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THE REAL-VALUED MODEL OF HIERARCHICAL CLASSES

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The real-valued model of hierarchical classes

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Abstract

A novel hierarchical classes model (RV-HICLAS) for two-way two-mode data is introduced. As the other members of the HICLAS family, the new model implies simultaneous hierarchically organized classifications of all modes involved in the data. A distinctive feature of the novel model, however, reads that it yields continuous, real-valued reconstructed data; this considerably broadens the potential application range of the HICLAS family. Estimates of RV-HICLAS models are found by minimizing an L_p-norm based loss function. In order to solve the associated optimization problem, a two-stage algorithm combining a simulated annealing and an alternating local descent stage is proposed. This algorithm is subsequently evaluated in a simulation study. Finally, the new RV-HICLAS model is applied to an empirical data set on anger.

1 Introduction

Data sets collected in many research domains can be regarded as a mapping from the Cartesian product of N sets of entities to some value set (for example, the set of reals $\mathbb{R}$ or the Boolean set $\mathbb{B} = \{0, 1\}$). If all sets in the Cartesian product are distinct, the data set is referred to as N-way N-mode (Carroll & Arabie, 1980).

A challenge for the data analyst is to capture the structural information that is present in N-way N-mode data. HICLAS models try to achieve this goal by capturing this information by means of simultaneous overlapping clusterings for several or all modes involved in the data. These clusterings are further hierarchically organized, in terms of (generalized) if-then type rules between partition classes that can be derived from the overlapping clusterings. Furthermore, the whole of the clusterings, possibly together with an N-way linking array, allows for an approximate reconstruction of the data. As such, HICLAS models always imply two- or multiway data with the associated aim of reconstructing the actual data values, rather than of summarizing dependency information, as implied by a two- or multiway contingency table, or of summarizing interaction information, as implied by two- or multiway data on the value of a criterion variable associated with all combinations of values of a number of categorical predictor variables. Finally, HICLAS models typically go with comprehensive graphical representations.

Up to now, only HICLAS models have been developed that imply two- or three-way binary or rating-valued reconstructed data (De Boeck & Rosenberg, 1988; Leenen, Van Mechelen, De Boeck, & Rosenberg, 1999; Ceulemans, Van Mechelen, & Leenen, 2003; Van Mechelen, Lombardi, & Ceulemans, in press). Yet, often it may be desirable to have models at one's disposal that include real-valued reconstructed data values, and this in at least two types of cases. First, in some cases it may be desirable to allow for real-valued reconstructed data, whereas the actual data are not real-valued; for example, modeling a binary data set with reconstructed data values in the interval

[0, 1] may allow the reconstructed data to be interpreted in terms of probabilistic association strength. Second, in several research domains, the observed data are not of a categorical type, but rather are values on a continuous scale; examples include response times, intensity of brain waves, muscle tensions and gene expression strengths; in order to deal with such data properly, often it may be desirable to approximate them by reconstructed data that take values from the same set, $\mathbb{R}$. Although the transition from binary/rating-valued to real-valued may seem to involve only a minor challenge, expanding the HICLAS family to real values implies the need for a new mathematical framework and a new algorithmic approach for model estimation.

In this paper, we will propose a novel hierarchical classes model that implies real-valued reconstructed data, the real-valued hierarchical classes model (RV-HICLAS); subsequently we will propose and evaluate an algorithm to estimate it.

The remainder of this paper is organized as follows: In Section 2, to make this paper self-contained, we will briefly recapitulate two important existing members of the HICLAS family. In Section 3 we will then introduce the novel RV-HICLAS model and discuss its estimation. Section 4 presents the results of a simulation study, an illustrative application is discussed in Section 5 and some concluding remarks are given in Section 6.

2 HICLAS and HICLAS-R

In this section, we briefly recapitulate two important representatives of the family of HICLAS models: the original (disjunctive) hierarchical classes model (HICLAS) as introduced by De Boeck and Rosenberg (1988) and the rating-valued hierarchical classes model (HICLAS-R) as introduced by Van Mechelen et al. (in press).

2.1 HICLAS

2.1.1 model

The original HICLAS model (De Boeck & Rosenberg, 1988) has been introduced as a model for two-mode $I \times J$ binary object by attribute data matrices $\mathbf{D}$. These data are approximated by an $I \times J$ matrix $\mathbf{M}$ of binary reconstructed data values that can be represented by a rank R HICLAS model. Such a model includes a binary $I \times R$ matrix $\mathbf{A}$ and a binary $J \times R$ matrix $\mathbf{B}$. The columns in $\mathbf{A}$ and $\mathbf{B}$ represent (possibly overlapping) clusters of objects and attributes, which will further be called bundles; correspondingly, $\mathbf{A}$ and $\mathbf{B}$ will be called bundle matrices.

Three types of relations implied by $\mathbf{M}$ are represented by the bundle matrices: equivalence, hierarchy and association. To illustrate, in Table 1, we will make use of the hypothetical reconstructed data matrix $\mathbf{M}$ and the rank 2 HICLAS model for these reconstructed data in Table 2.

Equivalence relations are defined on both the objects and attributes as follows: Each object (attribute) corresponds to a row (column) in $\mathbf{M}$; two objects are equivalent iff they correspond to identical rows in $\mathbf{M}$, a similar definition holds for the attributes. In Table 1, objects o_1 and o_3 are equivalent, as are attributes a_2 and a_4. Equivalence relations are represented by the bundle matrices in terms of identical binary row patterns for two equivalent objects (attributes). By the representation of the equivalence relations and their implied equivalence classes, the HICLAS model includes a partition of the two modes of the data.

Hierarchical relations are also defined on the elements of both modes of $\mathbf{M}$. These are if-then type relations and can be considered as quasi-orders on the elements, or as partial orders on the corresponding equivalence classes. Object i is hierarchically below object i' if the row in $\mathbf{M}$ corresponding to object i is a subset of the row corresponding to object i', a similar definition holds for the attributes. In Table 1, object o_2 is hierarchically below object o_1, and attribute

a_1 is hierarchically below attribute a_3. The hierarchical relations are represented by the bundle matrices of the HICLAS model in terms of subset-superset relations between the binary patterns corresponding to two objects (attributes). By the representation of the hierarchical relations, the classifications included in a HICLAS model turn into hierarchically organized partitions.

The *association relation* is the binary relation that links the objects and the attributes. It is represented by the decomposition rule of the HICLAS model:

$$m_{ij} = \bigoplus_{r=1}^{R} a_{ir} b_{jr} \qquad \forall i, j \tag{1}$$

where $\bigoplus$ denotes the Boolean sum, a_{ir} is the entry in the $i-th$ row and the $r-th$ column of the bundle matrix $\mathbf{A}$ and b_{jr} is the entry in the $j-th$ row and the $r-th$ column of the bundle matrix $\mathbf{B}$. The decomposition rule in (1) implies that object i is associated to attribute j iff they share at least one corresponding bundle.

Any HICLAS model goes along with a comprehensive and insightful graphic representation. Figure 1 illustrates this for the HICLAS model in Table 2. The upper half of the figure represents the partition of the objects, and the lower half that of the attributes. In the partition of the objects, hierarchical relations are represented by downward paths between the boxes that denote the equivalence classes. In the partition of the attributes, they are represented by upward paths between the equivalence classes. The association relation between object i and attribute j is represented by a path that includes a dashed line between that object-attribute pair.

2.1.2 data analysis

The goal of a HICLAS analysis is to find, given a data matrix $\mathbf{D}$, a reconstructed data matrix $\mathbf{M}$ that can be represented by a HICLAS model of a prespecified rank, such that $\mathbf{M}$ approximates the data $\mathbf{D}$ as closely as possible. In particular, the following loss function is minimized:

$$f(\mathbf{M}) = \sum_{i=1}^{I} \sum_{j=1}^{J} |d_{ij} - m_{ij}| \tag{2}$$

Note that in the binary case this loss function can be considered to be both of a least squares and of a least absolute deviations type.

To minimize loss function (2), De Boeck and Rosenberg (1988) proposed an algorithm that consists of two routines: In the first routine, bundle matrices are looked for that combine by decomposition rule (1) to a model matrix $\mathbf{M}$ for which (2) is minimal. The second routine then transforms the bundle matrices so as to make them represent the set-theoretical relations of equivalence and hierarchy in $\mathbf{M}$ correctly.

In particular, the first routine is of an alternating least-squares type. Assuming an initial configuration for one of the bundle matrices, the procedure re-estimates, by means of Boolean regressions, the rows of the companion bundle matrix, conditionally upon the other. This is repeated until further updates do not improve the loss function (2).

In the second routine, the set-theoretical relations are added to the bundle matrices obtained at the end of the first routine. This is accomplished by applying a closure operation (Barbut & Monjardet, 1970; Birkhoff, 1940) to the bundle matrices, implying that all individual entries of the bundle matrices with value 0 are changed to 1 if this modification does not alter $\mathbf{M}$. As shown by De Boeck and Rosenberg (1988), this operation ensures that the bundle matrices correctly represent the equivalence and hierarchy relations in $\mathbf{M}$.

2.2 HICLAS-R

2.2.1 model

Van Mechelen et al. (in press) introduced the HICLAS-R model for rating-valued two-mode $I \times J$ object by attribute data matrices $\mathbf{D}$. These data are approximated by an $I \times J$ matrix $\mathbf{M}$ of rating-valued reconstructed data entries that can be represented by a rank (R, S, T) HICLAS-R model. This model includes a binary $I \times R$ matrix $\mathbf{A}$, a binary $J \times S$ matrix $\mathbf{B}$ and a $R \times S$ rating-valued linking matrix $\mathbf{G}$ that takes T distinct nonzero values. $\mathbf{A}$ and $\mathbf{B}$ are called object and attribute bundle matrices, $\mathbf{G}$ the core. In general one may note that in HICLAS-R, unlike in HICLAS, there is no longer a one-to-one correspondence between object and attribute bundles, with the number of object bundles R further possibly being different from the number of attribute bundles S.

As in the original HICLAS model, three types of relations implied by $\mathbf{M}$ are represented by the HICLAS-R model: equivalence, hierarchy and association. To illustrate, we will make use of a hypothetical reconstructed data matrix $\mathbf{M}$ in Table 3 and the $(3, 3, 3)$ HICLAS-R model for these reconstructed data in Table 4.

Equivalence relations are defined and represented in the same way as in the binary case. Again they are represented by equivalent elements taking identical bundle patterns. In Table 3, objects o_2 and o_5 are equivalent.

Hierarchical relations are in the rating-valued case generalized if-then type relations: Object i is hierarchically below object i' if all the entries of the row in $\mathbf{M}$ pertaining to object i are less than or equal to the corresponding entries of the row in $\mathbf{M}$ pertaining to object i', a similar definition holds for the attributes. In Table 3, object o_1 is hierarchically below object o_3, and attribute a_4 is hierarchically below attribute a_3. Hierarchical relations again can be considered as quasi-orders on the elements, or as partial orders on the corresponding equivalence classes, and in the HICLAS-R model they are represented by subset-superset relations between bundle patterns.

The *association relation* is the mapping that links each object-attribute pair to its corresponding value in $\mathbf{M}$. This relation is represented by the following decomposition rule:

$$m_{ij} = \max_{r=1}^{R} \max_{s=1}^{S} a_{ir} b_{js} g_{rs} \qquad \forall i, j \tag{3}$$

where max denotes the maximum operator, a_{ir} is the entry in the $i-th$ row and the $r-th$ column of the bundle matrix $\mathbf{A}$, b_{js} is the entry in the $j-th$ row and the $s-th$ column of the bundle matrix $\mathbf{B}$ and g_{rs} is the entry in the $r-th$ row and the $s-th$ column of the core matrix $\mathbf{G}$. Rule (3) implies that object i is associated to attribute j with strength g_{rs} iff g_{rs} is the largest value in

G for which it holds that object i and attribute j belong to bundles r and s, respectively.

Figure 2 is a graphic representation of the HICLAS-R model in Table 4. Equivalence and hierarchy relations may be read from this figure in the same way as in Figure 1. The association relation between object i and attribute j is represented by the largest value contained in the hexagons which are included in a path between that object-attribute pair. For example, the rating value associated to object o_7 and attribute a_3 is the maximum of 3, 1 and 2, that associated to object o_2 and attribute a_1 is simply 1. By comparing Figure 2 to Figure 1, it should stand out that in Figure 2 one object bundle may be linked, via a hexagon, to more than one attribute bundle, and vice versa.

2.2.2 data analysis

For a given rating-valued data matrix **D**, a HICLAS-R model is estimated by minimizing the sum of absolute deviations between a rating-valued reconstructed data matrix **M** and **D**. The mathematical expression of the loss function is again (2). Note, however, that in the rating-valued case this loss function can no longer be considered of a least squares type as well.

To minimize the loss function, Van Mechelen et al. (in press) proposed an algorithm that consists of three steps. In the first step, the two-way two-mode rating data matrix **D** is mapped into a three-way three-mode binary array $\mathbf{t(D)}$ by a dummy recoding according to an ordinal coding scheme, which preserves the relations of equivalence and hierarchy. Next, a three-mode extension of the HICLAS algorithm, Tucker3-HICLAS (Ceulemans et al., 2003), is applied to the three-way three-mode binary array $\mathbf{t(D)}$. Finally, the Tucker3-HICLAS solution is recoded back, yielding a reconstructed matrix **M** of rating values that can be represented by a HICLAS-R model. Note that the fact that in the data-analytic process the rating-valued data matrix **D** is recoded into a binary three-way three-mode array underscores the inherently discrete nature of the HICLAS-R model.

3 RV-HICLAS

3.1 model

In this section, we propose a novel HICLAS model, RV-HICLAS, for positive real-valued two-mode $I \times J$ object by attribute data matrices $\mathbf{D}$. These data (which include binary and rating-vlued data as special cases) are approximated by an $I \times J$ matrix $\mathbf{M}$ of positive real-valued reconstructed data entries that can be represented by a rank (R, S) RV-HICLAS model. This model includes a binary $I \times R$ matrix $\mathbf{A}$, a binary $J \times S$ matrix $\mathbf{B}$ and a $R \times S$ positive real-valued linking matrix $\mathbf{G}$, which are called the object and attribute bundle matrices, and the core, respectively.

Equivalence relations are defined and represented in the same way as in the rating-valued case.

Hierarchical relations are again generalized if-then type relations that in the real-valued case are defined and represented in the same way as in the rating-valued case.

The *association relation* is the mapping that links each object-attribute pair to its corresponding value in $\mathbf{M}$. This relation is represented by the decomposition rule:

$$m_{ij} = \max_{r=1}^{R} \max_{s=1}^{S} a_{ir} b_{js} g_{rs} \qquad \forall i, j \tag{4}$$

A graphic representation of the RV-HICLAS model is analogous to that of HICLAS-R, except for the fact that the hexagons linking the bundles may contain real values. This implies that the relations of equivalence, hierarchy and association can be read from a RV-HICLAS graphic in the same way as for HICLAS-R. An example of such a graphic representation may be found in Section 5 for an empirical anger data set (Figure 4).

Note that g_{rs} is now positive real-valued, which implies that decomposition (4) takes place in the mathematical structure $(\mathbb{R}^+, \max, \times)$. This tropical semiring and its isomorphic algebraic structure, the max-plus algebra, have recently been the subject of intensive study (see, e.g., Baccelli, Cohen, Olsder, & Quadrat, 1993; Gaubert & Max Plus, 1997; De Schutter, Blondel, De Vries, &

De Moor, 1998). Note further that the rank of the RV-HICLAS model is indicated by the couple (R, S), implying that the restriction to only T distinct nonzero values in the core as in HICLAS-R is relaxed.

The novel RV-HICLAS implies several mathematical questions and challenges. Below, we discuss three of these more in detail: (1) the fact that only positive real-valued data are reconstructed, (2) existence of the RV-HICLAS model and (3) uniqueness.

(1) Positive-valued reconstructed data.

The RV-HICLAS model implies reconstructed data entries that take values from the set of positive reals $\mathbb{R}^+$ including 0. As we will explain, this is desirable both from a data-analytical and as from a set-theoretical point of view.

From a data-analytical perspective, negative values could be considered on the level of the reconstructed data as well as on the level of the core entries. In this regard, if there would be negative values in $\mathbf{G}$ only and not in $\mathbf{M}$, it is easy to see that these negative core values may always be increased to zero, without affecting the reconstructed data entries. On the other hand, if some $m_{ij} < 0$, then this implies that the bundle patterns of object i and attribute j contain 1's only and that all entries in the core are necessarily negative. It is straightforward then to derive that $\mathbf{M}$ contains only two possible values: 0 and the largest entry in $\mathbf{G}$, which is undesirable from a data-analytical perspective, since in general $\mathbf{D}$ contains many more than two values.

From a set-theoretical perspective, the restriction to positive values is necessary. Indeed, in case some $m_{ij} < 0$ it can be deduced that the subset-superset relation between the bundle pattern of object i and any other object i' with a different bundle pattern does not represent the hierarchical relation between i and i' in $\mathbf{M}$ correctly. This follows immediately from the fact that the bundle pattern for object i necessarily contains all 1's, and that the bundle pattern for object i' therefore is a subset of that for object i, although $m_{i'j} \geq 0$ and hence $m_{i'j} > m_{ij}$.

One may note that the restriction to positive real values is linked to the existence of a neutral and absorbing element. In particular, 0, which is one of the binary values being used in the bundle matrices, is neutral with respect to max and absorbing with respect to $\times$ in $(\mathbb{R}^+, \max, \times)$. It is easy to see that if we include negative values, as in $(\mathbb{R}, \max, \times)$, 0 is no longer neutral with respect to the maximum operator. Moreover, a null element in this case does not exist.

(2) Existence.

Given an $n \times m$ positive real-valued matrix $\mathbf{D}$, an exact RV-HICLAS decomposition of $\mathbf{D}$ always exists. To clarify this, we first rewrite decomposition (4) in an equivalent matrix notation:

$$\mathbf{M} = \mathbf{A} \otimes \mathbf{G} \otimes \mathbf{B}' \tag{5}$$

where $'$ denotes matrix transpose and $\otimes$ denotes the max-$\times$ matrix product (which is similar to the normal matrix product in linear algebra except for the fact that addition is replaced by max). Then, it is easy to see that an exact RV-HICLAS decomposition exists under the form of $\mathbf{D} = \tilde{\mathbf{I}}_n \otimes \mathbf{D} \otimes \tilde{\mathbf{I}}_m'$, where $\tilde{\mathbf{I}}_x$ denotes the closure of the $x \times x$ identity matrix.

(3) Uniqueness.

HICLAS models do not suffer from a general type of nonuniqueness, except for permutations of the bundles. For particular reconstructed data matrices $\mathbf{M}$, however, decomposition (4) may be nonunique. To be sure that this is not the case it is of interest to identify those characteristics of the reconstructed values that yield such a unique decomposition. For the binary HICLAS models, sufficient conditions for uniqueness have been given (Ceulemans & Van Mechelen, 2003). In Schepers and Van Mechelen (2007) these sufficient uniqueness conditions are generalized to RV-HICLAS. We recapitulate here the central result and refer to Schepers and Van Mechelen (2007) for a proof.

Theorem. *If a (R, S) RV-HICLAS decomposition of an $I \times J$ real-valued matrix $\boldsymbol{M}$ exists, such that (1) all bundle specific object (resp. attribute) classes are non-empty, and (2) no object (attribute) plane of $\boldsymbol{G} \leq$ the elementwise maximum of the other object (attribute) planes of $\boldsymbol{G}$, this decomposition is unique upon a permutation of the object and attribute bundles.*

If a solution violates this uniqueness condition, nonidentifiability may exist in the binary as well as in the real-valued part of the model. With respect to the latter, part of this nonuniqueness is removed by retaining only the maximal solution, $\mathbf{G}_{\max}$. Note that this is related to the closure operation applied to the bundle matrices (as explained in 2.1.2) and can also be considered a case of finding the largest subsolution, a topic in residuation theory in max-plus algebra (see Baccelli et al., 1993).

3.2 data analysis

3.2.1 Loss function

The aim of a RV-HICLAS analysis is to look for a model matrix $\mathbf{M}$, that can be represented by an RV-HICLAS model of rank (R, S), and that minimizes the following L_p-norm based loss function:

$$f(\mathbf{M}) = (\sum_{i=1}^{I} \sum_{j=1}^{J} |d_{ij} - m_{ij}|^p)^{1/p} \tag{6}$$

In particular, we will focus on the cases $p = 1$ (least absolute deviations) and $p = 2$ (least squares). Note that the estimation of HICLAS-R exclusively relied on a least absolute deviations loss function. This relates to the fact that the estimation in question relies on an equivalent reformulation of the HICLAS-R model into a binary Tucker3-HICLAS model (Ceulemans et al., 2003). For RV-HICLAS, we will consider the more familiar least squares loss function as well, allowing for better comparisons with other data-analytic methods.

3.2.2 Algorithm

Within the HICLAS family the optimization of (6) implies a new kind of problem: Whereas the estimation of all existing HICLAS models comes down to a discrete optimization problem, the estimation of the RV-HICLAS model involves a mixed-integer optimization problem. In particular, the estimation of $\mathbf{A}$ and $\mathbf{B}$ involves an optimization over the Boolean spaces $\mathbb{B}^{I\times R}$ and $\mathbb{B}^{J\times S}$, respectively, whereas the estimation of $\mathbf{G}$ involves an optimization over the real space ($\mathbb{R}^{R\times S}$).

In order to find the solution that minimizes (6) for $p = 1$ or $p = 2$, we propose an algorithm consisting of two stages. The first stage is a simulated annealing (SA) step and the second one a deterministic local descent (LD) that starts from the solution returned by the SA stage. Using such a two-stage procedure ensures that at least a locally optimal solution is obtained (Aarts & Lenstra, 1997) since the LD stage may act as a (quick) local optimum check in case no improvement was reached, or it may improve the value of the loss function to a (local) minimum. In the study of a different model Brusco (2001) found in this regard that the combination of SA and LD showed good results.

Every run of the two-stage algorithm proposed here starts from a randomly chosen initial solution. As discussed above, the algorithm may end up in a local optimum. Therefore, it is desirable to run it multiple times, each time starting from a different initial solution. In particular, we used 50 independently drawn initial solutions in such a multistart strategy, retaining only the best outcome as the estimated solution.

First stage: Simulated annealing.

For a general introduction, see Aarts and Lenstra (1997). The *basic architecture* of the SA stage is the following: Given a current solution for (6), a trial solution is generated and evaluated to see whether its loss function value is smaller than that of the current solution. If this is the case, the current solution is always replaced by the trial solution; if the trial solution does not improve the loss function value the current solution is replaced by it with probability

$$P = e^{\frac{f_t - f_c}{\tau}} \qquad (7)$$

with τ denoting the current temperature of the annealing process, and f_c and f_t the values of the loss function corresponding to the current and trial solutions, respectively. During the annealing process, the temperature τ is gradually decreased in a series of steps (chains), resulting in an expected decrease of the probability parameter (7) during the annealing process. Within each chain, τ is kept constant.

To estimate the RV-HICLAS model, the following specifications and metaparameters have been chosen for the SA stage of the algorithm. First, the *initial solution* is generated by drawing the entries of the bundle matrices **A** and **B** *iid* from a Bernoulli distribution with parameter $\pi = .5$, subject to the restriction that no empty bundles are present. The entries in the initial core matrix **G** are further drawn *iid* from a uniform distribution with lower and upper bound equal to d_{min} and d_{max}, respectively, as those can be easily shown to be the theoretical minimum and maximum for the core values. To generate *trial solutions* the following stochastic mechanism is used given a current solution $(\mathbf{A}, \mathbf{B}, \mathbf{G})^c$. A trial solution $(\mathbf{A}, \mathbf{B}, \mathbf{G})^t$ is generated by altering the value of one arbitrarily selected single entry of **G**, or one arbitrarily selected row pattern in **A** or **B**, making use of a discrete uniform distribution. For the binary bundle matrices, altering the value of an object (resp. attribute) row pattern implies that it is replaced by a pattern drawn uniformly from the set of all 2^R (resp. 2^S) binary row patterns, whereas for the real-valued core matrix **G**, altering an entry implies that its current value is replaced by a value drawn uniformly from the real interval $[d_{min}, d_{max}]$. Third, an *initial temperature* is chosen such that the annealing process accepts a high number of trial solutions in the early stages of the process. For this purpose, one chain is generated in which all trial solutions are accepted. For every pair of successive solutions, the difference $\triangle f = f_{n-1} - f_n$ between the corresponding loss function values is stored if this difference is smaller than zero (or, in other words, if the new solution is worse). After a complete pass through this initial chain, the estimated initial temperature τ_{init} is calculated as:

$$\tau_{init} = \frac{\text{average} \triangle f}{\ln(0.8)} \tag{8}$$

resulting in an average acceptance probability for worse solutions of .8 at τ_{init} (see, e.g., Murillo, Fernando Vera, & Heiser, 2005). Fourth, the *chain length*, that is, the number of generated solutions within one chain, was set equal to $I \times 2^R + J \times 2^S$. Fifth, with regard to the cooling scheme, each time the algorithm has passed through one complete chain, the current temperature of the annealing process (τ_c) is lowered to $\tau_{new} = .975 \times \tau_c$. Finally, the final temperature τ_{final} was set equal to 10^{-6}. This implies that

$$TD = \frac{\log(\tau_{final}) - \log(\tau_{init})}{\log(.975)} \tag{9}$$

chains will be passed through during the whole annealing process (Brusco, 2001), after which the algorithm stops. The best overall solution encountered during the whole process is finally retained and returned as the estimated solution after completion of the SA algorithm. Note that in most cases, the last generated trial solution is the same as the best overall solution.

Second stage: Alternating local descent.

In the second stage of the algorithm, trial solutions worse than the current solution are no longer accepted. In particular, starting with initial values ($\mathbf{A}^0$,$\mathbf{B}^0$,$\mathbf{G}^0$), which are provided by the simulated annealing stage, alternatingly, the best fitting $\mathbf{G}^w$, given $\mathbf{A}^{w-1}$ and $\mathbf{B}^{w-1}$, the best fitting $\mathbf{A}^w$, given $\mathbf{B}^{w-1}$ and $\mathbf{G}^w$, and the best fitting $\mathbf{B}^w$, given $\mathbf{A}^w$ and $\mathbf{G}^w$ are looked for ($w = 1, 2, ...$), until no more improvement in the value of the loss function is observed.

The conditional estimation of, for example, the object bundle matrix $\mathbf{A}$, given $\mathbf{B}$ and the core

G, comes down to the following optimization problem:

$$\min_{a_{ir}\in\{0,1\}} (\sum_{i=1}^{I}\sum_{j=1}^{J} |d_{ij} - \max_{r=1}^{R}\max_{s=1}^{S} a_{ir}b_{js}g_{rs}|^{p})^{1/p}, \tag{10}$$

Since (10) satisfies a separability property, conditionally optimal estimates for **A** can be obtained by optimizing the individual rows of **A** separately. To this end, for each row separately, an enumerative evaluation of all binary patterns is performed; in case of ties, the solution with the largest number of ones is retained, such that the set-theoretical relations in **M** are necessarily represented correctly by the bundle matrices. A conditionally optimal estimate of the attribute bundle matrix **B** is obtained similarly.

The conditional estimation of the real-valued core matrix **G** comes down to the following continuous optimization problem:

$$\min_{g_{rs}\in\mathbb{R}^{+}} (\sum_{i=1}^{I}\sum_{j=1}^{J} |d_{ij} - \max_{r=1}^{R}\max_{s=1}^{S} a_{ir}b_{js}g_{rs}|^{p})^{1/p} \tag{11}$$

Locally optimal estimates of (11) can be obtained by applying multivariate continuous optimization procedures such as Quasi-Newton, Levenberg-Marquardt or Sequential Quadratic Programming (SQP) (see Nocedal and Wright (1999) for detailed information on these optimization procedures). We propose to use a quasi-Newton line-search SQP approach, which also allows to provide the algorithm with the theoretical lower and upper bounds for the core entries, i.e., d_{min} and d_{max}, respectively. Note that as an initial value the previous estimate $\mathbf{G}^{w-1}$ is used. This implies that the algorithm ($\mathbf{A}^{w-1}\mathbf{B}^{w-1}\mathbf{G}^{w-1}\mathbf{A}^{w}\mathbf{B}^{w}\mathbf{G}^{w}\mathbf{A}^{w+1}\mathbf{B}^{w+1}$...) converges monotonically to a (possibly local) minimum.

4 Simulation study

In this section, we present a simulation study to examine the performance of the proposed algorithm with respect to the minimization of the loss function (4.2.1) and with respect to the extent to which the optimal solutions recover the truth underlying the data (4.2.2).

4.1 Design

In our simulation study three different types of real-valued $I \times J$ matrices must be distinguished: a true matrix $\mathbf{T}$, which can be represented by an RV-HICLAS model of a prespecified rank; a data matrix $\mathbf{D}$, which is $\mathbf{T}$ perturbed with error; and the model matrix $\mathbf{M}$ yielded by the algorithm, which can be represented by a RV-HICLAS model of the same rank as the true matrix $\mathbf{T}$.

The design of the simulation study was fully crossed, the factors being as follows:

(1) the *Size*, $I \times J$, of $\mathbf{T}$, $\mathbf{D}$, and $\mathbf{M}$, at 4 levels: 20×20, 40×40, 80×40, 150×20;

(2) the *Rank*, (R, S) of the two-mode RV-HICLAS model for $\mathbf{T}$ and $\mathbf{M}$, at 4 levels: $(2, 2)$, $(3, 3)$, $(4, 2)$, $(4, 4)$;

(3) the *Error*, ε, which is the expected proportion of variance in $\mathbf{D}$ due to error, at 4 levels: .00, .05, .15, .30;

For each combination of these three independent variables, 20 replicates were studied, yielding 20 $\times$ 4 (*Size*) $\times$ 4 (*Rank*) $\times$ 4(*Error*) = 1280 simulated data sets.

For each combination of the levels of *Size*, *Rank* and *Error*, the 20 true matrices $\mathbf{T}$ corresponding to the 20 replicates were constructed as follows: Bundle matrices $\mathbf{A}$ and $\mathbf{B}$ were randomly generated with entries that were independent realizations of a Bernoulli variable with probability parameter equal to .5, subject to the restriction that no empty columns were present. The entries in the core matrix **G** were independent realizations of a uniformly distributed variable on the real interval [0,1]. The true matrix **T** resulted from combining **A**, **B** and **G** by (4). Subsequently, a data matrix **D** was constructed by adding error to each true matrix **T** using the following expression:

$$d_{ij} \quad = \quad \max_{r=1}^{R} \max_{s=1}^{S} a_{ir} b_{js} g_{rs} + e_{ij} \qquad \forall i, j \tag{12}$$

where e_{ij} was sampled from $N(0, \sigma_\epsilon^2)$ with $\sigma_\epsilon^2 = \frac{\epsilon}{1-\epsilon}\sigma_{\mathrm{T}}^2$, ($\sigma_{\mathrm{T}}^2$ denoting the variance across all matrix entries of **T**).

Finally, all data matrices **D** were analyzed in the true rank (P, Q) with a loss function based on the L_2-norm by the RV-HICLAS algorithm. Each analysis of a data matrix **D** yielded one model matrix **M**; therefore, in total 20 (*replicates*) $\times$ 4 (*Size*) $\times$ 4 (*Rank*) $\times$ 4 (*Error*) different triplets (**T**,**D**,**M**) were obtained.

4.2 Results

4.2.1 Local Optima

In absence of knowledge about the global optimum, for each solution **M** we evaluated whether the loss value of **M** was less than or equal to the loss value of the truth. Note that the loss value of the truth equals

$$f(\mathbf{T}) = (\sum_{i=1}^{I} \sum_{j=1}^{J} |d_{ij} - t_{ij}|^2)^{1/2} \tag{13}$$

A loss value of **M** greater than that of the truth implies certainty that the obtained solution is a local optimum. This, however, happened in only one case, in particular, for a data set in the condition in which *Size* equalled 150×20, *Rank* 4×2 and *Error* .30. Therefore, in general the algorithm appears to succeed in minimizing the loss function (6), or, at least, does not yield suspect solutions.

4.2.2 Recovery of underlying truth

In order to assess how well the estimated models recover the underlying truth we calculated the relative badness-of-recovery (RBOR) of the returned solution for each simulated data set:

$$\text{RBOR} = \frac{\sum_{i=1}^{I}\sum_{j=1}^{J}(m_{ij} - t_{ij})^2}{\sum_{i=1}^{I}\sum_{j=1}^{J} t_{ij}^2} \tag{14}$$

On average, RBOR equalled .004 with a standard deviation of .007 and a range of $[0, .088]$. We further analyzed the effect of the independent variables on RBOR by means of an analysis of variance, retaining only effects with $\eta > .15$. Only for *Error* a sizeable effect was observed ($\eta = .41$). Figure 3 shows that the value of RBOR increases with increasing amounts of error in the data, implying that the estimates get further away from the underlying truth when the proportion of noise in the data increases.

insert Figure 3 somewhere here

Note that, taking into account the values of the overall mean and the range of RBOR, the overall discrepancy between the estimated model matrix $\mathbf{M}$ and the underlying true matrix $\mathbf{T}$ is always relatively small; this implies an excellent recovery of the underlying truth by the RV-HICLAS algorithm.

5 Illustrative application

In this section, we apply the RV-HICLAS model to a problem in the domain of componential emotion theory. In this domain, emotions are not treated as monolithic unities but rather as sets of components, including situational appraisals (e.g., "I feel attacked by someone else") and emotional meta-experiences (e.g., "I feel angry"). A challenge for researchers in this area is to understand the interrelations (including implicational if-then relations) between these emotional components (see, e.g., Kuppens, Van Mechelen, Smits, & De Boeck, 2003).

To study these relations with regard to the emotion of anger, we will make use of a data set in which 357 participants were asked to what degree they experienced a collection of 14 different emotion components in a set of 24 possibly anger-eliciting situations (Kuppens & Van Mechelen, 2007) (see Tables 5 and 6 for the full lists of emotion components and situations, respectively). In the present reanalysis of these data we will only focus on the general psychological question: How does the average person react in different situations? We therefore will proceed with the 24×14 situation by emotion component matrix $\mathbf{D}$ as obtained after averaging the raw data across participants.

RV-HICLAS models were fitted to $\mathbf{D}$, in ranks ranging from $(1,1)$ to $(5,5)$, yielding a set of 25 solutions. Based on a generalized scree-plot (Ceulemans & Kiers, 2006) and on the interpretability of the different solutions, the solution in rank $(3,3)$ was selected; this solution accounted for 65.89% of the variance in $\mathbf{D}$. Figure 4 shows the corresponding graphic representation.

In order to gain insight in the anger-eliciting process, we first focus on the hierarchy of the situation classes. To build an interpretation we consecutively examine the bottom classes along with all hierarchically higher situated classes, and look for distinctive characteristics for the corresponding sets of classes. For example, the empty leftmost bottom class along with its two hierarchically higher classes, contains situations such as CD-PLAYER and LET DOWN that all seem to indicate the presence of a deliberate infliction of harm (*INTENTIONALLY*). The middle bottom class (including situations such as SWIM) along with its hierarchically higher classes (including CD-PLAYER, LET DOWN and COMA) contains situations that all involve the presence of someone else rather than the participant under study (*OTHER INVOLVED*). Finally, the rightmost bottom class (including situations such as FAIL EXAM) along with its two hierarchically higher classes (including COMA and LET DOWN) involves situations with a large negative impact (*LARGE*

DAMAGE). Note that the empty bottom class in the *INTENTIONALLY* set reflects the logical relation that intentionality requires the presence of someone else.

Second, we consider the hierarchy of the emotion component classes. This hierarchy contains three non-empty bottom classes, and one class that spans these three. The top class mainly consists of emotional meta-experiences such as "I feel angry". The three bottom classes in their turn represent channels through which the emotion of anger can be triggered. Specifically, a person may feel angry because he/she is being attacked (*ATTACK*), because his/her goal is being obstructed (*GOAL BLOCKING*), and/or because someone else is to blame (*BLAME*).

Third, we may consider the link between the situation and emotion component hierarchies. For this purpose, we look at the hexagons that link the two hierarchies, and that contain linkage strength values. In Figure 4, to facilitate the interpretation, the values in the hexagons are also visualized in terms of grayscale levels (with higher values corresponding to darker gray levels). It can be seen that *LARGE DAMAGE* is almost exclusively linked to *GOAL BLOCKING*, and *OTHER INVOLVED* almost exclusively to *BLAME*, whereas *INTENTIONALLY* is linked to *GOAL BLOCKING*, *BLAME* as well as *ATTACK*. It can further be deduced that the highest levels of anger are elicited on the one hand by *LARGE DAMAGE* (which triggers anger through the *GOAL BLOCKING* channel) and on the other hand by *INTENTIONALLY* (which triggers anger primarily through *BLAME* but also to some lesser extent through the other two channels).

6 Conclusion and discussion

In this paper, a novel hierarchical classes model has been proposed that includes positively real-valued reconstructed data. As such it implied the need for a new mathematical framework and a new algorithmic estimation approach. With respect to the latter, unlike for the other members of the HICLAS family, the corresponding optimization problem is no longer purely discrete but mixed discrete-continuous. In order to solve it, a two-stage algorithm, consisting of a simulated annealing and an alternating local descent stage, was proposed. In a simulation study, this algorithm showed excellent performance with respect to both minimizing the loss function and recovery of the underlying truth. Finally, the application of RV-HICLAS to data from a study within the componential emotion domain made clear that the novel HICLAS model may yield meaningful and well interpretable results.

The model proposed in this paper is an unconstrained real-valued hierarchical classes model. It may, however, be sensible to develop constrained versions of the model. In this regard, a particularly interesting constraint could be to enforce $\mathbf{G}$ to be diagonal. Linking up with a framework developed by Ceulemans, Van Mechelen, and Kuppens (2004), this may be classified as a value constraint. It can be included in a straightforward way in the estimation approach as proposed in this paper. Note that a diagonal RV-HICLAS core implies a one-to-one correspondence between object and attribute bundles, such as in the original disjunctive binary HICLAS model for binary data (De Boeck & Rosenberg, 1988). An example in which such a constrained model may be particularly useful is in the case of a person by item data matrix on the quality of the solution that each person arrives at for each item. The bundles as yielded by a diagonal core RV-HICLAS analysis could be interpreted as underlying solution strategies. In particular, on the person side the bundles then indicate, for each individual, whether he or she masters the corresponding strategies or not; whereas on the item side, the bundles denote whether a particular strategy is appropriate to solve each item or not. The diagonal elements of the core then represent the quality of the solutions associated with each of the solution strategies. Furthermore, if a certain person then masters two or more solution strategies through each of which a particular item can be solved, then the quality of the ultimate solution arrived at will be that associated to the best of all strategies in question.

Several further extensions of the RV-HICLAS model can be considered; three of these will be discussed here somewhat more in detail. First, real-valued HICLAS models for three-way three-mode data can be developed. Such models could be considered real-valued counterparts for Tucker3-HICLAS (Ceulemans et al., 2003), Tucker2-HICLAS (Ceulemans & Van Mechelen, 2004) and INDCLAS (Leenen et al., 1999), in which the core is allowed to contain positively real-valued entries (with in the INDCLAS case, the core further being forced to take a superdiagonal form). One field of application in which such models could be useful is the contextualized study of personality (Mischel & Shoda, 1998; Vansteelandt & Van Mechelen, 1998; Kuppens, Van Mechelen, Smits, De Boeck, & Ceulemans, in press), in which three-mode person by situation by behavior data are a key object of research. Second, the model as described in the present paper is based on the maximum operator and, as such, belongs to the class of (generalized) disjunctive HICLAS models. It is possible, however, to formulate a dual, conjunctive variant of the model. Such a variant would rely on the Min- rather than on the Max-operator and its decomposition rule would take place in the mathematical structure $(\mathbb{R}^-, \min, \times)$. Third, it is possible to include offset terms to the model. Such terms could be estimated simultaneously with the other part of the model, in line with the approach taken by Kiers (2006) for the family of three-way component models.

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Table 1: Hypothetical reconstructed binary data matrix $\mathbf{M}$

	attributes			
objects	a_1	a_2	a_3	a_4
o_1	1	1	1	1
o_2	1	0	1	0
o_3	1	1	1	1
o_4	0	0	0	0
o_5	0	1	1	1
o_6	0	1	1	1
o_7	0	0	0	0

Table 2: HICLAS model for $\mathbf{M}$ in Table 1

Bundle matrices					
	Object bundle			Attribute bundle	
Objects	OB_1	OB_2	Attributes	AB_1	AB_2
o_1	1	1	a_1	0	1
o_2	0	1	a_2	1	0
o_3	1	1	a_3	1	1
o_4	0	0	a_4	1	0
o_5	1	0			
o_6	1	0			
o_7	0	0			

Table 3: Hypothetical reconstructed rating-valued data matrix $\mathbf{M}$

	attributes			
objects	a_1	a_2	a_3	a_4
o_1	3	2	3	1
o_2	1	3	3	1
o_3	3	3	3	1
o_4	0	1	2	2
o_5	1	3	3	1
o_6	3	3	3	2
o_7	3	0	3	1

Table 4: HICLAS-R model for $\mathbf{M}$ in Table 3

Bundle matrices								**G**			
	Object bundle				Attribute bundle						
Objects	OB_1	OB_2	OB_3	Attributes	AB_1	AB_2	AB_3		AB_1	AB_2	AB_3
o_1	1	0	0	a_1	1	0	0	OB_1	3	1	2
o_2	0	1	0	a_2	0	0	1	OB_2	1	1	3
o_3	1	1	0	a_3	1	1	1	OB_3	0	2	1
o_4	0	0	1	a_4	0	1	0				
o_5	0	1	0								
o_6	1	1	1								
o_7	1	0	0								

(1)	I am capable of undertaking action against it. (ACTION)
(2)	I think someone else does not take enough consideration of me. (NO CONSIDERATION)
(3)	I feel attacked by someone else. (ATTACKED)
(4)	I think someone else is responsible. (SOMEONE ELSE RESPONSIBLE)
(5)	I find the situation frustrating. (FRUSTRATION)
(6)	I feel angry. (ANGRY)
(7)	I am being treated unrespectfully. (NO RESPECT)
(8)	I think someone has bad intentions towards me. (BAD INTENTIONS)
(9)	My self-esteem is being threatened. (SELF-ESTEEM)
(10)	My plans/goals are being obstructed (OBSTRUCTION)
(11)	It really affects me as a person. (AFFECT PERSONALLY)
(12)	It is important to me. (IMPORTANT)
(13)	I think someone else is to blame. (SOMEONE ELSE TO BLAME)
(14)	I feel desperate. (DESPERATE)

Table 5: Description of all fourteen emotion components.

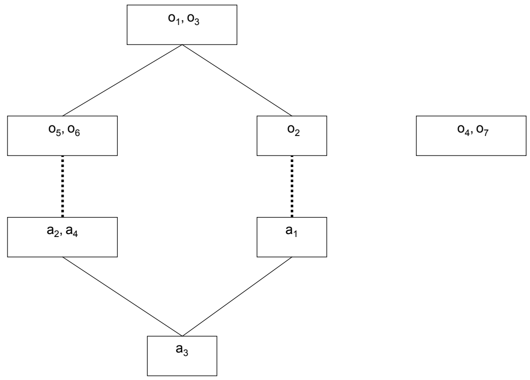

Figure 1: Graphic representation of the rank 2 HICLAS solution of Table 2.

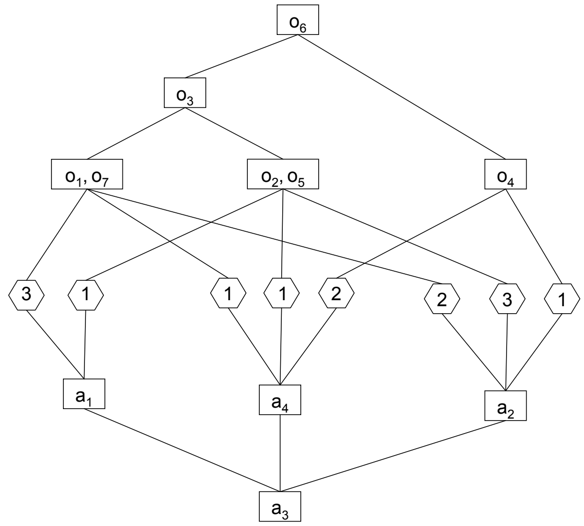

Figure 2: Graphic representation of the rank $(3, 3, 3)$ HICLAS-R solution of Table 4.

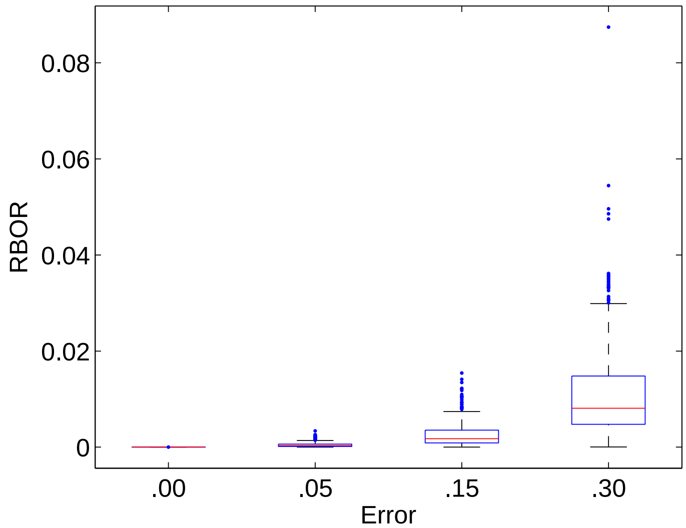

Figure 3: Box plot of relative badness-of-recovery (RBOR) for each level of *Error*.

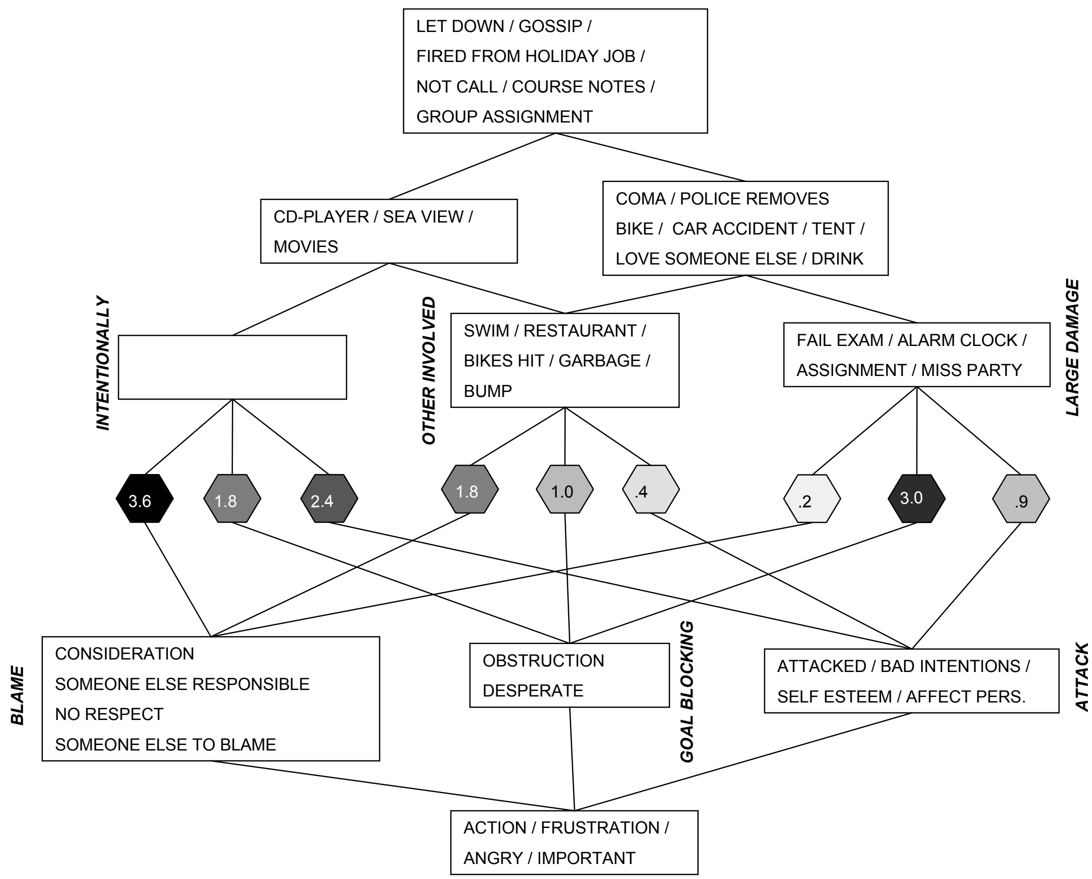

Figure 4: Graphic representation of the rank $(3, 3)$ RV-HICLAS solution for anger data.

(1)	Your friend is in a coma after an accident. (COMA)
(2)	A friend lets you down on a date, and calls you the following day to let you know that he/she didn't feel like meeting with you and went out with other people instead. (LET DOWN)
(3)	A friend returns your CD player, claiming that everything is OK, but it turns out to be broken afterwards. (CD-PLAYER)
(4)	A swimming appointment is cancelled because one of your friends falls ill. (SWIM)
(5)	The waiter in a restaurant informs you that it may take a while before you can eat because it is a busy evenening. Finally, you are served after 50 minutes of waiting. (RESTAURANT)
(6)	Upon leaving class, you notice that a police officer is removing your bike because it was illegally parked. (POLICE REMOVES BIKE)
(7)	You are hit by a car on your way to an important appointment, causing you to miss the appointment. (CAR ACCIDENT)
(8)	You arrange with a good friend to go out together, and he/she will contact you to meet each other. You don't hear from him/her. (NOT CALL)
(9)	On holiday with friends, you arrange that each, in turn, has to carry the heavy tent gear. One day, the tent gear is missing. (TENT)
(10)	You are hit on your bike by another biker. He/she apologizes, and proposes to pay back the damage to your bike. (BIKES HIT)
(11)	You have arranged for a hotel room with sea-view. Upon arrival, you are given a room without a sea-view. (SEA VIEW)
(12)	You are in love with someone but he/she is more interested in someone else. (LOVE SOMEONE ELSE)
(13)	You didn't study hard enough for an exam, and you fail the exam. (FAIL EXAM)
(14)	Your clock failed to wake you up in the morning and you miss the final class of a course. (ALARM CLOCK)
(15)	You arrange with your roommates that each in turn has to put out the garbage. When it is someone else's turn you noticed that he/she didn't clean up. (GARBAGE)
(16)	A floppy disk holding an important school assignment is destroyed by your computer. (FLOPPY)
(17)	You hear that a friend is spreading gossip about you. (GOSSIP)
(18)	You miss a popular party because you fall asleep at home. (MISS PARTY)
(19)	You are fired from your holiday job. (FIRED FROM HOLIDAY JOB)
(20)	A fellow student fails to return your notes when you need them for studying. (COURSE NOTES)
(21)	You bump into someone on the street. (BUMP)
(22)	You have a group assignment with some fellow students. They don't work hard, and you all get a bad grade. (GROUP ASSIGNMENT)
(23)	You're out for a drink after a hard day's work, and you have to wait 30 minutes before you are served. (DRINK)
(24)	Your roommates went to the movies without informing you. (MOVIES)

Table 6: Description of all twenty-four situations.