62 are influential was found particularly by the measures $\frac{d}{d\varepsilon}\sum_i \theta_i$ and $\theta_i^{(1)}$. Note that the former was obtained without using the perturbation theory of

Tabel 3.4 The result of sensitivity analysis.

No	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)
1	-0.1888	-0.8811	-0.8292	-0.0519	0.0413	0.0306	0.0615	0.0472
2	1.0306	1.8762	0.4507	1.4256	0.0547	0.0322	0.0774	0.0457
3	-0.5546	-1.1608	-0.4525	-0.7083	0.0375	0.0250	0.0590	0.0385
4	0.5618	1.1970	0.4878	0.7092	0.0387	0.0345	0.0562	0.0511
5	0.9960	1.5498	0.0696	1.4802	0.0303	0.0291	0.0430	0.0456
6	-0.4988	-1.2837	-0.7399	-0.5438	0.0396	0.0281	0.0709	0.0422
7	-0.8376	-1.2927	-0.0436	-1.2491	0.0379	0.0230	0.0545	0.0352
8	-0.2416	-0.4775	-0.1581	-0.3195	0.1162	0.0325	0.1641	0.0494
9	-0.9715	-1.3786	0.1171	-1.4957	0.0680	0.0131	0.0963	0.0221
10	-0.7492	-1.1889	-0.0844	-1.1045	0.0329	0.0215	0.0484	0.0332
11	0.6499	1.1151	0.1896	0.9254	0.0386	0.0289	0.0552	0.0454
12	-0.7430	-1.0904	0.0395	-1.1299	0.0356	0.0124	0.0510	0.0211
13	0.9168	1.7142	0.4637	1.2506	0.0291	0.0222	0.0436	0.0342
14	-0.0423	-0.5376	-0.6583	0.1208	0.0583	0.0250	0.0871	0.0409
15	1.0306	2.0169	0.6461	1.3708	0.0407	0.0299	0.0581	0.0446
16	-0.1945	-0.8065	-0.7137	-0.0928	0.0383	0.0282	0.0604	0.0444
17	-0.1088	-0.7845	-0.8624	0.0779	0.0532	0.0276	0.0792	0.0438
18	0.5653	1.2892	0.6085	0.6806	0.0563	0.0364	0.0798	0.0515
19	-0.0229	-0.3230	-0.4009	0.0778	0.0604	0.0207	0.0865	0.0368
20	1.2095	2.0778	0.3564	1.7214	0.0423	0.0255	0.0602	0.0364
21	-0.1820	-0.5158	-0.3359	-0.1799	0.0391	0.0242	0.0620	0.0379
22	-0.2813	-0.7633	-0.4720	-0.2913	0.0388	0.0246	0.0599	0.0381
23	-0.4883	-0.7064	0.0401	-0.7464	0.0317	0.0156	0.0469	0.0253
24	-0.7097	-1.0505	0.0253	-1.0758	0.0394	0.0180	0.0574	0.0285
25	0.8531	1.7977	0.7129	1.0848	0.0550	0.0421	0.0782	0.0616
26	-0.6026	-1.2957	-0.5396	-0.7561	0.0387	0.0260	0.0659	0.0395
27	0.0020	-0.2606	-0.3663	0.1057	0.0671	0.0204	0.0956	0.0366
28	0.0900	-0.0690	-0.2842	0.2152	0.0670	0.0196	0.0957	0.0359
29	-0.1330	-0.6895	-0.6797	-0.0097	0.0482	0.0275	0.0687	0.0437
30	0.5817	1.2978	0.5862	0.7116	0.0656	0.0372	0.0936	0.0526
31	-0.2547	-0.2156	0.2333	-0.4489	0.0678	0.0092	0.0973	0.0159
32	-0.0423	-0.5376	-0.6583	0.1208	0.0583	0.0250	0.0871	0.0409
33	-0.7199	-1.0407	0.0601	-1.1009	0.0602	0.0110	0.0859	0.0193
34	-0.3369	-0.2923	0.2986	-0.5910	0.0449	0.0257	0.0638	0.0407
35	-0.0436	-0.5007	-0.6045	0.1037	0.0655	0.0232	0.0931	0.0392
36	-0.8967	-1.2958	0.0755	-1.3713	0.0485	0.0122	0.0685	0.0209
37	-0.1232	-0.5565	-0.5153	-0.0412	0.0740	0.0231	0.1045	0.0390
38	-0.1732	-0.7330	-0.6561	-0.0769	0.0414	0.0289	0.0604	0.0453
39	0.8326	1.3998	0.2031	1.1967	0.1086	0.0381	0.1539	0.0613
40	-0.5546	-1.1608	-0.4525	-0.7083	0.0375	0.0250	0.0590	0.0385

Tabel 3.4 (Continued)

No	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)
41	-0.2303	0.1406	0.6772	-0.5366	0.0732	0.0283	0.1034	0.0445
42	-0.4004	-0.9013	-0.4146	-0.4867	0.0412	0.0244	0.0666	0.0380
43	-0.0989	-0.4885	-0.4717	-0.0167	0.0518	0.0237	0.0732	0.0396
44	0.6851	1.3855	0.4918	0.8937	0.0602	0.0320	0.0851	0.0453
45	-0.0278	0.3190	0.5012	-0.1823	0.0901	0.0244	0.1277	0.0404
46	-0.4883	-0.7064	0.0401	-0.7464	0.0317	0.0156	0.0469	0.0253
47	0.9464	1.8019	0.5236	1.2782	0.1363	0.0426	0.1929	0.0672
48	-0.8695	-1.3733	-0.0890	-1.2842	0.0501	0.0162	0.0710	0.0261
49	-0.2087	-0.8511	-0.7459	-0.1051	0.0431	0.0274	0.0612	0.0436
50	0.0119	-0.4218	-0.6108	0.1890	0.0627	0.0232	0.0934	0.0392
51	-0.0583	-0.5538	-0.6475	0.0937	0.0372	0.0288	0.0593	0.0452
52	-0.1732	-0.7330	-0.6561	-0.0769	0.0414	0.0289	0.0604	0.0453
53	-0.3857	-0.7475	-0.2316	-0.5159	0.0402	0.0242	0.0594	0.0380
54	0.0644	-0.1804	-0.3855	0.2051	0.0318	0.0242	0.0499	0.0380
55	-0.1814	-0.6079	-0.4651	-0.1428	0.0314	0.0243	0.0510	0.0379
56	-0.5363	-0.5977	0.2915	-0.8892	0.0521	0.0081	0.0737	0.0150
57	0.8289	1.7285	0.6674	1.0611	0.0350	0.0294	0.0526	0.0440
58	0.9176	1.7276	0.4806	1.2469	0.1173	0.0468	0.1657	0.0727
59	-0.2416	-0.4775	-0.1581	-0.3195	0.1162	0.0325	0.1641	0.0494
60	-0.2538	-0.4985	-0.1616	-0.3369	0.0393	0.0244	0.0588	0.0385
61	1.4752	3.2474	1.4257	1.8217	0.0849	0.0565	0.1226	0.0853
62	0.6005	4.3460	4.7818	-0.4358	0.1500	0.0219	0.2157	0.0379

Notes.

1) The measures are (1)$\frac{d}{d\varepsilon}(\prod_j \rho_j^2)$, (2)$\frac{d}{d\varepsilon}(\sum_j \rho_j^2)$, (3)$\frac{d}{d\varepsilon}\rho_1^2$, (4)$\frac{d}{d\varepsilon}\rho_2^2$, (5)$\|S(\varepsilon)-S\|/\|S\|$, (6)$\|T(\varepsilon)-T\|/\|T\|$, (7)$\|S(\varepsilon)S(\varepsilon)'-SS'\|/\|SS'\|$, (8)$\|T(\varepsilon)T(\varepsilon)'-TT'\|/\|TT'\|$.

2) The measures (5)~(8) are calculated by using unidimensional score (i.e. q=1).

eigenvalue problems. Therefore, if there are so many individuals that it is practically difficult to apply the perturbation theory n times, we may first select influential individuals roughly by the former measure and then investigate the precise influence of the selected individuals by the other measures.

Since $\tilde{\varepsilon}=\varepsilon/n$, the result for $\tilde{\varepsilon}=1/n$ (i.e. $\varepsilon=1$) just corresponds to the omission of a specified individual. To show the degree of approximation we compare the eigenvalues calculated by the perturbation method and the exact method. When we put $\tilde{\varepsilon}=1/62$ for the individual No. 1 and apply the perturbation theory of first order of $\tilde{\varepsilon}$, the relative errors of the two largest eigenvalues $|\theta_{asy}(\tilde{\varepsilon})-\theta_{exact}(\tilde{\varepsilon})|/\theta_{exact}(\tilde{\varepsilon})$ are 0.011 and 0.008, respectively. If the accuracy is not satisfactory, we must consider the order of $\tilde{\varepsilon}^2$ or more.

In our example the difference between the two eigenvalues is not small. However, in general if there exist some eigenvalues which are close to each other, the approximation becomes poor because of the terms $1/(\theta_s-\theta_i)$ in the second orders of the eigenvalues and the first and second orders of the eigenvectors. If $\theta_s\tilde{=}\theta_i$, the absolute value of $\{u_{js}^{(1)}\}$ and then the norm of $\{u_{js}+\tilde{\varepsilon}u_{js}^{(1)}\}$ become very large, though the constraints on the norms of eigenvectors are included in the formulation. In such cases we should use the perturbation theory under the assumption of multiple eigenvalues rather than under the assumption of simple eigenvalues. We shall discuss such computational problems in Chapter 5.

We usually express the scores t's and s's graphically in a

low dimensional vector space to grasp the relationship among the categories. In such figures we sometimes observe the phenomena that rotations occur also in the second method of quantification as shown in Tanaka(1984b) in the case of the third method. Such phenomena can be explained mathematically as follows.

When we assume simple eigenvalues, the scores $t(\tilde{\varepsilon})$'s calculated include the terms of $1/(\theta_s-\theta_i)$, $s\neq i$ in

$$u_{js}^{(1)} = \sum_{i\neq s} u_{ji}u_s'H^{(1)}u_i/(\theta_s-\theta_i).$$

If there exists a pair (θ_s,θ_i) such that $\theta_s\tilde{=}\theta_i$ among the eigenvalues of interest (i.e. $s,i\leq q$), the absolute values of $u_{js}^{(1)}$'s tend to be large as already mentioned. Then the coordinates of $\mathbf{t}(\tilde{\varepsilon})$ (or $\mathbf{s}(\tilde{\varepsilon})$) in the q-dimensional space move much from $\mathbf{t}$ (or $\mathbf{s}$).

Now let us consider the change of the configuration of $\mathbf{t}$'s (or $\mathbf{s}$'s). The (i,i)-th diagonal element of TT' indicates the squared Euclidean distance from the centroid to the i-th category and the (i,i')-th off diagonal element indicates the inner product of the two vectors from the centroid to the i-th and i'-th categories. Hence we can measure the change of the mutual relationship among the categories with some functions of $T(\tilde{\varepsilon})T(\tilde{\varepsilon})'-TT'$. This matrix can be rewritten as follows.

$$\begin{aligned} T(\tilde{\varepsilon})T(\tilde{\varepsilon})'-TT' &= \tilde{\varepsilon}(T^{(1)}T'+TT^{(1)}') + O(\tilde{\varepsilon}^2) \\ &= \tilde{\varepsilon}\{(S^{-1/2})^{(1)}UU'S^{-1/2}+S^{-1/2}UU'(S^{-1/2})^{(1)} \\ &\quad +S^{-1/2}(U^{(1)}U'+UU^{(1)}')S^{-1/2}\} + O(\tilde{\varepsilon}^2) \end{aligned}$$

In the expression of the right hand side only $U^{(1)}U'+UU^{(1)}'$ includes the terms $1/(\theta_s-\theta_i)$, $s\neq i$. However, it can be expressed by

$$U^{(1)}U'+UU^{(1)}',$$

$$= \sum_{s=1}^{q} \sum_{i>q} \{u_s u_i' H^{(1)} u_s u_i' + u_i u_s' H^{(1)} u_i u_s'\}/(\theta_s - \theta_i).$$

Notice that the right hand side does not include the terms $1/(\theta_s - \theta_i)$ for $1 \leq s, i \leq q$. Therefore, even if there are some pairs (s,i)'s such that $\theta_s \tilde{=} \theta_i$ among the eigenvalues of interest, the change of the configuration measured with $T(\tilde{\varepsilon})T(\tilde{\varepsilon})'-TT'$ is not large unless the smallest difference between the eigenvalues of interest and the remaining is not very small. Thus, when there are some close pairs (θ_s, θ_i) among the eigenvalues of interest $\{\theta_1, \ldots, \theta_q\}$ but the eigenvalues of interest are far from the remaining eigenvalues, it is expected that the change of the coordinates is large but the change of the mutual relationship among the categories is small. This means a rotation. When we assume multiple eigenvalues, the transformation from $(v_1, \ldots, v_k)$ to $(u_1, \ldots, u_k)$ suggests the same property.

As the number of individuals increase, the influence of each one individual decreases and the main concern becomes to detect influential sets of individuals. For investigation of the influence of multiple individuals it may not be practical to consider all possible combinations of individuals. But fortunately the first derivatives $H^{(1)}$, $U^{(1)}$, $T^{(1)}$ and $S^{(1)}$ for a set of individuals are equal to the summations of the corresponding derivatives for each individual belonging to the set. So the influence of a set of the individuals which have similar $T^{(1)}$ and/or $S^{(1)}$ values becomes large. To collect such individuals cluster analysis may be useful.

4 Sensitivity Analysis in Descriptive Multivariate Methods

As shown in Greenacre(1984) and Greenacre and Underhill (1982), a number of descriptive multivariate methods including the quantification methods (and correspondence analysis) are formulated by using the generalized singular value decomposition (GSVD). Since the GSVD leads to an eigenvalue problem, a unified method of sensitivity analysis can be constructed by using the perturbation theory of eigenvalue problems.

First in 4.2 we briefly explain a unified formulation of various descriptive methods based on the GSVD, which was discussed in Greenacre(1984). Then we develop a sensitivity analysis procedure of the generalized analysis to evaluate the influence of a small change of input data on the singular values, singular vectors and the corresponding row and/or column profiles by using the perturbation theory of eigenvalue problems.

We introduce several measures for the amount of influence. Numerical examples are shown to illustrate the usefulness of the proposed method, and finally discussion and summary are given.

4.1 Unified formulation of multivariate methods by the generalized singular value decomposition

Generalized singular value decomposition(GSVD): Suppose that A is a matrix of order n×p and of rank K and that Ω and Φ are positive definite matrices of order n×n and p×p, respectively. Then A can be decomposed as

$$(4.1) \quad A = ND_\alpha M' = \sum_{k=1}^{K} \alpha_k \mathbf{n}_k \mathbf{m}_k',$$

where

$$(4.2) \quad N'\Omega N = I, \quad M'\Phi M = I, \quad D_\alpha = \mathrm{diag}[\alpha_1, \ldots, \alpha_K],$$
$$N = [\mathbf{n}_1, \ldots, \mathbf{n}_K], \quad M = [\mathbf{m}_1, \ldots, \mathbf{m}_K].$$

It is known that the following general analysis procedure based on the GSVD includes various multivariate methods as special cases (Greenacre(1984)).

General analysis procedure

1) Transform the data matrix Y to the matrix A by preprocessing of some type of centering.
2) Apply the GSVD to the matrix A for given Ω and Φ and obtain the singular values $\{\alpha_k\}$ and the left and right singular vectors $\{\mathbf{n}_k\}$ and $\{\mathbf{m}_k\}$.
3) Compute the scores for rows and columns by

$$(4.3) \quad F = N_{(L)} D^a_{\alpha(L)}, \quad G = M_{(L)} D^b_{\alpha(L)},$$

where the matrices with the subscript (L) indicate the submatrices of L columns of the full matrices.

The methods such as principal component analysis, biplot, canonical correlation analysis, Hayashi's second and third methods of quantification and correspondence analysis are treated as special cases of the above general procedure with appropriate A, Ω, Φ, a and b. Here as a matter of convenience to develop sensitivity analysis we shall formulate those multivariate methods in somewhat generalized manner introducing weights for individuals. The result are summarized in Table 4.1.

Let the Cholesky decomposition of a positive definite matrix Ω (or Φ) be

(4.4) $\Omega = (\Omega^{1/2})(\Omega^{1/2})^T$,

or

(4.4)' $\Phi = (\Phi^{1/2})(\Phi^{1/2})^T$,

where $\Omega^{1/2}$ (or $\Phi^{1/2}$) is a lower triangular matrix and $\Omega^{-1/2}$ (or $\Phi^{-1/2}$) is its inverse. Then the generalized SVD problem is transformed into the following ordinary SVD problem.

(4.5) $B = UD_\alpha V^T$,

where

(4.6) $B = (\Omega^{1/2})^T A \Phi^{1/2}$,

(4.7) $U^TU = I, \quad V^TV = I.$

The matrices N and M are calculated as

(4.8) $N = (\Omega^{-1/2})^T U$,

(4.9) $M = (\Phi^{-1/2})^T V$.

From this ordinary SVD problem we obtain an eigenvalue problem such as

Table 4.1 Multivariate methods formulated by the generalized singular value decomposition.

Method	Transformed matrix A	Ω	Φ	a	b	Note
(1)Principal component analysis	$Y-\mathbf{1}\mathbf{1}^T D_w Y/\bar{n}$	$D_w/\bar{n}$	I	1	0	$D_w=\mathrm{diag}(w_1,\ldots,w_n)$ indicates weights for rows. $\bar{n}=\Sigma_k w_k$
(2)Biplot (Type 1)	$Y-\mathbf{1}\mathbf{1}^T D_w Y/\bar{n}$	$D_w/\bar{n}$	I	1	0	$\mathbf{1}=(1,\ldots,1)^T$
(Type 2 Covariance biplot)	〃	〃	〃	0	1	
(Type 3 Symmetric biplot)	〃	〃	〃	1/2	1/2	
(3)Quantification Ⅱ	$D_r^{-1}YD_c(\mathbf{w})^{-1}$	D_rD_w	$D_c(\mathbf{w})$	0	0	Y:data matrix $D_r=\mathrm{diag}(Y\mathbf{1})$ $D_c(\mathbf{w})=\mathrm{diag}(Y^TD_w\mathbf{1})$
(4)Correspondence analysis	$D_r^{-1}YD_c(\mathbf{w})^{-1}$	D_rD_w	$D_c(\mathbf{w})$	1	1	
(5)Canonical correlation analysis (Also, canonical discriminant analysis, Quantification Ⅱ)	$S_{11}^{-1}(\mathbf{w})S_{12}(\mathbf{w})S_{22}^{-1}(\mathbf{w})$	$S_{11}(\mathbf{w})$	$S_{22}(\mathbf{w})$	1	1	$S_{jk}(\mathbf{w})$:sample covariance matrix

(4.10) $H = VD_\alpha^2 V^T$,

where

(4.11) $H = (\Phi^{1/2})^T A^T \Omega A \Phi^{1/2}$.

Thus, to perform the general analysis procedure we should first solve the eigenvalue problem (4.10) and obtain the eigenvalues D_α^2 and eigenvectors (or the right singular vectors) V. Then after calculating U by the relation

(4.12) $U = BVD_\alpha^{-1}$,

we can get the coordinates F and G by the following equations.

(4.13) $F = (\Omega^{-1/2})^T U_{(L)} D_{\alpha(L)}^a$,

(4.14) $G = (\Phi^{-1/2})^T V_{(L)} D_{\alpha(L)}^b$.

4.2 Sensitivity analysis

4.2.0 Basic idea of sensitivity analysis

Here we consider to evaluate the influence of a small change of the input data to the result of analysis. Though we can treat various types of change, we discuss mainly the influence of the change of weights for a single or multiple individuals.

Let the weights for the individuals be

(4.15) $w_k = \begin{cases} 1-\varepsilon, & k=i, \\ 1 & k\neq i, \end{cases}$ (single individual case)

or

(4.16) $w_k = \begin{cases} 1-\varepsilon, & k\in I, \\ 1 & k\notin I, \end{cases}$ (multiple individual case)

where i and I are a specified individual and a specified set of

individuals, respectively. Then the matrix H in (4.11) can be expressed as a power series of ε as follows by Taylor expansion.

(4.17) $H(\varepsilon) = H + \varepsilon H^{(1)} + \varepsilon^2 H^{(2)} + O(\varepsilon^3)$,

where H is the value of $H(\varepsilon)$ for $\varepsilon=0$ and the matrices $H^{(1)}$ and $H^{(2)}$ can be easily calculated for each multivariate method.

When ε varies slightly, the matrix $H(\varepsilon)$ varies according to the expression (4.17). The problem is to evaluate efficiently how the eigenvalues D_α^2, the eigenvectors V and also the coordinates G and/or F vary correspondingly. Our basic idea is as follows. First calculate the change of the matrix H. Next evaluate the change of D_α^2 and V based on the perturbation theory of eigenvalue problems. Then obtain the change of the intermediate quantities U, N, M and finally the coordinates F, G by Taylor expansion.

4.2.1 Perturbation of the eigenvalues and the associated eigenvectors

It is known that, when the matrix $H(\varepsilon)=(h_{jj'}(\varepsilon))$ is expanded in a power series convergent in a neighborhood of $\varepsilon=0$, there exist power series of the eigenvalues $\theta_s(\varepsilon)$'s and the eigenvectors $\mathbf{v}_s(\varepsilon)$'s all convergent in a neighborhood of $\varepsilon=0$.

(4.18) $\theta_s(\varepsilon) = \theta_s + \varepsilon\theta_s^{(1)} + \varepsilon^2\theta_s^{(2)} + O(\varepsilon^3)$, $s=1,\ldots,K$.

(4.19) $\mathbf{v}_s(\varepsilon) = \mathbf{v}_s + \varepsilon\mathbf{v}_s^{(1)} + \varepsilon^2\mathbf{v}_s^{(2)} + O(\varepsilon^3)$, $s=1,\ldots,K$.

K denoting the number of dimensions of interest. The coefficients $\theta_s^{(1)}$, $\theta_s^{(2)}$, $\mathbf{v}_s^{(1)}$ and $\mathbf{v}_s^{(2)}$ are obtained by the lemmas in Chapter 2.

4.2.2 Perturbation of the singular values and the singular vectors

The singular values $\alpha_s(\varepsilon)$, the left singular vectors $N(\varepsilon)$ and the right singular vectors $M(\varepsilon)$ are expressed by using the Taylor series expansions as follows.

$$\alpha_s(\varepsilon) = \alpha_s + \varepsilon\alpha_s^{(1)} + \varepsilon^2\alpha_s^{(2)} + O(\varepsilon^3), \tag{4.20}$$

$$N(\varepsilon) = N + \varepsilon N^{(1)} + \varepsilon^2 N^{(2)} + O(\varepsilon^3), \tag{4.21}$$

$$M(\varepsilon) = M + \varepsilon M^{(1)} + \varepsilon^2 M^{(2)} + O(\varepsilon^3), \tag{4.22}$$

where

$$\begin{cases} \alpha_s = \theta_s^{1/2}, \\ \alpha_s^{(1)} = \theta_s^{(1)}/(2\alpha_s), \\ \alpha_s^{(2)} = \{\theta_s^{(2)}/\alpha_s - (\alpha_s^{(1)})^2/\alpha_s\}/2, \end{cases} \tag{4.23}$$

$$\begin{cases} N^{(1)} = A^{(1)}\Phi^{1/2}VD_\alpha^{-1} + A(\Phi^{1/2})^{(1)}VD_\alpha^{-1} \\ \qquad + A\Phi^{1/2}V^{(1)}D_\alpha^{-1} - A\Phi^{1/2}VD_\alpha^{-1}D_\alpha^{(1)}D_\alpha^{-1}, \\ N^{(2)} = A^{(2)}\Phi^{1/2}VD_\alpha^{-1} + A^{(1)}(\Phi^{1/2})^{(1)}VD_\alpha^{-1} \\ \qquad + A^{(1)}\Phi^{1/2}V^{(1)}D_\alpha^{-1} - A^{(1)}\Phi^{1/2}VD_\alpha^{-1}D_\alpha^{(1)}D_\alpha^{-1} \\ \qquad + A(\Phi^{1/2})^{(2)}VD_\alpha^{-1} + A(\Phi^{1/2})^{(1)}V^{(1)}D_\alpha^{-1} \\ \qquad - A(\Phi^{1/2})^{(1)}VD_\alpha^{-1}D_\alpha^{(1)}D_\alpha^{-1} - A\Phi^{1/2}V^{(1)}D_\alpha^{-1}D_\alpha^{(1)}D_\alpha^{-1} \\ \qquad + A\Phi^{1/2}V^{(2)}D_\alpha^{-1} + A\Phi^{1/2}V(D_\alpha^{-1})^{(2)}, \end{cases} \tag{4.24}$$

$$\begin{cases} M^{(1)} = (\Phi^{-1/2})^{(1)}T_V + (\Phi^{-1/2})T_V^{(1)}, \\ M^{(2)} = (\Phi^{-1/2})^{(2)}T_V + (\Phi^{-1/2})^{(1)}T_V^{(1)} + (\Phi^{-1/2})T_V^{(2)}, \end{cases} \tag{4.25}$$

$$(D_\alpha^{-1})^{(2)} = D_\alpha^{-1}D_\alpha^{(1)}D_\alpha^{-1}D_\alpha^{(1)}D_\alpha^{-1} - D_\alpha^{-1}D_\alpha^{(2)}D_\alpha^{-1}. \tag{4.26}$$

4.2.3 Perturbation of the coordinates of rows and columns

The coordinates $F(\varepsilon)$ and $G(\varepsilon)$ are expanded in power series of ε as follows.

$$F(\varepsilon) = F + \varepsilon F^{(1)} + \varepsilon^2 F^{(2)} + O(\varepsilon^3), \tag{4.27}$$

$$G(\varepsilon) = G + \varepsilon G^{(1)} + \varepsilon^2 G^{(2)} + O(\varepsilon^3), \tag{4.28}$$

where

$$\left\{\begin{aligned}
F &= A\Phi^{1/2}V_{(L)}D_{\alpha(L)}^{a-1}, \\
F^{(1)} &= A^{(1)}\Phi^{1/2}V_{(L)}D_{\alpha(L)}^{a-1} + A(\Phi^{1/2})^{(1)}V_{(L)}D_{\alpha(L)}^{a-1} \\
&\quad + A\Phi^{1/2}V_{(L)}^{\{1\}}D_{\alpha(L)}^{a-1} + (a-1)A\Phi^{1/2}V_{(L)}D_{\alpha(L)}^{a-2}D_{\alpha(L)}^{(1)}, \\
F^{(2)} &= A^{(2)}\Phi^{1/2}V_{(L)}D_{\alpha(L)}^{a-1} + A(\Phi^{1/2})^{(2)}V_{(L)}D_{\alpha(L)}^{a-1} \\
&\quad + A\Phi^{1/2}V_{(L)}^{\{2\}}D_{\alpha(L)}^{a-1} + (a-1)A\Phi^{1/2}V_{(L)}D_{\alpha(L)}^{a-2}D_{\alpha(L)}^{(2)} \\
&\quad + (a-1)(a-2)A\Phi^{1/2}V_{(L)}D_{\alpha(L)}^{a-3}(D_{\alpha(L)}^{(1)})^2 \\
&\quad + 2A^{(1)}(\Phi^{1/2})^{(1)}V_{(L)}D_{\alpha(L)}^{a-1} \\
&\quad + 2A^{(1)}\Phi^{1/2}V_{(L)}^{\{1\}}D_{\alpha(L)}^{a-1} \\
&\quad + 2(a-1)A^{(1)}\Phi^{1/2}V_{(L)}D_{\alpha(L)}^{a-2}D_{\alpha(L)}^{(1)} \\
&\quad + 2A(\Phi^{1/2})^{(1)}V_{(L)}^{\{1\}}D_{\alpha(L)}^{a-1} \\
&\quad + 2(a-1)A(\Phi^{1/2})^{(1)}V_{(L)}D_{\alpha(L)}^{a-2}D_{\alpha(L)}^{(1)} \\
&\quad + 2(a-1)A\Phi^{1/2}V_{(L)}^{\{1\}}D_{\alpha(L)}^{a-2}D_{\alpha(L)}^{(1)},
\end{aligned}\right. \tag{4.29}$$

$$\left\{\begin{aligned}
G &= (\Phi^{-1/2})^{T}V_{(L)}D_{\alpha(L)}^{b}, \\
G^{(1)} &= (\Phi^{-1/2})^{(1)T}V_{(L)}D_{\alpha(L)}^{b} + (\Phi^{-1/2})^{T}V_{(L)}^{\{1\}}D_{\alpha(L)}^{b} \\
&\quad + b(\Phi^{-1/2})^{T}V_{(L)}D_{\alpha(L)}^{b-1}D_{\alpha(L)}^{(1)}, \\
G^{(2)} &= (\Phi^{-1/2})^{(2)T}V_{(L)}D_{\alpha(L)}^{b} + (\Phi^{-1/2})^{T}V_{(L)}^{\{2\}}D_{\alpha(L)}^{b}
\end{aligned}\right. \tag{4.30}$$

$$
\left.
\begin{aligned}
&+ b(b-1)(\Phi^{-1/2})^{T}V_{(L)}D_{\alpha(L)}^{b-2}(D_{\alpha(L)}^{(1)})^{2} \\
&+ b(\Phi^{-1/2})^{T}V_{(L)}D_{\alpha(L)}^{b-1}D_{\alpha(L)}^{(2)} \\
&+ 2(\Phi^{-1/2})^{(1)}T_{V\{L\}}^{(1)}D_{\alpha(L)}^{b} \\
&+ 2b(\Phi^{-1/2})^{(1)}T_{V_{(L)}}D_{\alpha(L)}^{b-1}D_{\alpha(L)}^{(1)} \\
&+ 2b(\Phi^{-1/2})T_{V\{L\}}^{(1)}D_{\alpha(L)}^{b-1}D_{\alpha(L)}^{(1)} \cdot
\end{aligned}
\right\}
$$

The first and second order terms in the expansions of $\Omega(\varepsilon)^{-1/2}$ and $\Phi(\varepsilon)^{-1/2}$ are given by

$$
(4.31)\left\{
\begin{aligned}
(\Omega^{-1/2})^{(1)} &= (\Omega^{-1/2})' \\
&= -\Omega^{-1/2}(\Omega^{1/2})'\Omega^{-1/2}, \\
(\Omega^{-1/2})^{(2)} &= (1/2)(\Omega^{-1/2})'' \\
&= \Omega^{-1/2}(\Omega^{1/2})'\Omega^{-1/2}(\Omega^{1/2})'\Omega^{-1/2} \\
&\quad -(1/2)\Omega^{-1/2}(\Omega^{1/2})''\Omega^{-1/2},
\end{aligned}
\right.
$$

and

$$
(4.32)\left\{
\begin{aligned}
(\Phi^{-1/2})^{(1)} &= (\Phi^{-1/2})' \\
&= -\Phi^{-1/2}(\Phi^{1/2})'\Phi^{-1/2}, \\
(\Phi^{-1/2})^{(2)} &= (1/2)(\Phi^{-1/2})'' \\
&= \Phi^{-1/2}(\Phi^{1/2})'\Phi^{-1/2}(\Phi^{1/2})'\Phi^{-1/2} \\
&\quad -(1/2)\Phi^{-1/2}(\Phi^{1/2})''\Phi^{-1/2}.
\end{aligned}
\right.
$$

The differential coefficients of the matrices $\Omega^{1/2}$ and $\Phi^{1/2}$ can be calculated easily when these matrices are diagonal as in the case of PCA, biplot, Hayashi's third method of quantification and correspondence analysis. However, when they are not diagonal as in the case of canonical correlation analysis, we must apply Taylor expansion to the Cholesky decomposition.

4.2.4 Perturbation of the matrix H

We must consider the matrices H, A, Φ and Ω for each method.

(1)Principal component analysis

From Table 4.1 the matrix H is given as follows by using the weights $\mathbf{w}=(w_k)$ in the case of principal component analysis.

$$(4.33)\quad H(\mathbf{w}) = \frac{1}{n}(Y-\frac{1}{n}\mathbf{1}\mathbf{1}^T D_w Y)^T D_w (Y-\frac{1}{n}\mathbf{1}\mathbf{1}^T D_w Y)$$

Substituting (4.15) into (4.33) and expanding with respect to ε we obtain

$$(4.34)\quad h_{jj'}(\varepsilon) = h_{jj'} + \varepsilon h_{jj'}^{(1)} + \varepsilon^2 h_{jj'}^{(2)} + O(\varepsilon^3),$$

where

$$(4.35)\quad h_{jj'} = \frac{1}{n}\sum_{k=1}^{n}(y_{kj}-\bar{y}_j)(y_{kj'}-\bar{y}_{j'}) ,$$

$$(4.36)\quad h_{jj'}^{(1)} = h_{jj'}/n - (y_{ij}-\bar{y}_j)(y_{ij'}-\bar{y}_{j'})/n, \qquad \text{(single individual)}$$

$$= (m/n)\{h_{jj'} - \sum_{i\in I}(y_{ij}-\bar{y}_j)(y_{ij'}-\bar{y}_{j'})/m\}, \qquad \text{(multiple individuals)}$$

$$(4.37)\quad h_{jj'}^{(2)} = h_{jj'}/n^2 - 2(y_{ij}-\bar{y}_j)(y_{ij'}-\bar{y}_{j'})/n^2, \qquad \text{(single)}$$

$$= (m/n)^2\{h_{jj'} - \sum_{i\in I}(y_{ij}-\bar{y}_j)(y_{ij'}-\bar{y}_{j'})/m \qquad \text{(multiple)}$$

$$-(\sum_{i\in I} y_{ij}/m - \bar{y}_j)(\sum_{i\in I} y_{ij'}/m - \bar{y}_{j'})\}$$

$$(4.38)\quad \bar{y}_j = \sum_{k=1}^{n} y_{kj}/n .$$

Similarly, expanding the transformed matrix A(w) with respect to ε we get

$$(4.39)\quad a_{kj}(\varepsilon) = a_{kj} + \varepsilon a_{kj}^{(1)} + \varepsilon^2 a_{kj}^{(2)} + O(\varepsilon^3),$$

where

$$(4.40)\quad a_{kj} = y_{kj} - \bar{y}_j,$$

$$(4.41)\quad a_{kj}^{(1)} = \begin{cases} a_{ij}/n & k\neq i, \\ a_{ij}/n - a_{ij} & k=i, \end{cases} \qquad \text{(single)}$$

$$(4.42)\quad a_{kj}^{(1)} = \begin{cases} \sum_{i\in I} a_{ij}/n & k\notin I, \\ \sum_{i\notin I} a_{ij}/n - a_{kj} & k\in I, \end{cases} \qquad \text{(multiple)}$$

$$(4.43)\quad a_{kj}^{(2)} = \begin{cases} a_{ij}/n^2 & k\neq i, \\ a_{ij}/n^2 - a_{ij}/n & k=i. \end{cases} \qquad \text{(single)}$$

$$(4.44)\quad a_{kj}^{(2)} = \begin{cases} \sum_{i\in I} a_{ij}/n^2 & k\notin I, \\ \frac{m}{n^2}\sum_{i\notin I} a_{ij} - \sum_{i\in I} a_{kj}/n & k\in I, \end{cases} \qquad \text{(multiple)}$$

From Table 4.1,

$$(4.45)\quad \begin{cases} \Omega(\varepsilon) = (I-\varepsilon J_i)/(n-\varepsilon) \\ \qquad = (1/n)I + (1/n)\varepsilon\{(1/n)I - J_i\} \\ \qquad\quad + (1/n)^2\varepsilon^2\{(1/n)I - J_i\} + O(\varepsilon^3). \end{cases}$$

where J_i is a diagonal matrix with 1 in its (i,i) element and 0's in the other elements. Since the matrix $\Omega(\varepsilon)$ is diagonal, their differential coefficients are calculated as

$$(4.46)\quad \begin{cases} (\Omega^{1/2})' = (1/2)\Omega^{-1/2}\Omega', \\ (\Omega^{1/2})'' = (-1/4)\Omega^{-3/2}(\Omega')^2 + (1/2)\Omega^{-1/2}\Omega'', \end{cases}$$

and the differential coefficients Ω' and Ω'' are given by

$$(4.47)\quad \begin{cases} \Omega' = \{(1/n)I - J_i\}/n, \\ \Omega'' = 2\{(1/n)I - J_i\}/n^2. \end{cases}$$

Thus in the case of PCA or biplot we can evaluate the expansion (4.27) by substituting (4.47) into (4.46), (4.46) into (4.31), (4.31) into (4.29) and (4.30), and finally (4.29) into (4.27). Since the matrix Φ is a constant matrix, it is obvious that

(4.48) $(\Phi^{-1/2})(1) = (\Phi^{-1/2})(2) = 0.$

Substituting (4.48) into (4.31) and (4.31) into (4.28) we can evaluate the expression (4.28).

(2)Hayashi's third method of quantification and correspondence analysis

In the case of Hayashi's third method of quantification the matrix H(w) is given by

(4.49) $H(w) = D_C(w)^{-1/2} Y^T D_w D_r^{-1} Y D_C(w)^{-1/2},$

This matrix is expanded in a power series of ε as in (4.17), where the 0-th to 2nd order terms are given as

(4.50) $$h_{jj'} = \sum_{k=1}^{n} \frac{y_{kj}\ y_{kj'}}{r_k \sqrt{c_j c_{j'}}},$$

(4.51) $$h^{(1)}_{jj'} = \frac{h_{jj'}}{2}\left(\frac{y_{ij}}{c_j} + \frac{y_{ij'}}{c_{j'}}\right) - \frac{y_{ij}\ y_{ij'}}{r_i \sqrt{c_j c_{j'}}}, \qquad \text{(single)}$$

$$= \frac{h_{jj'}}{2} \sum_{i\in I}\left(\frac{y_{ij}}{c_j} + \frac{y_{ij'}}{c_{j'}}\right) - \sum_{i\in I} \frac{y_{ij}\ y_{ij'}}{r_i \sqrt{c_j c_{j'}}}, \qquad \text{(multiple)}$$

(4.52) $$h^{(2)}_{jj'} = h_{jj'}\left(\frac{1}{4}\frac{y_{ij}\ y_{ij'}}{c_j\ c_{j'}} + \frac{3}{8}\left(\frac{y_{ij}}{c_j}\right)^2 + \frac{3}{8}\left(\frac{y_{ij'}}{c_{j'}}\right)^2\right)$$

$$- \frac{1}{2}\left(\frac{y_{ij}}{c_j} + \frac{y_{ij'}}{c_{j'}}\right)\frac{y_{ij}\ y_{ij'}}{r_i \sqrt{c_j c_{j'}}}, \qquad \text{(single)}$$

$$= h_{jj'}\left\{\frac{1}{4}\left(\sum_{i\in I}\frac{y_{ij}}{c_j}\right)\left(\sum_{i\in I}\frac{y_{ij'}}{c_{j'}}\right)\right. \qquad \text{(multiple)}$$

$$\left. + \frac{3}{8}\left(\sum_{i\in I}\frac{y_{ij}}{c_j}\right)^2 + \frac{3}{8}\left(\sum_{i\in I}\frac{y_{ij'}}{c_{j'}}\right)^2\right\}$$

$$- \frac{1}{2} \left(\sum_{i \in I} \frac{y_{ij}}{c_j} + \sum_{i \in I} \frac{y_{ij'}}{c_{j'}} \right) \sum_{i \in I} \frac{y_{ij}\ y_{ij'}}{r_i \sqrt{c_j c_{j'}}} .$$

The transformed matrix A(w) is expanded as in the form of (4.39), where the coefficients are given by

(4.53) $a_{kj} = y_{kj}/(r_k c_j)$,

(4.54) $a_{kj}^{(1)} = a_{kj} \frac{y_{ij}}{c_j}$ $\quad k \neq i,$

(single)

$= a_{ij} \frac{y_{ij}}{c_j} + a_{ij}$ $\quad k = i,$

(4.55) $a_{kj}^{(1)} = a_{kj} \sum_{i \in I} \frac{y_{ij}}{c_j}$ $\quad k \notin I,$

(multiple)

$= a_{kj} \sum_{i \in I} \frac{y_{ij}}{c_j} + a_{kj}$ $\quad k \in I,$

(4.56) $a_{kj}^{(2)} = a_{kj} \left(\frac{y_{ij}}{c_j} \right)^2$ $\quad k \neq i,$

(single)

$= a_{ij} \left\{ \left(\frac{y_{ij}}{c_j} \right)^2 + \frac{y_{ij}}{c_j} + 1 \right\}$ $\quad k = i.$

(4.57) $a_{kj}^{(2)} = a_{kj} \left(\sum_{i \in I} \frac{y_{ij}}{c_j} \right)^2$ $\quad k \notin I,$

(multiple)

$= a_{kj} \left\{ \left(\sum_{i \in I} \frac{y_{ij}}{c_j} \right)^2 + \sum_{i \in I} \frac{y_{ij}}{c_j} + 1 \right\}$ $\quad k \in I.$

From Table 4.1, Ω and Φ are both diagonal matrices whose diagonal elements are given by

(4.58) $\omega_{kk}(\varepsilon) = r_k - \varepsilon r_i,$

(4.59) $\phi_{jj}(\varepsilon) = c_j - \varepsilon y_{ij}.$

The differential coefficients become

(4.60) $\omega'_{kk} = -r_i, \qquad \omega''_{kk} = 0,$

(4.61) $\phi'_{jj} = -y_{ij}, \qquad \phi''_{jj} = 0.$

Thus by using (4.60) and (4.61) we can obtain the first and second order terms of F and G. $((\Phi^{1/2})'$ and $(\Phi^{1/2})''$ are expressed with Φ, Φ' and Φ'' as in the case of $(\Omega^{1/2})'$ and $(\Omega^{1/2})''$ in (4.46).)

Correspondence analysis is equivalent to Hayashi's third method of quantification except for the normalization of coordinates.

(3)Canonical correlation analysis (CCA)

The matrix H(w) is expressed by

$$(4.62)\quad H(w)=S_{22}(w)^{-1/2}S_{21}(w)S_{11}(w)^{-1}S_{12}(w)(S_{22}(w)^{-1/2})^T,$$

which is expanded as in (4.3), where the 0-th to 2nd order terms are given as follows.

$$(4.63)\quad \begin{cases} H^{(1)} = R^{(1)}QR^T + RQ^{(1)}R^T + RQR^{(1)T} \\ H^{(2)} = R^{(2)}QR^T + RQ^{(2)}R^T + RQR^{(2)T} \\ \qquad + R^{(1)}Q^{(1)}R^T + R^{(1)}QR^{(1)T} + RQ^{(1)}R^{(1)T} \end{cases}$$

where

$$(4.64)\quad \begin{cases} Q = S_{21}S_{11}^{-1}S_{12} \\ Q^{(1)} = S_{21}^{(1)}S_{11}^{-1}S_{12} - S_{21}S_{11}^{-1}S_{11}^{(1)}S_{11}^{-1}S_{12} + S_{21}S_{11}^{-1}S_{12}^{(1)} \\ Q^{(2)} = S_{21}^{(2)}S_{11}^{-1}S_{12} - S_{21}^{(1)}S_{11}^{-1}S_{11}^{(1)}S_{11}^{-1}S_{12} + S_{21}^{(1)}S_{11}^{-1}S_{12}^{(1)} \\ \qquad + S_{21}S_{11}^{-1}S_{11}^{(1)}S_{11}^{-1}S_{11}^{(1)}S_{11}^{-1}S_{12} - S_{21}S_{11}^{-1}S_{11}^{(2)}S_{11}^{-1}S_{12} \\ \qquad - S_{21}S_{11}^{-1}S_{11}^{(1)}S_{11}^{-1}S_{12}^{(1)} + S_{21}S_{11}^{-1}S_{21}^{(2)} \end{cases}$$

$$(4.65)\quad \begin{cases} R = S_{22}^{-1/2} \\ R^{(1)} = -S_{22}^{-1/2}(S_{22}^{1/2})^{(1)}S_{22}^{-1/2} \end{cases}$$

$$\left\{ \begin{aligned} R^{(2)} &= S_{22}^{-1/2}(S_{22}^{1/2})^{(1)}S_{22}^{-1/2}(S_{22}^{1/2})^{(1)}S_{22}^{-1/2} \\ &\quad - S_{22}^{-1/2}(S_{22}^{1/2})^{(2)}S_{22}^{-1/2} . \end{aligned} \right.$$

The transformed matrix $A(\mathbf{w})$ is expanded as in the form of (4.39), where the coefficients are given by

$$(4.66)\quad A = S_{11}^{-1}S_{12}S_{22}^{-1},$$

$$(4.67)\quad A^{(1)} = -S_{11}^{-1}S_{11}^{(1)}S_{11}^{-1}S_{12}S_{22}^{-1} + S_{11}^{-1}S_{12}^{(1)}S_{22}^{-1} - S_{11}^{-1}S_{12}S_{22}^{-1}S_{22}^{(1)}S_{22}^{-1},$$

$$\begin{aligned}(4.68)\quad A^{(2)} &= (S_{11}^{-1})^{(2)}S_{12}S_{22}^{-1} + S_{11}^{-1}S_{12}^{(2)}S_{22}^{-1} \\ &\quad + S_{11}^{-1}S_{12}(S_{22}^{-1})^{(2)} - S_{11}^{-1}S_{11}^{(1)}S_{11}^{-1}S_{12}^{(1)}S_{22}^{-1} \\ &\quad + S_{11}^{-1}S_{11}^{(1)}S_{11}^{-1}S_{12}S_{22}^{-1}S_{22}^{(1)}S_{22}^{-1} \\ &\quad - S_{11}^{-1}S_{12}^{(1)}S_{22}^{-1}S_{22}^{(1)}S_{22}^{-1}.\end{aligned}$$

The covariance matrices can be expressed as

$$(4.69)\quad S_{11}(\mathbf{w}) = S_{11}(\varepsilon) = S_{11} + \varepsilon S_{11}^{(1)} + \varepsilon^2 S_{11}^{(2)} + O(\varepsilon^3),$$

$$(4.70)\quad S_{12}(\mathbf{w}) = S_{12}(\varepsilon) = S_{12} + \varepsilon S_{12}^{(1)} + \varepsilon^2 S_{12}^{(2)} + O(\varepsilon^3),$$

$$(4.71)\quad S_{22}(\mathbf{w}) = S_{22}(\varepsilon) = S_{22} + \varepsilon S_{22}^{(1)} + \varepsilon^2 S_{22}^{(2)} + O(\varepsilon^3),$$

where

$$(4.72)\quad S_{11}^{(1)} = (m/n)\{S_{11} - (1/m)\sum_{i\in I}(\mathbf{x}_i-\bar{\mathbf{x}})(\mathbf{x}_i-\bar{\mathbf{x}})'\},$$

$$\begin{aligned}(4.73)\quad S_{11}^{(2)} &= (m/n)^2\{S_{11} - (1/m)\sum_{i\in I}(\mathbf{x}_i-\bar{\mathbf{x}})(\mathbf{x}_i-\bar{\mathbf{x}})', \\ &\qquad - ((1/m)\sum_{i\in I}\mathbf{x}_i-\bar{\mathbf{x}})((1/m)\sum_{i\in I}\mathbf{x}_i-\bar{\mathbf{x}})'\},\end{aligned}$$

$$(4.74)\quad (S_{11}^{-1})^{(2)} = S_{11}^{-1}S_{11}^{(1)}S_{11}^{-1}S_{11}^{(1)}S_{11}^{-1} - S_{11}^{-1}S_{11}^{(2)}S_{11}^{-1}.$$

$S_{12}^{(1)}$, $S_{12}^{(2)}$, $S_{22}^{(1)}$ and $S_{22}^{(2)}$ denoting the similar formula with respect to the covariance matrices between the first and second group of variables and within the second group of variables. $(S_{22}^{1/2})^{(1)}$ and $(S_{22}^{1/2})^{(2)}$ are calculated by the differentiation of

the Cholesky decomposition shown later.

Canonical discriminant analysis (CDA) is included in CCA where the variables of the first group are the dummy variables expressing the mutually exclusive categories of an item. Hayashi's second method of quantification is a special case of CDA where the variables of the second group are also given as the dummy variables expressing the categories of several items.

Differential coefficients of Cholesky decomposition

A positive definite symmetric matrix A can be decomposed into the product of a lower triangular matrix G and its transpose G^T, i.e.

(4.75) $A = GG^T$.

The elements of G are calculated by

$$
(4.76)\begin{cases}
g_{11} = (a_{11})^{1/2}, & \\
g_{j1} = a_{j1}/g_{11}, & j>1, \\
g_{ii} = (a_{ii} - \sum_{s=1}^{i-1} g_{is}^2)^{1/2}, & i>1 \\
g_{ji} = (a_{ji} - \sum_{s=1}^{i-1} g_{is}g_{js})/g_{ii}, & i<j \\
g_{ji} = 0, & i>j.
\end{cases}
$$

From (4.76) we easily obtain the differential coefficients.

$$
\begin{cases}
g'_{11} = a_{11}^{-1/2}a'_{11}/2, & \\
g''_{11} = -a_{11}^{-3/2}(a'_{11})^2/4 + a_{11}^{-1/2}a''_{11}/2, & \\
g'_{j1} = a'_{j1}/g_{11} - a_{j1}g'_{11}/(g_{11})^2, & j>1 \\
g''_{j1} = a''_{j1}/g_{11} - (2a'_{j1}g'_{11}+a_{j1}g''_{11})/(g_{11})^2 & j>1
\end{cases}
$$

$$
(4.77)\quad
\begin{aligned}
&\quad + 2a_{j1}(g'_{11})^2/(g_{11})^3, \\
g'_{ii} &= \tfrac{1}{2}(a'_{ii} - 2\sum_{s=1}^{i-1} g'_{is}g_{is})/g_{ii}^{1/2} && i>1 \\
g''_{ii} &= \tfrac{1}{2}\{a''_{ii} - 2\sum_{s=1}^{i-1}(g'^{2}_{is} + g_{is}g''_{is})\}/g_{ii}^{1/2} && i>1 \\
&\quad - \tfrac{1}{4}\{a'_{ii} - 2\sum_{s=1}^{i-1} g'_{is}g_{is})g'_{ii}/g_{ii}^{3/2} \\
g'_{ji} &= \{a'_{ji} - \sum_{s=1}^{i-1}(g'_{is}g_{js}+g_{is}g'_{js})\}/g_{ii} && i<j \\
&\quad - (a_{ji} - \sum_{s=1}^{i-1} g_{is}g_{js})g'_{ii}/(g_{ii})^2, \\
g''_{ji} &= \{a''_{ji} - \sum_{s=1}^{i-1}(g''_{is}g_{js}+2g'_{is}g'_{js}+g_{is}g''_{js})\}/g_{ii} && i<j \\
&\quad - 2\{a'_{ji} - \sum_{s=1}^{i-1}(g'_{is}g_{js}+g_{is}g'_{js})\}g'_{ii}/(g_{ii})^2 \\
&\quad - (a_{ji} - \sum_{s=1}^{i-1} g_{is}g_{js})g''_{ii}/(g_{ii})^2 \\
&\quad +2(a_{ji} - \sum_{s=1}^{i-1} g_{is}g_{js})(g'_{ii})^2/(g_{ii})^3.
\end{aligned}
$$

4.3 Measures of the amount of influence

To express the amount of influence we can consider the following measures.

(1) Differential coefficient of the sum of eigenvalues(squared singular values)

$$\frac{d}{d\varepsilon}\sum_k \theta_k(\varepsilon)\Big|_{\varepsilon=0} = \mathrm{tr}\, H^{(1)}$$

(2) Differential coefficient of the product of eigenvalues

(squared singular values)

$$\frac{d}{d\varepsilon}\prod_k \theta_k(\varepsilon)\Big|_{\varepsilon=0} = |H|\mathrm{tr}(H^{-1}H^{(1)})$$

(3) Differential coefficient of each singular value

$$\alpha_k^{(1)} = \frac{d}{d\varepsilon}\alpha_k(\varepsilon)\Big|_{\varepsilon=0}$$

(4) Euclidean norm of the differential coefficients of the coordinates F (or G) normalized by $\|F\|$ (or $\|G\|$)

$$\|F^{(1)}\| / \|F\| , \qquad \|G^{(1)}\| / \|G\|$$

(5) Euclidean norm of the differential coefficient of the configurations FF^T (or GG^T) normalized by $\|FF^T\|$ (or $\|GG^T\|$)

$$\|F^{(1)}F^T + FF^{(1)T}\| / \|FF^T\|$$

$$\|G^{(1)}G^T + GG^{(1)T}\| / \|GG^T\|$$

In the above we used the differential coefficients to measure the amounts of influence for the sake of simplicity. When we apply the second or higher order perturbation we should use the difference such as $\theta_k(\varepsilon)-\theta_k(0)$ and $\alpha_k(\varepsilon)-\alpha_k(0)$ instead of the differential coefficients such as $\frac{d}{d\varepsilon}\theta_k(\varepsilon)\Big|_{\varepsilon=0}$ and $\frac{d}{d\varepsilon}\alpha_k(\varepsilon)\Big|_{\varepsilon=0}$.

4.4 Numerical examples

(1) Principal component analysis

As an illustration we analyzed the data given in Table 4.2, which is a part of the result of a survey on food acceptance

Table 4.2 Food acceptance data : acceptance patterns of 12 drinks in 10 groups
(mean values in 9 point rating scale).

	Category									
Individual	1	2	3	4	5	6	7	8	9	10
1	4.6	5.0	6.0	5.4	5.4	4.7	4.2	4.2	4.1	4.4
2	4.6	5.1	6.7	7.2	6.5	3.3	3.6	4.2	4.3	3.6
3	6.1	6.3	7.1	6.8	6.6	6.5	6.8	7.2	6.8	7.4
4	6.1	6.7	6.6	5.8	5.5	5.8	6.0	6.0	5.7	5.8
5	6.2	6.8	6.2	6.6	5.5	5.0	6.3	6.3	6.2	5.8
6	7.4	7.3	6.8	6.7	6.8	6.3	6.3	5.0	6.4	5.2
7	8.1	6.8	6.7	6.3	5.9	7.8	7.0	6.3	6.7	6.1
8	7.8	6.6	6.4	6.2	5.8	7.6	6.6	5.9	5.9	5.2
9	7.0	5.3	5.3	4.8	4.2	6.7	5.1	4.7	4.2	4.3
10	6.9	6.9	6.2	5.6	5.0	5.6	5.8	4.5	3.9	3.3
11	7.6	6.6	5.8	5.3	5.3	6.9	6.4	5.5	5.5	5.7
12	7.0	5.6	4.3	4.3	4.2	6.5	5.7	5.3	4.8	4.2

Notes.
(1)Individuals(drinks): 1.wine, 2.beer, 3.green tea, 4.black tea, 5.coffee, 6.milk, 7.Calpis(lactic acid drink), 8.orange juice, 9.powdered juice, 10.coke, 11.soda pop, 12.Nectar(fruit juce).

(2)Categories(groups): 1.male -15, 2.male 16-20, 3.male 21-30, 4.male 31-40, 5.male 41-, 6.female -15, 7.female 16-20, 8.female 21-30, 9.female 31-40, 10.female 41-.

(Toda and Tanaka(1968)). Each value in the table means to what degree each of 12 drinks is accepted in each of 10 groups defined by age and sex. In order to investigate the mutual relationship among 10 groups and/or 12 drinks, we applied principal component analysis to these data. The result is shown in Fig. 4.1. From the configuration of the points we can construct some clusters of rows (individuals, in this case foods) and/or columns(categories, in this case groups)

Next to investigate the stability of the above result we applied the sensitivity analysis. The measures of the amount of influence defined in section 3 are calculated by changing the weight for each individual from 1 to $1-\varepsilon$ in turn. The results are shown in Table 4.3. Since the individual No. 2 looks relatively influential, according to this table, we evaluated the influence of the individual No. 2 precisely. Fig. 4.2 shows the changes of coordinates of rows and columns due to a small change of the weights for the individual No. 2 from 1 to $1-\varepsilon$ ($\varepsilon=0.3$). Though a small clockwise rotation is observed in this figure, the influence is so small that it does not affect the interpretation.

(2) Hayashi's third method of quantification

We applied Hayashi's third method of quantification to the data given in Table 4.4, which is also a part of the result of the survey on food acceptance. Each mark in the table means whether each of 12 foods is accepted(1) or not(0) in each of 10 groups. The result is shown in Fig. 4.3. Here the coordinates are normalized so that the variance in each dimension is equal to

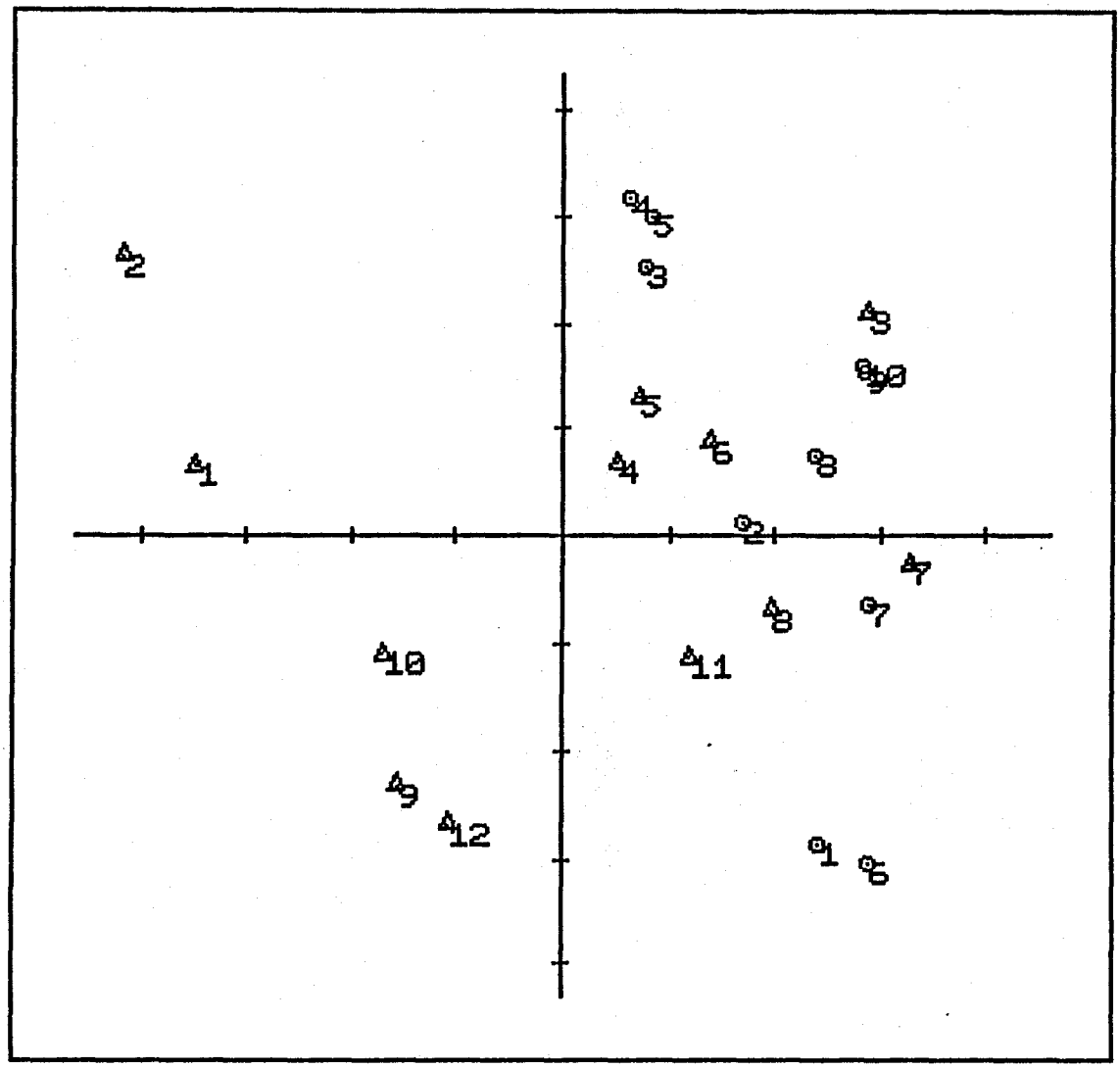

Fig.4.1 Column profiles(circle) and row profiles(triangles) between the first and the second axis. (Principal component analysis)

Table 4.3 The amount of influence of each drink (Principal component analysis).

No	$\alpha_1^{(1)}$	$\alpha_2^{(1)}$	$\|F^{(1)}\| / \|F\|$	$\|FF^T\|$	$\|G^{(1)}\| / \|G\|$	$\|GG^T\|$
1	-0.12656	0.05502	0.10732	0.14814	0.07606	0.10775
2	-0.22018	-0.11471	0.50171	0.69883	0.34506	0.48108
3	-0.05548	-0.04978	0.29677	0.42626	0.22680	0.31843
4	0.09098	0.05450	0.03981	0.05745	0.02787	0.03763
5	0.08614	0.02165	0.08436	0.12208	0.07404	0.09970
6	0.06043	0.04626	0.07911	0.11121	0.07763	0.11134
7	-0.10014	0.06423	0.04302	0.06089	0.02893	0.04159
8	0.02453	0.05329	0.07256	0.10286	0.05041	0.07267
9	0.05186	-0.07470	0.20171	0.27874	0.13197	0.18527
10	0.04397	0.03356	0.11047	0.15276	0.10409	0.14837
11	0.06952	0.03222	0.08478	0.12188	0.04683	0.06617
12	0.07492	-0.12154	0.20062	0.27851	0.16546	0.23712

Note. $\|FF^T\|$ and $\|GG^T\|$ mean $\|F^{(1)}F^T+FF^{(1)T}\| / \|FF^T\|$ and $\|G^{(1)}G^T+GG^{(1)T}\| / \|GG^T\|$, respectively.

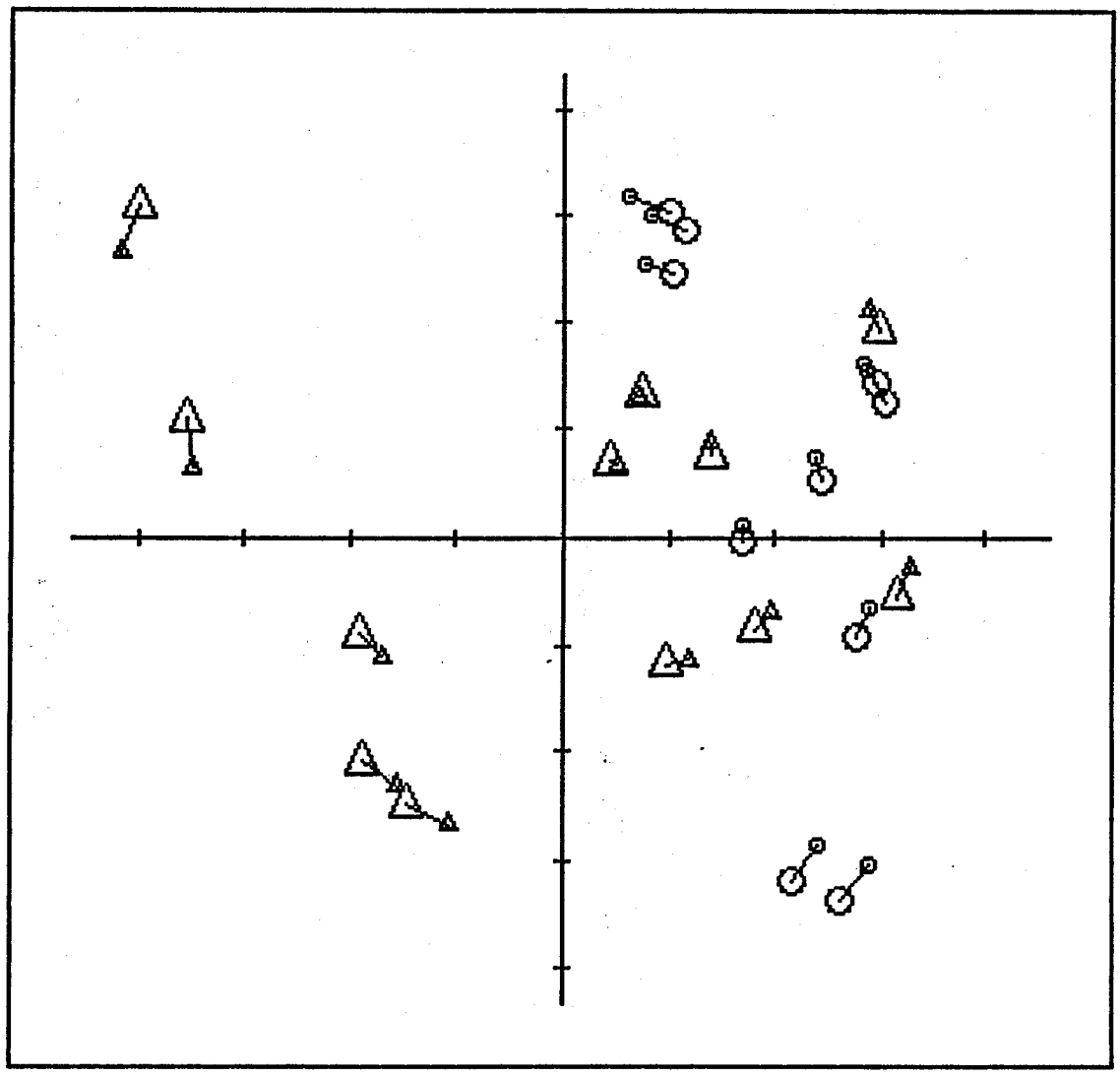

Fig.4.2 Changes of the row and column profiles when the weight for individual 2 is slightly changed form 1 to 1-ε (ε=0.3).
Small marks indicate the profiles for the original data, and large marks indicate the profiles for the perturved data. (Principal component analysis)

Table 4.4 Food acceptance data : acceptance patterns of 12 foods in 10 groups.

Individual	Category 1	2	3	4	5	6	7	8	9	10
1	1	1	1	0	0	1	1	1	1	0
2	0	0	0	0	1	1	0	0	0	1
3	1	1	1	1	0	1	1	1	1	0
4	0	1	1	1	1	1	1	1	1	1
5	1	1	1	1	1	1	1	1	1	1
6	1	1	0	0	0	1	1	0	0	0
7	1	1	1	1	0	1	1	0	1	0
8	0	1	1	1	1	0	1	1	1	1
9	1	1	1	1	1	0	0	0	0	1
10	1	1	0	1	1	1	0	1	1	1
11	0	0	1	1	0	0	1	1	1	1
12	0	1	1	1	1	0	1	1	1	1

Notes.

(1)Individuals(foods): 1.curry and rice, 2.iced noodles, 3.flield noodles, 4.miso soup, 5.sukiyaki, 6.croquette, 7.ham, 8.sliced raw fish, 9.broiled eel, 10.Japanese hotchpotch, 11.Chinese cooked vegetables, 12.cooled tofu.

(2)Categories(groups): 1.male -15, 2.male 16-20, 3.male 21-30, 4.male 31-40, 5.male 41-, 6.female -15, 7.female 16-20, 8.female 21-30, 9.female 31-40, 10.female 41-.

(3)The figure "1" indicates that the food is accepted in the group in the sense that the mean scores using a 9-point scale is larger than 6.0 and figure "0" indicates the opposite.

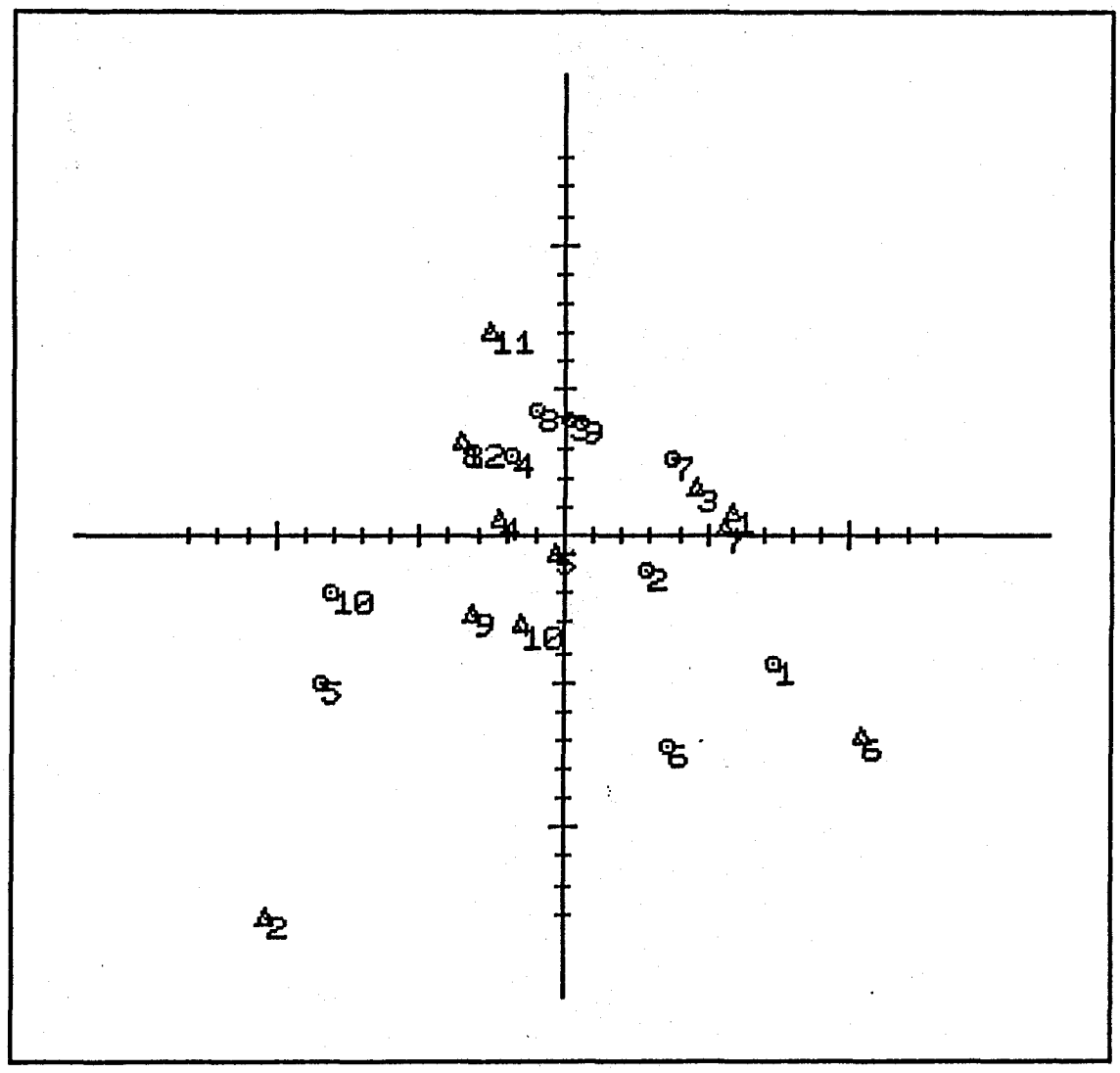

Fig.4.3 Column profiles(circle) and row profiles(triangles) between the first and the second axis. (Hayashi's third method of quantification)

the corresponding eigenvalue as in correspondence analysis. Also in this analysis we may construct some clusters of the points of rows and/or columns.

Next we applied the sensitivity analysis. Table 4.5 shows the measures of the amount of influence calculated by changing the weight for each individual in turn. According to this table the individual No. 2 looks influential. So we evaluate the influence of the individual No. 2 precisely. Fig. 4.4 shows the changes of coordinates of rows and columns when the weight for the individual No. 2 is slightly changed from 1 to $1-\varepsilon$ ($\varepsilon=0.3$). Also in this case we can observe a rotation. However, mutual relationship among points seems stable.

4.5 Discussion and summary

Our concern is how the result of analysis changes when the weight for a single or multiple individuals changes slightly. Our sensitivity analysis procedure is as follows.

Step 1. Evaluate the influence of each individual in turn by changing its weight form 1 to $1-\varepsilon$ and summarize the result in a table.

Step 2. Find influential individuals by checking the table.

Step 3. Show the influence of a single or multiple influential individuals graphically, and judge how it affects the interpretation.

In step 1 we must calculate the influence of each individual

Table 4.5 The amount of influence of each food (Hayashi's third method of quantification).

No	$\alpha_1^{(1)}$	$\alpha_2^{(1)}$	$\|F^{(1)}\| / \|F\|$	$\|FF^T\|$	$\|G^{(1)}\| / \|G\|$	$\|GG^T\|$
1	-0.01799	0.01698	0.31761	0.43181	0.22560	0.21346
2	-0.01998	-0.06012	1.05495	1.13861	0.86456	0.42685
3	-0.00894	0.01578	0.34883	0.37623	0.28163	0.18620
4	0.01576	0.01965	0.15369	0.20508	0.16321	0.22235
5	0.02748	0.02199	0.07456	0.14373	0.12980	0.25876
6	-0.04151	-0.01582	0.73377	0.78745	0.55648	0.26463
7	-0.01504	0.01604	0.27783	0.40187	0.17792	0.19534
8	0.00719	0.00222	0.40792	0.33359	0.35367	0.20694
9	0.01675	0.00388	0.16598	0.28537	0.20292	0.30475
10	0.02375	0.00883	0.18457	0.27547	0.18662	0.26529
11	0.00533	-0.03165	0.41789	0.45864	0.32476	0.21517
12	0.00719	0.00222	0.40792	0.33359	0.35367	0.20694

Note. $\|FF^T\|$ and $\|GG^T\|$ mean $\|F^{(1)}F^T+FF^{(1)T}\| / \|FF^T\|$ and $\|G^{(1)}G^T+GG^{(1)T}\| / \|GG^T\|$, respectively.

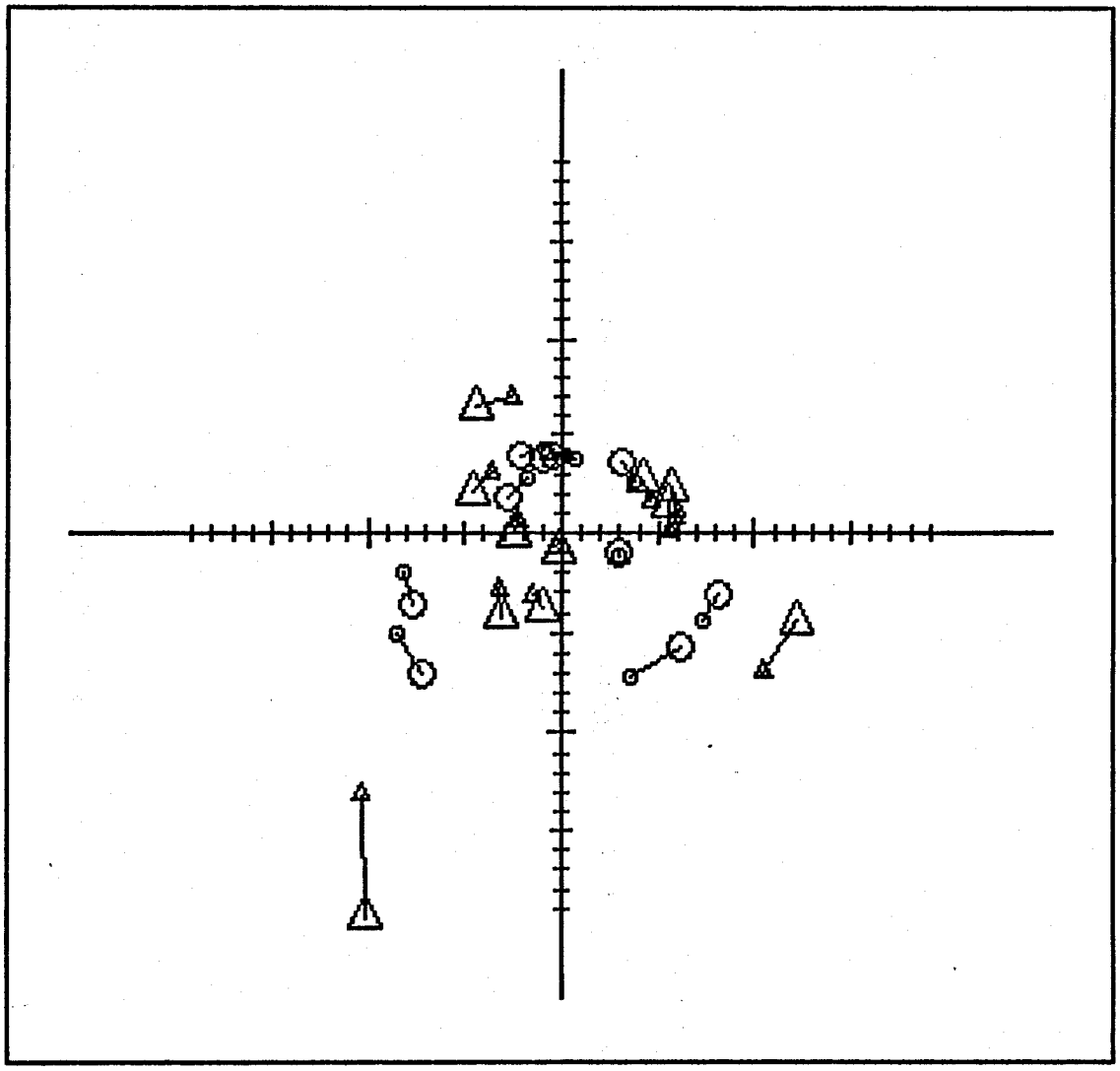

Fig.4.4 Changes of the row and column profiles when the weight for individual 2 is slightly changed form 1 to 1-ε (ε=0.3).
Small marks indicate the profiles for the original data, and large marks indicate the profiles for the perturved data. (Hayashi's third method of quantification)

in turn. When the number of individuals increases the amount of calculation becomes large. Therefore it is very important practically to use a numerical method which is as efficient as possible. From such viewpoint we avoided to apply exact methods to solve eigenvalue problems, and instead we used the perturbation theory of eigenvalue problems.

The formulation of the perturbation theory are different depending on whether we can assume the eigenvalues of interest are all simple or not. The precise computational problems are fully discussed in Chapter 5.

For evaluation of the stability of the result so called jackknife method and bootstrap method are also useful. If we put $\varepsilon=1$ our method just corresponds to the jackknife method. The bootstrap method requires, in general, much computing time. Therefore, if a large scale computer is available and if the evaluation of the stability is a critical problem we should use the bootstrap method.

5 Computational Aspect of Sensitivity Analysis

In this chapter we discuss the computational aspect of sensitivity analysis in multivariate methods which are formulated as eigenvalue problems of symmetric matrices.

Since we must evaluate the eigenvalues and eigenvectors of slightly different matrices many times in order to search for influential observations, we should use a computing method which is as efficient as possible. From such a viewpoint we applied the perturbation theory in our sensitivity analysis. But the perturbation methods are different, depending on whether the eigenvalues of interest are all simple or not. Of course in actual data analysis the eigenvalues of interest are usually all simple in the strict sense. However, if there are close eigenvalues we should better apply the perturbation method under the assumption of multiple eigenvalues to get the result with high accuracy, because the method under the assumption of simple eigenvalues does not work well in such cases. The problem whether we should use the first order approximation or second order approximation is another problem.

We investigate six computational methods based on the

perturbation theory and compare their degrees of accuracy numerically, and discuss the switching policies among those methods of computation.

5.1 Computational methods

For the computation of eigenvalues and eigenvectors of each matrix $H(\varepsilon)$ we may apply the following methods.

(EM) Exact method to solve each eigenvalue problem of $H(\varepsilon)$ by an ordinary numerical procedure.

(PS1) Perturbation method of first order assuming simple eigenvalues based on Lemma 1 in Chapter 2.

(PS2) Perturbation method of second order assuming simple eigenvalues based on Lemma 1 in Chapter 2.

(PM1) Perturbation method of first order assuming multiple eigenvalues based on Lemma 2-1 in Chapter 2.

(PM2) Perturbation method of second order assuming multiple eigenvalues based on Lemma 2-2 in Chapter 2.

(PM'1) Modification of PM1. The method to compute eigenvalues of first order approximation by using Lemma 3 in Chapter 2 and obtain eigenvectors by solving linear simultaneous equations.

(PM'2) Modification of PM2. The method to compute eigenvalues of second order approximation by using Lemma 3 in Chapter 2 and obtain eigenvectors by solving linear simultaneous

equations.

As is mentioned before there are various sources which bring small changes of the matrix H, and, in general, we must evaluate the eigenvalues and eigenvectors of slightly different matrices many times. Therefore, it is practically important to choose the procedure which is as efficient as possible, if its computation error is not so large. So if the result of any one perturbation method is accurate we should better choose it.

In applying the perturbation methods the appropriateness of the assumption of simple eigenvalues depends on the closeness of the eigenvalues of interest. The choice between the first order perturbation or second order perturbation depends on the size of ε. In order to investigate the effects of the closeness of the eigenvalues of interest and the size of ε we performed numerical experiments as shown below. The data are generated according to the following model.

Model:

$$H(\varepsilon) = H + \varepsilon H^{(1)} + \varepsilon^2 H^{(2)},$$

where

$$H = \theta_1 u_1 u_1' + \ldots + \theta_4 u_4 u_4',$$

$$u_1 = (1/2 \;\; 1/2 \;\; -1/2 \;\; -1/2)',$$

$$u_2 = (1/2 \;\; -1/2 \;\; 1/2 \;\; -1/2)',$$

$$u_3 = (1/2 \;\; -1/2 \;\; -1/2 \;\; 1/2)',$$

$$u_4 = (1/2 \;\; 1/2 \;\; 1/2 \;\; 1/2)'.$$

$$\theta_1 = 3+\Delta, \quad \theta_2 = 3-\Delta, \quad \theta_3 = 0.5, \quad \theta_4 = 0,$$

$$H^{(\ell)}=(h_{ij}^{(\ell)}),\quad h_{ij}^{(\ell)} : [-1,1] \text{ uniform random number.}$$
$$\ell=1,2$$

First, to investigate the effect of the closeness of eigenvalues, we generated ten sets of $H(\varepsilon)$'s by putting $\varepsilon=0.1$ (fixed) and $\Delta=0.01,0.05,0.10(0.10)0.50$, and calculated their eigenvalues and eigenvectors by the above EM~PM'2 methods. The results are summarized in Table 5.1. From this table we find that,

① when Δ is large, the eigenvalues and eigenvectors are calculated accurately by all of the PS, PM and PM' methods, but

② when Δ decreases, the accuracy of the PS method grows worse while the PM and PM' methods are still satisfactorily accurate, and

③ there is no clear difference in accuracy between the PM and PM' methods.

From (2.5)-(2.6) we can interpret that the main source of the errors due to the closeness of eigenvalues is the term $\theta_s-\theta_r$ in the denominator in the second equation of (2.5). So, when some eigenvalues are close to each other the first order terms of the eigenvectors will be inaccurate and in consequence the second order terms of the eigenvalues and eigenvectors will be also inaccurate. In such cases the norms of the eigenvectors $\|\mathbf{v}_s\|$'s will deviate from 1.0 though the equations (2.5)-(2.6) are formulated under the constraint $\|\mathbf{v}_s\|=1$. From this standpoint we drew the scatter diagram of the norm and the error of eigenvector in Fig. 5.1. It seems that the norms of eigenvectors actually

Table 5.1 Relationship between the amount of errors and the closeness of eigenvalues(Δ).
— Simulation study based on ten sets of artificially generated data —

ε=0.1 Δ		Eigenvalue *1)						Eigenvector *2)					
		PS1	PS2	PM1	PM2	PM'1	PM'2	PS1	PS2	PM1	PM2	PM'1	PM'2
0.50	Mean	0.01724	0.00068	0.01417	0.00080	0.01417	0.00081	0.01188	0.00170	0.01122	0.00241	0.00822	0.00093
	S.D.	0.00701	0.00028	0.00648	0.00047	0.00648	0.00047	0.00385	0.00139	0.00346	0.00101	0.00299	0.00052
	Max	0.03181	0.00122	0.02524	0.00173	0.02524	0.00173	0.02064	0.00560	0.01718	0.00482	0.01315	0.00199
	Min	0.00629	0.00015	0.00629	0.00015	0.00629	0.00015	0.00607	0.00047	0.00572	0.00131	0.00409	0.00030
0.40	Mean	0.01453	0.00077	0.01238	0.00078	0.01238	0.00079	0.01439	0.00268	0.00964	0.00188	0.01084	0.00106
	S.D.	0.01014	0.00043	0.00721	0.00077	0.00721	0.00078	0.00791	0.00295	0.00592	0.00157	0.00647	0.00103
	Max	0.03873	0.00151	0.02337	0.00228	0.02337	0.00231	0.03171	0.00866	0.02388	0.00585	0.02625	0.00305
	Min	0.00345	0.00016	0.00299	0.00011	0.00299	0.00009	0.00530	0.00032	0.00445	0.00083	0.00381	0.00010
0.30	Mean	0.01591	0.00122	0.01354	0.00087	0.01354	0.00091	0.02283	0.00411	0.00974	0.00130	0.01327	0.00153
	S.D.	0.00812	0.00074	0.00724	0.00062	0.00724	0.00061	0.01424	0.00258	0.00327	0.00050	0.00720	0.00104
	Max	0.02645	0.00312	0.02637	0.00200	0.02637	0.00201	0.05025	0.00868	0.01511	0.00225	0.02971	0.00336
	Min	0.00288	0.00040	0.00229	0.00018	0.00229	0.00025	0.00625	0.00118	0.00427	0.00060	0.00521	0.00045
0.20	Mean	0.02374	0.00329	0.01463	0.00046	0.01463	0.00048	0.04744	0.01726	0.00656	0.00059	0.02372	0.00133
	S.D.	0.01379	0.00362	0.00478	0.00026	0.00478	0.00025	0.02947	0.01216	0.00145	0.00025	0.01715	0.00074
	Max	0.05470	0.01085	0.02123	0.00088	0.02123	0.00088	0.09702	0.04395	0.00863	0.00112	0.06398	0.00293
	Min	0.00465	0.00008	0.00536	0.00014	0.00536	0.00014	0.00781	0.00265	0.00462	0.00026	0.00660	0.00028

*1) Sum of the absolute errors of the largest two eigenvalues. The differences between the results of a perturbation method and the exact method are considered to be errors.
*2) Sum of Euclidean norms of the errors of the eigenvectors associated with the largest two eigenvalues.

Table 5.1 (Continued)

ε=0.1 Δ		Eigenvalue *1)						Eigenvector *2)					
		PS1	PS2	PM1	PM2	PM'1	PM'2	PS1	PS2	PM1	PM2	PM'1	PM'2
0.10	Mean	0.02742	0.01642	0.01210	0.00101	0.01210	0.00034	0.37323	0.33245	0.01175	0.00294	0.09832	0.01008
	S.D.	0.01507	0.01921	0.00637	0.00162	0.00637	0.00019	0.42703	0.51279	0.01537	0.00745	0.11682	0.02251
	Max	0.05598	0.05899	0.02488	0.00583	0.02488	0.00071	1.22139	1.68054	0.05727	0.02527	0.43106	0.07686
	Min	0.01174	0.00045	0.00234	0.00011	0.00234	0.00009	0.00939	0.00046	0.00317	0.00010	0.01294	0.00014
0.05	Mean	0.03258	0.03148	0.01602	0.00052	0.01602	0.00044	0.64984	0.99899	0.00727	0.00095	0.07162	0.00391
	S.D.	0.04085	0.03988	0.00698	0.00039	0.00698	0.00030	0.65737	1.24536	0.00223	0.00077	0.06749	0.00313
	Max	0.14137	0.14351	0.03579	0.00159	0.03579	0.00112	2.37088	4.15922	0.01141	0.00265	0.22549	0.01019
	Min	0.00600	0.00055	0.00928	0.00022	0.00928	0.00013	0.03677	0.01965	0.00387	0.00023	0.00771	0.00065
0.01	Mean	0.06729	0.25404	0.01436	0.00073	0.01436	0.00056	5.60250	19.94530	0.01220	0.00138	0.16730	0.01500
	S.D.	0.05092	0.33403	0.00861	0.00043	0.00861	0.00031	2.85429	14.28540	0.00938	0.00167	0.11001	0.01549
	Max	0.19501	1.15268	0.03116	0.00134	0.03116	0.00115	11.79850	45.68990	0.03823	0.00633	0.40762	0.05500
	Min	0.01776	0.00663	0.00467	0.00010	0.00467	0.00019	0.71216	1.32382	0.00356	0.00044	0.03192	0.00274

*1) Sum of the absolute errors of the largest two eigenvalues. The differences between the results of a perturbation method and the exact method are considered to be errors.

*2) Sum of Euclidean norms of the errors of the eigenvectors associated with the largest two eigenvalues.

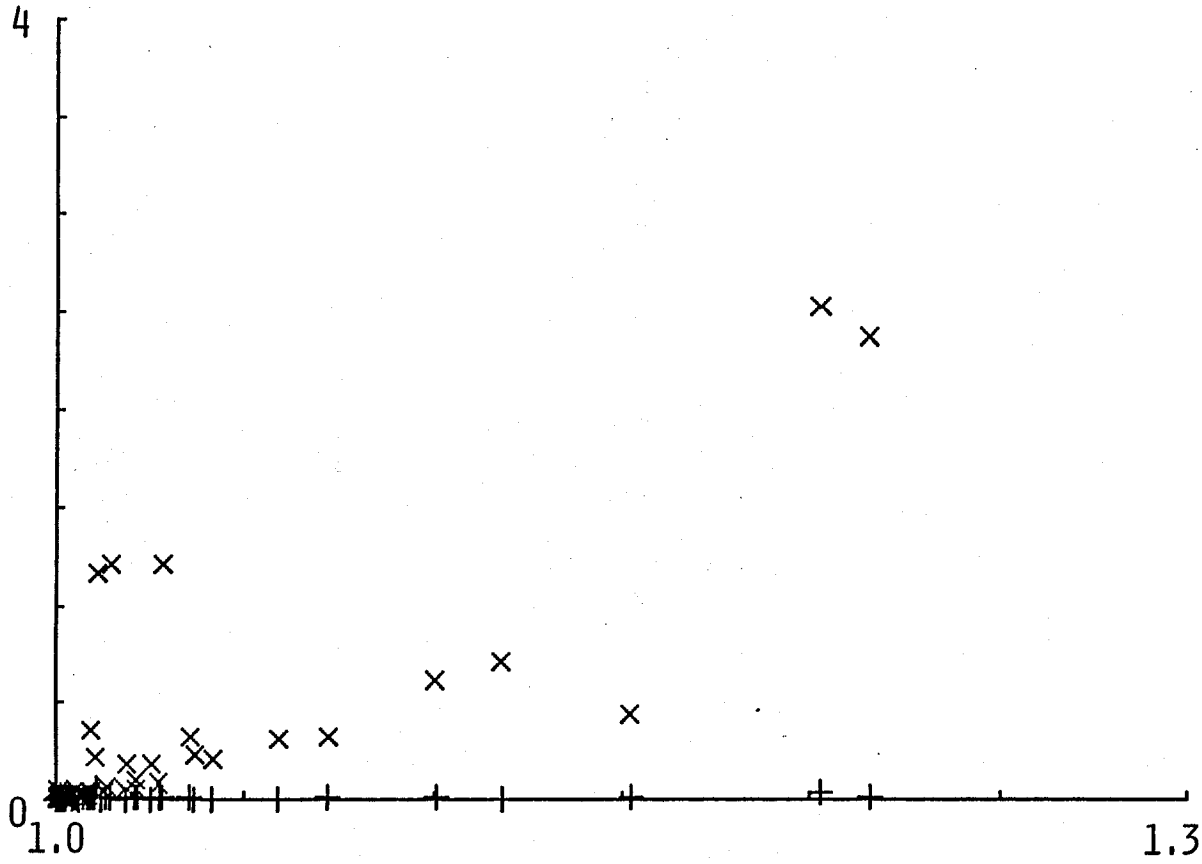

Fig. 5.1 Relationship between the norm and the amount of error of eigenvector.

Notes.

(1) The x- and y- axes indicate the maximum of the norms of eigenvectors and the sum of the Euclidean norms of errors of eigenvectors, respectively.

(2) The marks x and + indicate the results of the perturbation assuming simple eigenvalues (PS1) and those assuming multiple eigenvalues (PM1), respectively.

(3) The points whose x-values are more than 1.3 are omitted in the above figure.

deviate from 1.0 in most cases when the errors of eigenvectors are large. So we may find whether the error of the PS method is large or not by checking the norms of eigenvectors. In Fig. 5.1 there are three cases where the norms of eigenvectors do not deviate much from 1.0 but the values have large errors. The rotations of axes of the first and second eigenvectors are observed in these three cases.

Next, to investigate the effect of the size of ε, we generated ten sets of $H(\varepsilon)$'s by putting $\Delta=0.5$(fixed) and $\varepsilon=0.01,0.05,0.10,0.20$, and calculated the eigenvalues and eigenvectors. The results are shown in Table 5.2. From this table we can see the following.

④ When ε is small, the eigenvalues and eigenvectors are calculated accurately by both of the first order and second order perturbation methods.

⑤ When ε increases, the accuracies of the both methods grow worse. However, the rate of growing worse is a little slower in the case of the second order perturbation.

Fig. 5.2 shows the relationship between $\theta_s^{(2)}$ and the error of the eigenvector based on the PS1 method. This figure suggests that we can find the case where the error of first order perturbation of eigenvector is large by checking $\theta_s^{(2)}$.

Table 5.2. Relationship between the amount of errors and the perturbation parameter(ε).
— Simulation study based on ten sets of artificially generated data —

Δ=0.5		Eigenvalue *1)						Eigenvector *2)					
ε		PS1	PS2	PM1	PM2	PM'1	PM'2	PS1	PS2	PM1	PM2	PM'1	PM'2
0.01	Mean	0.00012	0.00000	0.00011	0.00001	0.00011	0.00001	0.00015	0.00002	0.00108	0.00022	0.00014	0.00002
	S.D.	0.00007	0.00000	0.00005	0.00000	0.00005	0.00000	0.00012	0.00001	0.00017	0.00004	0.00007	0.00001
	Max	0.00028	0.00000	0.00018	0.00002	0.00018	0.00002	0.00047	0.00006	0.00143	0.00030	0.00030	0.00005
	Min	0.00004	0.00000	0.00004	0.00001	0.00004	0.00001	0.00006	0.00000	0.00089	0.00017	0.00006	0.00001
0.05	Mean	0.00287	0.00009	0.00290	0.00013	0.00290	0.00013	0.00331	0.00012	0.00415	0.00076	0.00330	0.00018
	S.D.	0.00147	0.00006	0.00126	0.00007	0.00126	0.00007	0.00173	0.00005	0.00104	0.00019	0.00134	0.00008
	Max	0.00482	0.00019	0.00488	0.00031	0.00488	0.00031	0.00621	0.00023	0.00596	0.00098	0.00571	0.00036
	Min	0.00024	0.00002	0.00116	0.00004	0.00116	0.00004	0.00125	0.00007	0.00210	0.00039	0.00121	0.00008
0.10	Mean	0.01546	0.00158	0.01216	0.00070	0.01216	0.00071	0.01878	0.00236	0.00910	0.00183	0.00832	0.00085
	S.D.	0.00825	0.00191	0.00638	0.00056	0.00638	0.00056	0.01496	0.00191	0.00535	0.00122	0.00373	0.00065
	Max	0.03109	0.00519	0.02685	0.00174	0.02685	0.00174	0.04399	0.00547	0.01822	0.00399	0.01832	0.00199
	Min	0.00567	0.00010	0.00564	0.00006	0.00564	0.00006	0.00443	0.00026	0.00226	0.00035	0.00463	0.00006
0.20	Mean	0.07711	0.00677	0.06559	0.00409	0.06559	0.00417	0.03778	0.01142	0.02707	0.00530	0.03019	0.00495
	S.D.	0.02393	0.00643	0.03099	0.00297	0.03099	0.00301	0.02172	0.00975	0.01121	0.00277	0.01604	0.00355
	Max	0.11764	0.01955	0.11764	0.00847	0.11764	0.00855	0.08836	0.03855	0.04293	0.01037	0.07178	0.01103
	Min	0.04030	0.00088	0.01290	0.00072	0.01290	0.00072	0.01648	0.00146	0.00845	0.00211	0.01071	0.00102

*1) Sum of the absolute errors of the largest two eigenvalues. The differences between the results of a perturbation method and the exact method are considered to be errors.
*2) Sum of Euclidean norms of the errors of the eigenvectors associated with the largest two eigenvalues.

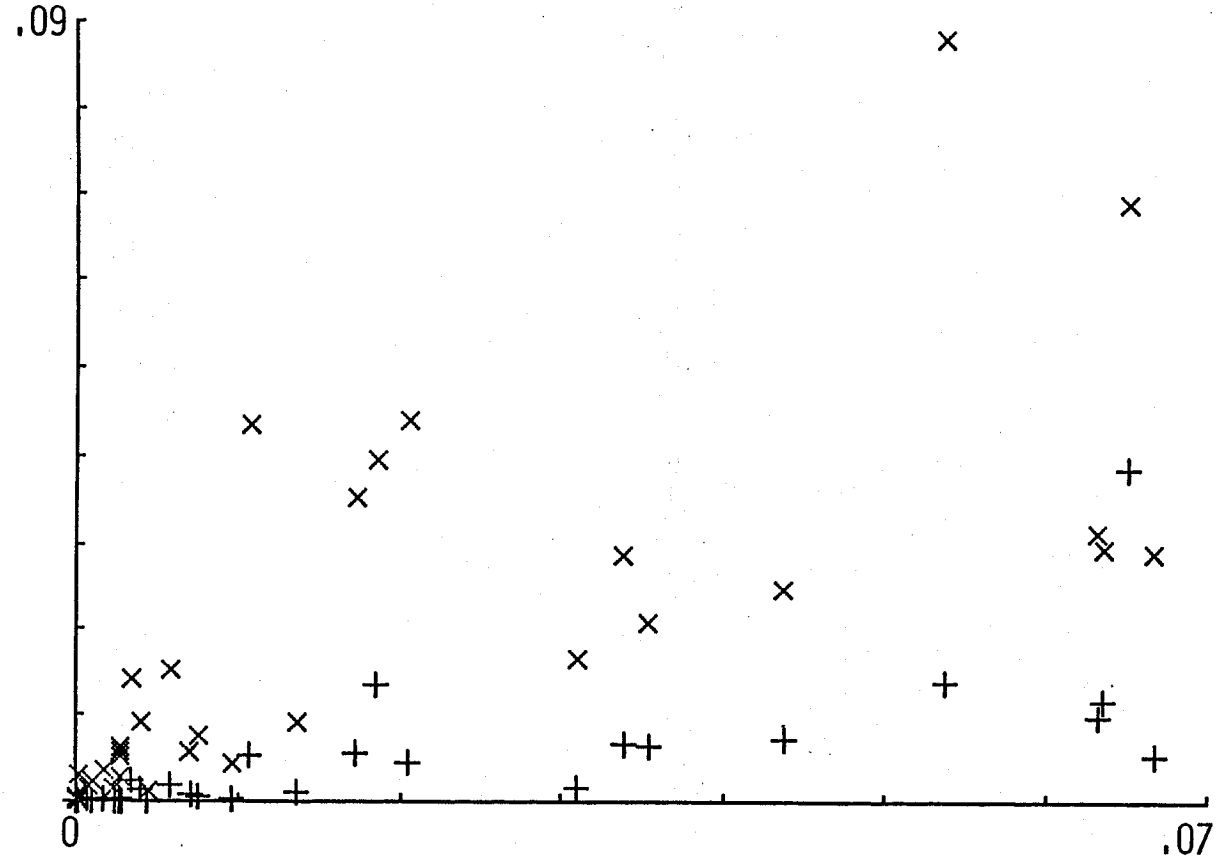

Fig. 5.2 Relationship between $|\varepsilon^2\theta^{(2)}|$ and the amount of error of eigenvector.

Notes.

(1) The x- and y- axes indicate the maximum of $|\varepsilon^2\theta_s^{(2)}|$, s=1,2 and the sum of the Euclidean norms of errors of eigenvectors, respectively.

(2) The marks x and + indicate the results of the first order perturbation (PS1) and those of the second order perturbation (PS2), respectively.

5.2 Discussion and summary

We considered six computational methods based on the perturbation theory assuming simple or multiple eigenvalues. Then we applied them to the artificially generated matrices $H(\varepsilon)$ and compared their degrees of accuracy. The results showed that, when there are close eigenvalues among those of interest, the methods assuming simple eigenvalues do not work well and that, when ε is large, the second order perturbation is a little better than the first order perturbation.

From the viewpoint of computing speed the PS1 method is the best. So we recommend to use the PS1 method in the ordinary case. When the closeness of eigenvalues causes the inaccuracy of the PS1 method, the norm of eigenvector usually deviates from 1.0. Therefore we can switch over to the PM1 method in such cases.

Comparing with the difference between PS and PM the difference between the 1st and 2nd orders is relatively small. However, if we wish to switch from the 1st to the 2nd or vice versa we may consider as follows. When we have already obtained $\theta_s^{(1)}$ and $\mathbf{v}_s^{(1)}$, it is easy to compute $\theta_s^{(2)}$ in addition to $\theta_s^{(1)}$ and $\mathbf{v}_s^{(1)}$. If we compute $\theta_s^{(2)}$ in the first order perturbation additionally and to check the value of $\varepsilon^2\theta_s^{(2)}$ or $\varepsilon\theta_s^{(2)}/\theta_s^{(1)}$, we can find the case when the first order perturbation gives poor approximation.

In our sensitivity analysis we first search for influential observations by checking each individual in turn and then

investigate the effects of the influential observations precisely by the aid of graphical representation. Usually we must evaluate the eigenvalues and eigenvectors of slightly different matrices many times at the first step. So we recommend to use the approximate method such as PS1 or PM1 especially at the first step from the viewpoint of computing speed. We may use the exact method at the second step when we need the result with high accuracy even if it requires much time.

Acknowledgment

The author wishes to thank Professor M. Okamoto of Osaka University for his valuable suggestions and helpful comments. He is also grateful to Professor Y. Tanaka of Okayama University, who is the coauthor of the papers which include the contents of Chapter 2, 3 and 5, for his advice and continual encouragement.

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