Linear Latent Structure Analysis: from Foundations to Algorithms and Applications

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Abstract

A new statistical technique for constructing linear latent structure (LLS) models from available data, supported by well established theoretical results and an efficient algorithm, is presented. The method reduces the problem of estimating LLS model parameters to a sequence of linear algebra problems. This assures a low computational complexity and an ability to handle large scale data that involve thousands of variables. An overall computational scheme and all its components are discussed in detail. Simulation experiments demonstrate the excellent performance of the algorithm in reconstructing model parameters. Step-by-step analysis of a demographic survey is presented as an example.

The technique is useful for the analysis of high-dimensional categorical data (e.g., demographic surveys, gene expression data) where the detection, evaluation, and interpretation of a underlying latent structure are required.

Key words: Latent structure analysis, mixing distributions, high-dimensional categorical data, simulation experiments, methods of linear algebra

1 Introduction

Categorical data often occur in behavior sciences, epidemiology, genetics, education, and marketing. A common feature of modern categorical data collection (e.g., demographic surveys or gene expression data) is their high dimensionality with respect to both to sample size and the numbers of categorical variables measured for each individual.
Limited numbers of categorical variables may not precisely characterize an object. This can be due to the stochastic nature of observed objects, their heterogeneity, or measurement error. Often the phenomenon of interest cannot be observed directly, so a series of measures has to be made, each related to latent variables of interest. As a consequence, the set of categorically scored measurements is strongly related. Researchers analyzing such data have to: i) extract the signal from data with a large stochastic component, ii) extract a latent (unobservable) structure, related to the categorical data, and iii) parameterize the latent structure to interpret it substantively. The identification and description of a latent structure are not sufficient when estimation of individual parameters are required. Such problems are informally solved by a physician making a diagnosis: he/she estimates an unobservable variable of interest (presence of a disease) based on categorical measures (description of symptoms and answers to physician’s questions) and estimated population characteristics (physician’s professional experience). Likewise, having a set of categorical measurements (e.g., a demographic survey) made on individuals, a researcher would like to discover i) properties of the population and ii) properties of the individuals. Methods which attempt to achieve these simultaneously are known as latent structure analysis.

One of the best known such methods is the latent class model (LCM), which can be characterized as a statistical method for finding subtypes of related cases (latent classes) from multivariate categorical data (Lazarsfeld and Henry, 1968; Goodman, 1974; Clogg, 1995). In LCM, individuals are assigned to one of several homogeneous classes. This requires estimation of the individual latent variable (class number). Other specific models of this family such as item response theory and Rasch models, discrete latent class models (Heinen, 1996), latent distribution analysis (Mislevy, 1984; Uebersax & Grove, 1993; Qu, Tan & Kutner, 1996), differ by the assumptions made about the latent variable(s). One method for identifying the latent structure in large categorical data sets with simultaneous evaluation of individual scores in a state space is Grade of Membership (GoM) analysis. GoM was introduced in Woodbury and Clive (1974); see Manton et al. (1994) for a detailed exposition and additional references. Statistical properties of GoM models were analyzed by Tolley and Manton (1992).

All these models belong to the family of latent structure analysis that considers a number of categorical variables measured on each individual in a sample with the intent of discovering the properties of both a population and individuals composing the population. Different approaches to this general problem, and recent developments, are described in reports collected in Hagaenars and McCutcheon (2002). The relation of specific latent structure models is discussed by Uebersax (1997) and Erosheva (2005). Comparative analyses of methods of LSA and traditional statistical approaches (Agresti 2002) attempting to find the correspondence of population parameters of interest and sample statistics
are presented by Powers and Xie (2000).

Methods of latent structure analysis can be reformulated in terms of statistical mixtures and mixing distributions. Bartholomew (2002) noted the theory of mixing distributions as a common mathematical framework of latent structure models with abilities “to clarify, simplify, and unify the disparate developments spanning over a century.” The main assumption of the latent structure analysis is the local independence assumption. Being formulated in terms of the theory of mixing distributions, it states that the observed joint distribution (of categorical random variables) can be described as a mixture of independent distributions. The mixing distribution is considered as a distribution of the latent variable(s) that contains latent information regarding the phenomenon under study. Specific models of latent structure analysis vary by assumptions regarding properties of the mixing distribution.

LCM, GoM, and many other methods of latent structure analysis use maximum likelihood for parameter estimation. Although a part of parameters describing a latent structure are regular (structural) parameters, parameters corresponding to individual states are so-called “nuisance” parameters, the number of which may increase with sample size. There are a series of non-trivial mathematical tasks which have to be solved to estimate such individual parameters. First is the problem of identifiability, which is especially difficult for large samples and a large number of estimated parameters. Second is the problem of consistency, which is very difficult to prove when structural and nuisance parameters are estimated simultaneously. Third is the availability and quality of algorithms to perform estimations. Often additional assumptions not required by a model are made to facilitate likelihood maximum. No general theorems are available to address these questions, so all of these points have to be considered separately for each task involved in dealing with nuisance parameters (e.g., Haberman, 1995; Erosheva, 2002).

Recently Linear Latent Structure (LLS) analysis has been proposed to model high dimensional categorical data (Kovtun et al., 2005a,b,c). LLS has been formulated using mixing distribution theory. Similar to other latent structure analyses, the goal of LLS analysis is to derive both the properties of a population and individuals using discrete measurements. LLS, however, does not use a maximum likelihood approach for parameter estimation. Instead, it uses a new estimator, where LLS parameter estimates are solutions of a quasilinear system of equations. For this estimator, it is possible to prove consistency, to formulate conditions for identifiability, and to formulate a high-performance algorithm allowing one to handle datasets involving thousands of categorical variables.

The LLS approach is briefly reviewed in Section 2. Specifically, the structure of the data base, the LLS problem formulations, their basic properties, and two
examples are discussed. A detailed description of the LLS algorithm and its implementation is in Section 3. Attention is paid not only to the components of LLS analysis, but also to auxiliary algorithms, and to procedures for choosing a basis which may require prior information about the study phenomenon. Section 4 is devoted to applications, and has two parts. The first contains a description of simulation experiments designed to check the quality of reconstruction of model components. The second discusses how the model is applied to a specific dataset. Section 5 summarizes results and includes discussion and conclusions.

2 Linear Latent Structure Analysis

2.1 Structure of datasets and population characteristics.

The typical dataset analyzed by methods of latent structure analysis can be represented by the \( I \times J \) matrix constituted by categorical outcomes \( X_{ij} \) of \( J \) measurements on \( I \) individuals, where \( i = 1, \ldots, I \) and \( j = 1, \ldots, J \) run over individuals and measurements, respectively. Each row in the matrix corresponds to an individual and contains an individual response pattern, i.e., a sequence of \( J \) numbers with the \( j \)th number running from 1 to the number of responses \( L_j \) for that variable. In most cases \( L_j \) ranges from 2 to 5-10, and rarely exceeds several dozens. Thus, the results of a survey are represented by \( I \) measurements of random variables \( X_1, \ldots, X_J \), with the set of outcomes of the \( j \)th measurement being \( \{1, \ldots, L_j\} \). The joint distribution of random variables \( X_1, \ldots, X_J \) can be described by the elementary probabilities,

\[
p_\ell = P(X_1 = \ell_1 \text{ and } \cdots \text{ and } X_J = \ell_J),
\]

where \( \ell = (\ell_1, \ldots, \ell_J) \) is an individual response pattern and \( \ell_j \in \{1, \ldots, L_j\} \). To include into consideration marginal probabilities, we allow some components of \( \ell \) to be 0’s. For example, for three binary variables,

\[
p_{(2,0,1)} = P(X_1 = 2 \text{ and } X_3 = 1) = p_{(2,1,1)} + p_{(2,2,1)}
\]

Values of these probabilities \( p_\ell \) (and only these) are directly estimable from the observations. If \( I_\ell \) is the number of individuals with pattern \( \ell \), consistent estimates for \( p_\ell \) are given by frequencies \( f_\ell = I_\ell / I \).
2.2 LLS task: statistical, geometrical, and mixing distribution points of view.

The problem in LLS analysis is to evaluate dimension of a hidden space, identify its location in the space of larger dimension, and to evaluate hidden individuals’ characteristics (coordinates in the latent sub-space) from the data. The LLS analysis is based on two assumptions. The first is the assumption about “local independence”, which is common for all methods of latent structure analysis. The second is specific for LLS analysis. It is about existence of low-dimensional linear subspace associated with the latent structure. We present LLS in terms of the theory of mixing distributions, and then discuss its specific assumption from statistical and geometrical points of view.

Population characteristics are completely described by the joint distribution of random variables $X_1, \ldots, X_J$ presented by probabilities (1). Among all possible joint distributions, one can distinguish independent distributions, i.e. distributions satisfying,

$$p_\ell = P(X_1 = \ell_1 \mbox{ and } \cdots \mbox{ and } X_J = \ell_J) = \prod_j P(X_j = \ell_j).$$  (2)

The description of an independent distribution law requires only knowing $P(X_j = \ell_j)$ denoted below as $\beta_{jl}$. Vectors of probabilities $\beta = (\beta_{11}, \ldots, \beta_{jL_j})$ belong to vector space $R^{L_j}$, where $|L| = \sum_j L_j$. Indexes of the vector components run over all possible pairs of $jl$, i.e., corresponding to probabilities of the first outcome to the first question, of the second outcome to the first question, and so on. Requirements for $\beta_{jl}$ to be probabilities restricts their domain in the vector space by

$$\sum_{l=1}^{L_j} \beta_{jl} = 1 \quad \mbox{and} \quad \beta_{jl} \geq 0.$$  (3)

This domain represents the direct product of $J$ unit simplex of dimensions $L_j$.

Since variables $X_1, \ldots, X_J$ in general case are not independent, the observed distribution $\{p_\ell\}$ cannot be described by the product of independent distributions, but it can be exactly described as a mixture of independent distributions. This means that each set of independent probabilities contributes to observed distribution with a weight function. This weight function is called mixing distribution. It is defined in the space of independent distributions, i.e. for each vector of probabilities $\beta$ satisfying (3). Let $F(\beta)$ be the cumulative distribution function of the mixing distribution. Probabilities $p_\ell$ are represented as,

$$p_\ell = \int dF(\beta) \prod_{j=1}^{L_j} \beta_{jl}.$$  (4)

Thus, latent structure analysis searches for a representation of the observed distribution as a mixture of independent distributions.
Any distribution \(\{p_\ell\}\) can be represented as a mixture, so representation (4) does not restrict the family of distributions and further specifications are required. They are formulated as restrictions on the support of mixing distribution or, equivalently, on a set of mixed independent distributions. The LLS specific assumption is that this set is restricted to be a \(K\)-dimensional linear subspace of the space of independent distributions, i.e., the mixing distribution is supported by the linear subspace spanned by \(K\) basis vectors \(\lambda^1, \ldots, \lambda^K\). Below this LLS assumption is considered from the point of view of pure statistical analysis and the geometry of the task.

Individual characteristics are described by individual probabilities \(\beta^i_{jl} = P(X^i_j = l)\) of specific outcomes \((i = 1, \ldots, I\) runs over individuals).

The LLS assumption about the existence of a low-dimensional linear subspace supporting the mixing distribution is essentially equivalent to the assumption that there exists a \(K\)-dimensional random vector \(G\) such that for every \(j\) a regression of \(Y_{jl}\) (random variable \(Y_{jl}\) equaling 1 if \(X_j = l\) and 0 otherwise) on \(G\) is linear. The regression equation relates the expectation of \(Y_{jl}\), which is \(\beta_{jl}\), to the random vector \(G\). If a specific value of \(G\) is associated with individual \(i\) (so-called LLS scores \(g_{ik}\)), then the regression takes the form,

\[
\beta^i_{jl} = \sum_{k=1}^{K} g_{ik} \lambda^k_{jl}. \tag{5}
\]

The sense of the regression coefficients \(\lambda^k_{jl}\) and model restrictions is clarified by analyzing the geometry of the LLS task.

Vectors of individual probabilities \(\beta^i = \{\beta^i_{jl}\}\), of individual responses \(Y^i = \{Y^i_{jl}\}\) and the regression coefficients \(\lambda^i = \{\lambda^k_{jl}\}\) lie in the permitted domain (3) of the space of independent distributions. From a geometric point of view, LLS searches a \(K\)-dimensional subspace (represented by \(\lambda^k_{jl}\)) in this space, which is the “closest” to the set of \(I\) points representing individual outcomes \(Y^i_{jl}\). This linear subspace is defined by its basis \(\lambda^1, \ldots, \lambda^K\), so to find the \(K\)-dimensional subspace means finding a basis, \(\lambda^k_{jl}\), \((k = 1, \ldots, K)\). Every basis \(\lambda^1, \ldots, \lambda^K\) defines a family of regression coefficients and vice versa. The complete set of restrictions in the LLS task allowing to consider \(\beta^i_{jl}\) and \(\lambda^k_{jl}\) as probabilities, is,

\[
\sum_{l=1}^{L_j} \lambda^k_{jl} = 1, \quad \lambda^k_{jl} \geq 0, \quad \sum_{k=1}^{K} g_{ik} = 1 \quad \text{and} \quad \sum_{k} g_{ik} \lambda^k_{jl} \geq 0. \tag{6}
\]

LLS scores \(g_{ik}\) characterizing an individual \(i\) are then estimated as the expectation of vector \(G\), conditional on the respondent’s answers. Basis vectors of the subspace can be interpreted as probabilities and can define the “pure types” (Manton et al., 1994). In this sense, the model decomposition (5) has the interpretation of a decomposition over pure types or over “ideal persons” whose individual probabilities are basis vectors of the subspace.
Summarizing, one can say that the LLS model approximates the observed
distribution of $X_1, \ldots, X_J$ by a mixture of independent distributions with a
mixing distribution supported by a $K$-dimensional subspace of the space of
independent distribution. To specify such a model distribution it is sufficient
to define the following LLS parameters:

1. A basis $\lambda_1, \ldots, \lambda_K$ of the space that supports the mixing distribution.
2. Conditional moments $E(G|X = \ell)$.

This set of model parameters is not the only set possible. We chose it because
of a number of useful properties listed below.

**Property 1.** The mixing distribution can be estimated in the style of an
empirical distribution, i.e., when the estimator is a distribution concentrated
in points $E(G|X = \ell)$ with weights $f_\ell$.

**Property 2.** The conditional expectations $E(G|X = \ell)$ provide knowledge
about individuals. These conditional expectations can be considered as co-
ordinates in a phase space, to which all individuals belong. The ability to
discover the phase space and determine individual positions in it is a valuable
feature of LLS analysis.

**Property 3.** When the number of measurement, $J$, tends to infinity, the
individual conditional expectations $g_i = E(G|X = \ell^{(i)})$, where $\ell^{(i)}$ is the vector
of responses of individual $i$, converge to the true value of the latent variable
for this individual, and estimates of the mixing distribution converge to the
true one, provided some regularity conditions (Kovtun et al., 2005d).

### 2.3 Moment matrix and the main system of equations.

Parameter estimation is based on two facts (Kovtun et al., 2005a,b) formulated in terms of the conditional and unconditional moments of the mixing
distribution. The first is that columns of moment matrix belong exactly to
the desired linear space. The second is that they obey the main system of
equations.

#### 2.3.1 Unconditional moments and the moment matrix

The first set of values in which we are interested consists of the unconditional
moments of the mixing distribution $F(\beta)$,

$$M_\ell = \int dF(\beta) \prod_{j: \ell_j \neq 0} \beta_j \ell_j p_\ell$$

(7)
Note an important fact regarding the above equation. The value on the left-hand-side, \( M_\ell \), is a moment of *mixing distribution*, while the value on the right-hand-side, \( p_\ell \), comes from the *joint distribution of* \( X_1, \ldots, X_J \); the equality of these values is a direct corollary of the definition of mixture. The existence of their connection between two distinct distributions is crucial for LLS analysis.

The first corollary of eq. (7) is that the unconditional moments are directly estimable from data and, therefore, the frequencies \( f_\ell \) of response patterns \( \ell \) observed in a sample are consistent and efficient estimators for conditional moments \( M_\ell \).

Recall that we allow some components of response pattern \( \ell \) to be 0. In this case \( p_\ell \) are marginal probabilities. In the definition of \( M_\ell \) the multipliers, corresponding to 0 components of \( \ell \), are excluded from the product. Thus, the order of moment \( M_\ell \) is equal to the number of non-zero components in \( \ell \).

All moments defined in (7) are estimable by frequencies; however, this definition does not cover all moments of a certain order. For example, moments of second order with \( \beta_{jl1} \) and \( \beta_{jl2} \), (i.e., with the same \( j \)) are not estimable. This arises because the data do not include double answers to the same question. One can notice that i) all moments of first order are estimable, ii) the proportion of estimable moments decreases with the increase of order, and iii) no moments of order \( J + 1 \) and higher are estimable.

The moment matrix is constructed from moments of order up to \( J \) using the following formal rules:

1. Rows of the moment matrix are indexed by response patterns containing exactly one non-zero component or, equivalently, by pair indexes \( jl \). Thus, the moment matrix contains \( |L| \) rows, and their columns can be considered as vectors in \( R^{|L|} \).
2. Columns of the moment matrix are indexed by all possible response patterns, including a response pattern containing all 0’s. The first column is indexed by response pattern \((0, \ldots, 0)\); the next \( |L| \) columns are indexed by response patterns containing one non-zero component, and so on.
3. The element on the intersection of row \( \ell' \) and column \( \ell'' \) is \( M_{\ell' + \ell''} \), if \( \ell'' \) has 0 at the position of the only non-zero component of \( \ell' \) (in this case, \( \ell' + \ell'' \) is a meaningful response pattern; otherwise, the question mark is placed on the position of intersection of row \( \ell' \) and column \( \ell'' \)). For example, the element of the moment matrix in row \((1, 0, 0)\) and column \((0, 2, 2)\) is \( M_{1,2,2} \), and element in row \((1, 0, 0)\) and column \((1, 0, 2)\) is a question mark.

Equation (8) gives an example of a portion of the moment matrix for the case
of $J = 3$ dichotomous variables, i.e., \( L_1 = L_2 = L_3 = 2 \).

\[
\begin{pmatrix}
M_{(100)} & ? & ? & M_{(110)} & M_{(120)} & M_{(101)} & M_{(102)} & ? & \cdots \\
M_{(200)} & ? & ? & M_{(210)} & M_{(220)} & M_{(201)} & M_{(202)} & ? & \cdots \\
M_{(010)} & M_{(110)} & M_{(210)} & ? & ? & M_{(011)} & M_{(012)} & ? & \cdots \\
M_{(020)} & M_{(120)} & M_{(220)} & ? & ? & M_{(021)} & M_{(022)} & ? & \cdots \\
M_{(001)} & M_{(101)} & M_{(201)} & M_{(011)} & M_{(021)} & ? & ? & M_{(111)} & \cdots \\
M_{(002)} & M_{(102)} & M_{(202)} & M_{(012)} & M_{(022)} & ? & ? & M_{(112)} & \cdots \\
\end{pmatrix}
\]

In this example, places for inestimable moments are filled by question marks. The first column of the moment matrix contains moments of the first order, when only one specific outcome of one specific question is taken into account. There are no inestimable moments in the first column. Elements of this column can be denoted as components of vectors in \( \mathbb{R}^{|L|} \), i.e., as \( M_{jl} \). The next six (\( |L| \) in general) columns correspond to second-order moments. Blocks of diagonal elements are not estimable. Second-order moments can be also denoted via pair \( jl \) of indexes as \( M_{jl} \); \( j' l' \). The last shown column corresponds to third order moments. The notation \( M_{jl} \) and \( M_{jl}; j' l' \) is used below for specific columns of the moment matrix.

The part of the moment matrix consisting of second-order moments (which is \( |L| \times |L| \) square matrix) together with the column of first-order moments is of special interest. A well-know fact is that if a distribution in an \( n \)-dimensional Euclidean space is carried by a \( k \)-dimensional linear manifold, then the rank of the covariance matrix is equal to \( k \), and the position of the manifold can be derived from the covariance matrix. This fact is the cornerstone of principal component analysis. Our method is based on similar ideas, adapted to having an incomplete set of second-order moments. For a small \( J \) (as in the example), there is a relatively large fraction of non-estimable components in the second-order part of the moment matrix. For increasing \( J \), this fraction rapidly decreases.

For a moment matrix \( M \) let its completion \( \bar{M} \) be a matrix obtained from \( M \) by replacing question marks with arbitrary numbers. The main fact with respect to the moment matrix is that the moment matrix always has a completion in which all columns belong to the supporting plane \( \Lambda \). Thus, if the estimable part of the moment matrix has sufficient rank (which is the case in nondegenerate situations,) a basis in \( \Lambda \) may be obtained from this matrix. As we have a consistent estimator of the moment matrix in the form of a frequency matrix, the supporting plane may be consistently estimated.

The mixing distribution in the LLS model is supported by the intersection of the linear subspace with the polyhedron defined by (3). This intersection \( P_\beta \)
can be parameterized by \(g\)'s in accordance with (5). In Appendix, we demonstrate that integrals in (7) over \(P_\beta\) can be reduced to integrals in the linear subspace over the polyhedron \(P_g\), and how distribution functions \(F(\beta)\) and \(F(g)\) relate to each other. Then unconditional moments \(M_\ell\) can be formally represented as

\[
M_\ell = p_\ell = \int dF(g) \prod_{j,l_j \neq 0} \sum_k g_k \lambda_{j,l_j} \tag{9}
\]

Representation (9) helps to illustrate the main properties of the moment matrix: i) the rank of the matrix is \(K\) and ii) all columns of the matrix belong to a linear subspace with a basis represented by vectors \(\lambda^k\). Indeed, since \(j,l\) indexes running in each column of the moment matrix are only involved in \(\lambda\)'s, which are independent of integration variable \(g\), and, therefore, which can be removed from the integral. The remaining integration over \(g\) is common for all elements of the moment matrix of a certain order. The first column and second order matrix are represented,

\[
M_{jl} = \int dF(g) \sum_k g_k \lambda^k_{jl} = \sum_k \left( \int dF(g) g_k \right) \cdot \lambda^k_{jl} = \sum_k I_k \lambda^k_{jl} \tag{10}
\]

\[
M_{j\ell,j'\ell'} = \int dF(g) \left[ \sum_k g_k \lambda^k_{j\ell} \right] \left[ \sum_{k'} g_{k'} \lambda^k_{j'\ell'} \right] = \sum_{kk'} \lambda^k_{j\ell} \lambda^k_{j'\ell'} \int dF(g) g_k g_{k'}
\]

\[
= \sum_k \left( \sum_{k'} \lambda^k_{j'\ell'} \int dF(g) g_k g_{k'} \right) \cdot \lambda^k_{j\ell} = \sum_k I_{k,j'\ell'} \lambda^k_{j\ell}
\]

where \(I_k\) and \(I_{k,j'\ell'}\) are some numeric coefficients. From (10) we see that each column of moment matrix can be represented as a linear combination of \(K\) vectors \(\lambda^k\).

### 2.3.2 Unconditional moments and main system of equations

Another set of the values of interest are the conditional moments \(E(G_k|X=\ell)\), which express knowledge of the state of individuals based on measurements. They are not directly estimable from observations. The goal of LLS analysis is to obtain estimates for these conditional moments. Explicit expressions for those of the lowest order are obtained using the Bayes theorem (Kovtun et al. 2005a),

\[
E(G_n|X=\ell) = \int dF(g) g_n \frac{\prod_{j,l_j \neq 0} \sum_k g_k \lambda^k_{j,l_j}}{M_\ell(\mu_\beta)} \tag{11}
\]

Analogously, higher conditional moments, including products of components of \(G\), can be constructed. As can be seen explicitly from (34) and (11), the relation of conditional and unconditional moments in LLS analysis can be described as,

\[
\sum_k \lambda^k_{j\ell} \cdot E(G_k|X=\ell) = \frac{M_{\ell+l_j}}{M_\ell} \tag{12}
\]
where vector \( \ell \) contains 0 in position \( j \), and \( \ell + l_j \) contains \( l \) in this position. Similar equations can be written for conditional moments of higher orders. We refer to the system of equations relating conditional and unconditional moments as the main system of the equation. Kovtun et al, (2005a) proved the following properties of solutions of the main system of equations: i) any basis \( \lambda^k_{jl} \) of \( \Lambda \) together with conditional moments \( E(G_k|X = \ell) \) calculated on this basis give a solution of the main system of equation; and ii) under regular conditions, every solution of the main system of equations gives a basis of \( \Lambda \) and conditional moments calculated in this basis. Note, that equation (12) is linear with respect to conditional moments.

The described properties of the moment matrix and solutions of the main system of equations suggest an efficient algorithm to obtain LLS estimates. First, a basis of the supporting plane can be obtained from the moment matrix, and second, conditional moments can be found by solving a linear system of equations. An important property of conditional moments is that (Kovtun et al., 2005d): if a population is represented by a set of true LLS scores, then unconditional moments give good approximation for them for finite \( J \), and converge to true LLS scores when \( J \rightarrow \infty \).

### 2.4 Two illustrative examples.

Before going into detail for the algorithm and to realistic tasks of data analysis, we consider two simple illustrative examples. For both of them, assume \( K = 2 \), three dichotomous variables \( (J = 3) \), and the basis vectors are \( \lambda^1 = (1, 0; 1, 0; 1, 0) \) and \( \lambda^2 = (1/2, 1/2; 0, 1; 0, 1) \). Then the independent distributions being mixed are defined by vectors:

\[
\beta = g_1 \lambda^1 + g_2 \lambda^2 = g_1 \lambda^1 + (1 - g_1)\lambda^2, \quad 0 \leq g_1 \leq 1. \tag{13}
\]

Thus, a mixing distribution can be given one dimensional p.d.f. \( \rho(g_1) \). For the first task, we assume that the mixing distribution is uniform \( (\rho(g_1) = 1 \cdot \theta(g_1) \cdot \theta(1-g_1)) \). In the second case we assume the mixing distribution is concentrated at two points with \( g_1 = 0.1 \) and \( g_1 = 0.4 \) \( (\rho(g_1) = 1/2[\delta(g_1 - 1/10) + \delta(g_1 - 2/5)]) \). Unconditional moments are calculated using (7). Moment matrices for both
cases are

\[
\begin{pmatrix}
3 & 7 & 12 & 4 & 1 & 1 & 5 & 1 \\ 4 & 12 & 6 & 2 & 1 & 4 & 12 & 3 \\
5 & 12 & 1 & 8 & 1 & 12 & 1 & 6 \\
1 & 8 & 1 & 8 & 1 & 12 & 1 & 6 \\
7 & 1 & 1 & 16 & 16 & 16 & 8 & 4 \\
16 & 1 & 1 & 16 & 16 & 8 & 1 & 4 \\
1 & 12 & 1 & 8 & 1 & 12 & 1 & 6 \\
1 & 8 & 1 & 12 & 1 & 8 & 1 & 6 \\
\end{pmatrix}
\]  \quad \text{and}  \quad
\begin{pmatrix}
5 & 317 & 183 & 451 & 549 & 67 & 183 \\ 8 & 800 & 800 & 1600 & 1600 & 400 & 800 \\
3 & 183 & 117 & 249 & 351 & 33 & 117 \\
8 & 800 & 800 & 160 & 1600 & 400 & 400 \\
7 & 451 & 249 & 653 & 249 & 101 & 249 \\
16 & 1600 & 1600 & 3200 & 3200 & 800 & 800 \\
9 & 549 & 351 & 747 & 1053 & 99 & 351 \\
16 & 1600 & 1600 & 3200 & 3200 & 800 & 800 \\
1 & 67 & 33 & 101 & 99 & 17 & 33 \\
4 & 400 & 400 & 800 & 800 & 200 & 200 \\
3 & 183 & 117 & 249 & 351 & 33 & 117 \\
4 & 400 & 400 & 800 & 800 & 200 & 200 \\
\end{pmatrix}
\]

(14)

Since these matrices were constructed from mixing distributions known a priori, diagonal blocks in the sub-matrix of the second order are calculable (marked by the italic font in (14)). As one can see, the rank of both these matrices is 2. Conditional moments are calculated for an outcome pattern. Choose \( \ell = (001) \) and \( \ell + l_1 = (101) \). Using (11) we have,

\[
E(G_1 | X = (001)) = 2/3 \quad \text{and} \quad E(G_2 | X = (001)) = 1/3
\]

(15)

for the first example and,

\[
E(G_1 | X = (001)) = 17/50 \quad \text{and} \quad E(G_2 | X = (001)) = 33/50
\]

(16)

for the second. Using corresponding elements of \( M_\ell \) in (14) (marked by bold text) we can see that l.h.s. and r.h.s of eq. (12) equal to 5/6 for first example and 67/100 for the second:

\[
1 \cdot \frac{2}{3} + \frac{1}{2} \cdot \frac{1}{3} = \frac{5}{12} \quad \text{and} \quad 1 \cdot \frac{17}{50} + \frac{1}{2} \cdot \frac{33}{50} = \frac{67}{400}
\]

(17)

External indexes in this example are \( j = 1 \) and \( l = 1 \).

### 3 Algorithms of Linear Latent Structure Analysis

Parameter estimations in LLS models are based on properties of the moment matrix and the main system of equations. These properties allow us to reduce a problem of estimating model parameters to a sequence of linear algebra problems. The algorithm based on linear algebra methods assures a low computational complexity.

Data to be analyzed are represented by a set of measurements \( X_{ij} \) (See section 2.1). Finding a linear space and individual LLS scores is required. Estimation of the model includes four steps: i) estimating the rank of the frequency matrix, ii) finding the supporting plane, iii) choosing a basis in the found
plane, iv) calculating individual conditional expectations and estimating mixing distribution. The second and fourth steps are the essence of LLS parameter estimation problem. The first step is defined as separate because sometimes the desired dimensionality of the LLS model may be provided by a researcher, and this step may be skipped. The third step requires using prior information about the processes studied, so it is also examined separately.

3.1 Moment matrix calculation

An important preceding step that deserves special attention is the moment matrix calculation. The elements of the moment matrix given by $M_{\ell}$ are approximated by observable frequencies defined as $f_{\ell} = I_{\ell}/I$, where $I_{\ell}$ is the number of individuals with outcome pattern $\ell$, and $I$ is the total number of individuals having certain (not missing) outcomes for nonzero elements in $\ell$. Columns of a different order have different normalizations, e.g., the sum of first-order moments corresponding to question $j$ is one (e.g., $M_{(010)} + M_{(020)} = 1$), while sums of columns for this $j$ of the second-order sub-matrix are equal to corresponding first-order moment (e.g., $M_{(110)} + M_{(120)} = M_{(100)}$). General conditions of summations of the second order moments written in terms of notation defined after eq. (8) are,

$$\sum_{l'=1}^{L_{j'}} M_{jl; j' l'} = M_{jt}.$$  \hspace{1cm} (18)

Because of missing data, the property of normalization can be violated. This property, with or without the renormalization making the sums equaling to one, is required for the analysis. The renormalization could provide the property in the case of presence of missing data, however, this approximation can be true only assuming missing data are random. More detailed discussion of procedures to deal with missing data are discussed in Section 3.9.

In addition, a matrix containing standard errors (or confidence intervals) of estimates of frequencies is calculated for each element of the frequency matrix. Standard errors for binomial distribution, i.e. $\sigma_{\ell} = \sqrt{f_{\ell}(1-f_{\ell})/I_{\ell}}$, require generalization for patterns with small $I_{\ell}$ as discussed in Brown et al. (2001). A generalization based on Wilson’s approach (Brown et al., 2001) uses,

$$CI_W = \frac{I_{\ell} f_{\ell} + \frac{1}{2} z_{\alpha/2}^2}{I_{\ell} + z_{\alpha/2}^2} \pm \frac{z_{\alpha/2} \sqrt{T_{\ell}}}{I_{\ell} + z_{\alpha/2}^2} \sqrt{f_{\ell}(1-f_{\ell}) + \frac{z_{\alpha/2}^2}{4} \frac{4}{I_{\ell}}}.$$  \hspace{1cm} (19)

Eq. (19) recovers the standard Wald’s estimates of CIs, i.e., $CI_s = p_e \pm z_{\alpha/2} \sigma_E$; $z_{\alpha/2} = \Phi^{-1}(1-\alpha/2)$, where $\Phi(x)$ is the standard normal distribution function and $\alpha$ denotes the confidence level.
3.2 Computational rank of the frequency matrix

The frequency matrix can be presented as a sum of the moment matrix with rank $K$ and a matrix with a stochastic component. To define the dimensionality of the LLS problem, we have to estimate the rank of the frequency matrix eliminating the stochastic component. Specifically, we take the greatest minor of the frequency matrix that does not contain question marks. Then we calculate the singular value decomposition (SVD) and take $K$ equal to the number of singular values that are greater than a maximum of the total standard deviation estimated as the quadratic sum of standard errors of frequencies involved in the minor.

The choice of a minor does not essentially influence the computational rank of the frequency matrix. Indeed, the geometrically specific choice of a minor (e.g. a $n$-dimensional minor of maximal size in left low corner of moment matrix) corresponds to projection of a part of vectors onto $n$-dimensional linear subspace. If the real rank of the moment matrix is much less than $n$, it is clear that the rank of the projections does not change.

3.3 Finding the supporting plane

All columns of the moment matrix belong to the supporting plane, and as the frequency matrix is an approximation of the moment matrix, a natural way to search for the supporting plane is to search for a plane that minimizes the sum of distances from it to the columns of the frequency matrix. In our case, however, this way is complicated by: (a) the frequency matrix is incomplete; (b) the statistical inaccuracy of approximation of moments $M_\ell$ by frequencies $f_\ell$ varies considerably over elements of frequency matrix; and (c) a sought basis should exactly satisfy conditions $\sum_{\ell=1}^{L_j} \lambda_{k\ell}^j = 1$ for every $k$ and $j$. The current prototype of the code overcomes these obstacles by using some heuristic methods: (a) An iterative procedure for completion of the frequency matrix is used: after a basis of supporting plane is obtained, it is used to recalculate completion of the frequency matrix. A new frequency matrix is used for adjusting basis calculation etc. (b) Only the first and second order moments are examined, so statistical errors of different columns in this matrix are compatible. (c) Rotation of each simplex (corresponding to each question) to the hyperplane to eliminate one degree of freedom. Rotation, but not a simple projection, is required to provide the same distances between points in a simplex. Items (a) and (c) require explicit consideration.
3.3.1 Completion of the moment matrix

We consider the second-order moment matrix where for every \( j \) there are undefined elements corresponding to repeated answers to the same question. The intent of completion procedure is to approximate these elements, assuming that the supporting subspace \( \Lambda \) is found. Since only the completed frequency matrix is used for finding subspace \( \Lambda \), and since the completion procedure uses a basis in the sought subspace \( \Lambda \), it can be done within the iteration procedure. For one iteration step, it is required to find a symmetric matrix \( B_j \) of \( L_j \times L_j \)-dimension with positive elements and the required summation conditions such that the sum of elements in a column (or in a row) equals to the corresponding moment of the first order, i.e., \( \sum_l B_{j,tl} = M_{j,l} \). Since we know first- and second-order frequencies \( (f_{jl} and f_{jl,j',l'}; j \neq j') \), which only approximate exact moments \( (M_{jl} and M_{jl,j'l'}) \), special efforts are required to process the properties of \( B_j \). Columns of the second-order sub-matrix corresponding to question \( \bar{j} \) are presented using known frequencies \( f_{jl,\bar{j}l}; j \neq \bar{j} \) and inestimable elements \( B_{j,tl_{\bar{j}}} \),

\[
\begin{pmatrix}
  f_{11,\bar{j}1} & \cdots & f_{11,\bar{j}L_j} \\
  \vdots & \ddots & \vdots \\
  f_{1L_1,\bar{j}1} & \cdots & f_{1L_1,\bar{j}L_j} \\
  \vdots & \ddots & \vdots \\
  B_{j,11} & \cdots & B_{j,1L_j} \\
  \vdots & \ddots & \vdots \\
  B_{j_{L_j}1} & \cdots & B_{j_{L_j}L_j} \\
  \vdots & \ddots & \vdots \\
  f_{11,\bar{j}1} & \cdots & f_{1L_1,\bar{j}L_j} \\
  \vdots & \ddots & \vdots \\
  f_{jL_1,\bar{j}1} & \cdots & f_{jL_1,\bar{j}L_j} \\
  \vdots & \ddots & \vdots \\
  \end{pmatrix}
\]

(20)

The completion procedure is based on the fact that the rank of the moment matrix is \( K \), which is much smaller than the dimension of matrix \( |L| \). Therefore, only \( K \) columns are linearly independent. Each column of the moment matrix, being a vector in \( K \)-dimensional vector space, can be expanded over basis vectors \( \lambda^1, \ldots, \lambda^K \) available after finding the subspace \( \Lambda \). Known elements \( f_{j\bar{j}l} \) \((\bar{l} = 1, \ldots, L_{\bar{j}} \text{ and } j \neq \bar{j})\) of columns of the moment matrix corresponding to question \( j \) are expanded,

\[
f_{j\bar{j}l} = \sum_k C_{j\bar{j}}^{\bar{j}l} \lambda_{jl}^k \quad (j \neq \bar{j}).
\]

(21)
If coefficients $C_{k}^{ij}$ are found, matrix $B_{j}$ can be constructed as

$$B_{j} = \sum_{k} C_{k}^{ij} \lambda_{jk}^{i},$$

The number of known components of a vector $f_{jl}^{ji}$ is greater than the number of basis vectors, so coefficients $C_{k}^{ij}$ can be calculated by ordinary least squares methods minimizing residuals. Matrix $B_{j}$ has to be obtained exactly symmetric, using minimization with restrictions. Lagrangian $Lg_{j}$ are written for each $j$,

$$Lg_{j} = \sum_{jl;j \neq j} \left( f_{jl}^{ji} - \sum_{k} C_{k}^{ij} \lambda_{jk}^{i} \right)^{2} + \sum_{l,k} \rho_{lk} C_{k}^{ij} + \sum_{l} \rho_{l} \left( \sum_{k} C_{k}^{ij} - 1 \right) - \sum_{l \neq l'} \rho_{ll'} \sum_{k} \left( C_{k}^{ij} \lambda_{jk}^{i} - C_{k}^{ij} \lambda_{jk}^{i} \right)$$

where $\rho_{l}$ and $\rho_{ll'}$ are Lagrange multipliers for equality conditions, and $\rho_{lk}$ — for inequality conditions. The optimization task to find $C_{k}$ with a quadratic minimizing function and linear equality and inequality conditions are a quadratic programming problem. This problem is used by different parts of the algorithm (see eqs. (27) and (31)), so Section 3.7 is devoted to this calculation.

### 3.3.2 Removing restrictions

The restrictions $\sum_{l=1}^{L_{j}} \lambda_{jl}^{k} = 1$ are removed by reducing the number of rows by $J$ (one for every group of indexes $j1, \ldots, jL_{j}$). Specifically, we use a linear map from $R^{L_{j}}$ to $R^{L_{j}-J}$ represented by a block-diagonal matrix $A$ with $J$ blocks of size $L_{j} \times (L_{j} - 1)$:

$$A_{j} = \begin{pmatrix}
-\sqrt{L_{j}-1} & 1 & 0 & \ldots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
-\sqrt{L_{j}-1} & 1 & 0 & \ldots & 0
\end{pmatrix}$$

(23)

Geometrically, such a map provides isometric rotation ($\bar{\lambda}^{k} = A\lambda^{k}$) to the hyperplane with zero first coordinate, i.e., (every block $A_{j}$ defines a rotation of a unit simplex in $L_{j}$-dimensional space around a hypersurface opposite to the first vertex; the angle of this rotation is such that the first vertex moves to the point where the first coordinate equals 0). Explicitly, this rotation is $\bar{\lambda}_{jl-1}^{k} = A_{j} \lambda_{jl}^{k}$ in matrix form or $\bar{\lambda}_{jl-1}^{k} = \lambda_{jl}^{k} - \sqrt{L_{j}-1} \lambda_{jl}^{k}$ for $l = 2, \ldots, L_{j}$. New vectors $\lambda^{k}$ do not possess any ties. It is easy to ascertain that such a transformation really conserves distances between points in a simplex. The reverse transformation is,

$$\lambda_{jl}^{k} = \frac{1 - \sum_{l=2}^{L_{j}} \bar{\lambda}_{jl-1}^{k}}{\sqrt{L_{j}}}, \quad \bar{\lambda}_{jl}^{k} = \lambda_{jl-1}^{k} + \frac{\sqrt{L_{j}-1}}{L_{j}-1} \lambda_{jl}^{k}.$$  

(24)
3.3.3 Algorithm for identifying the subspace

The initial completion of the moment matrix is constructed in an arbitrary way, e.g., by the unitary diagonal matrix or completing by frequencies as \( f_{ij} = f_i f_j \).

The next preliminary step is the rotation of each simplex (corresponding to each question as described above) to the hyperplane to eliminate one degree of freedom. This produces \( n \) points \( c^1, \ldots, c^n \) (images of columns of frequency matrix) in \( m = (|L| - J) \)-dimensional space. The problem is to find an affine plane that minimally deviates from these points in the space of individual probabilities. First, we find the center of gravity of this system

\[
c^0 = \frac{1}{n} \sum_i c^i \tag{25}
\]

and then consider a new set of points \( \bar{c}^i = c^i - c^0 \), that corresponds to shifting the point of origin. Now we need to find a \( K \)-dimensional linear subspace in \( \mathbb{R}^m \) that minimally deviates from this set of points. The solution of this problem is well-known (see, e.g., chapter 43 of Kendall and Stuart, 1977): one has to consider an \( m \times m \) matrix \( X \) with components \( X_{rs} = \sum_i \bar{c}^r_i \bar{c}^s_i \); this matrix is symmetric and positively defined, and thus its normalized eigenvectors are composed of an orthonormal basis in \( \mathbb{R}^m \). Let \( \gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_m > 0 \) be eigenvalues of matrix \( X \), and let \( z^1, \ldots, z^m \) be corresponding eigenvectors. The plane of dimensionality \( K \) that minimizes the sum of squared distances from points \( \bar{c}^1, \ldots, \bar{c}^m \) is spanned by \( z^1, \ldots, z^K \), and the sum of squared distances is \( \text{tr} X - \sum_{k=1}^{K} \gamma_k \). Vectors \( c^0, c^0 + z^1, \ldots, c^0 + z^{K-1} \) give us an affine basis of the sought affine plane. Finally, we apply inverses of transformation (24) to \( c^0, c^0 + z^1, \ldots, c^0 + z^{K-1} \) to obtain the sought basis \( \lambda^1, \ldots, \lambda^K \) of the subspace \( \Lambda \).

3.4 Choice of a basis

The basis cannot be defined uniquely, and any convex combination keeping the LLS restrictions can be considered an alternative. A choice may be made using prior information about the process of interest. The appeal of prior information at this stage is reasonable because of the evident fact that the same dataset can be used for analyzing different (say, disability or CVD) processes.

The way how this information is used and how the procedure of specific choice of the basis is defined is a question of taste. We describe here two possible schemes implemented in the algorithm prototype.

A researcher specifies the characteristics of “ideal” individuals based on his/her experience in the research domain. Then he/she can construct vectors of probabilities for such ideal individuals or take these individuals from the sample
under consideration. The vectors of probabilities of these individuals are taken as basis vectors. If probability vectors are constructed by hand, they could be beyond polyhedron \( \mathcal{P}_g \), so they should be projected to \( \mathcal{P}_g \). The individual coordinates in this basis would represent “proximity” of the individual to the “ideal” ones.

In another scheme, the basis is obtained using assignment of LLS scores (calculated on some arbitrary basis) to \( K \) clusters, and then basis vectors \( \lambda^1, \ldots, \lambda^K \) are calculated as means of probabilities \( \beta^j_{il} \) over each cluster.

A researcher can develop his/her own scheme of basis selection. For example, he/she can simply use vectors already known from previous studies or construct a basis purely mathematically, e.g., from the condition of maximal linear independence of the vectors, or choose it from the set of the supportive polyhedron vertexes.

3.5 Calculation of individual conditional expectations.

When a basis of the supporting plane is found, the conditional expectations can be found from the main system of equations (12), which is a linear system after substituting the basis. The system, however, relates conditional expectations \( \mathbb{E}(G_k|X = \ell) \) for a pattern \( \ell \) with at least one 0 outcome. Thus exact system of equations (12) can be written for all patterns \( \ell \) except patterns where all outcomes are known. For the complete patterns, we can calculate \( J \) conditional expectations, subsequently excluding one of \( J \) questions (i.e., obtaining patterns \( \ell^{[i]} \), where \( \ell^{[i]} \) denotes vector \( \ell \) with \( j^{th} \) coordinate equal to 0), solving the exact system of equations for obtained patterns, and defining LLS score for complete pattern as mean over \( J \) solutions for conditional expectations for \( \ell^{[i]} \) patterns. This approach can be formalized by considering a system of \( J \) system of equations:

\[
\sum_k \lambda^k_{ji} \cdot g_{\ell k} \approx \frac{f_{\ell}}{f_{\ell}^{[i]}}
\]

This is a sparse overdetermined system; methods for solving such systems are well-elaborated (see, for example, Forsythe et al. (1977), Kahaner et al. (1988)). Since \( \sum_k g_{\ell k} = 1 \) and \( \sum_k \lambda^k_{ji} \cdot g_{\ell k} \geq 0 \) have to be satisfied for any \( \ell \), the Lagrangian for the optimization task has to include corresponding terms with Lagrange multipliers:

\[
L_{g_{\ell}} = \sum_j \left( \sum_k \lambda^k_{ji} \cdot g_{\ell k} - \frac{f_{\ell}}{f_{\ell}^{[i]}} \right)^2 + \sum_{ji} \rho_{ji} \sum_k \lambda^k_{ji} \cdot g_{\ell k} + \rho \left( \sum_k g_{\ell k} - 1 \right)
\]
This is a quadratic programming problem. We used the method of antigradient
projection to the polyhedron defined by the inequality and equality conditions
with iterations as described in Section 3.7. The initial point is defined as
g_{\ell k} = 1/K$. It is possible to show that this initial point always belongs to the
polyhedron.

LLS scores can deviate restrictions $\sum_k \lambda_{j\ell}^k \cdot g_{\ell k} \geq 0$ in limited numbers of cases;
e.g., for a relatively small number of questions $J < 100$. Options to solve the
optimization task without the inequality restriction are also included in the
program. Keeping in (28) Lagrange multipliers for equality conditions only we
have

$$L_{g_{\ell}} = \sum_j \left( \sum_k \lambda_{j\ell}^k \cdot g_{\ell k} - \frac{f_{\ell}}{f_{\ell j}} \right)^2 + \rho \left( \sum_k g_{\ell k} - 1 \right)$$  \hspace{1cm} (28)

The advantage of this task is that it can be solved explicitly, i.e.; without the
search procedures required for the quadratic programming problem. The simplest way to deal with the restriction is to just substitute the $K^{th}$ component
and apply SVD to a $J \times (K - 1)$-matrix $A_{jk} = \lambda_{j\ell_j}^k - \lambda_{j\ell_j}^K$. If SVD has explicit
form as $A_{jk} = \sum_{k'} \tilde{A}_{jk'} W_{k'} V_{k'}^{k}$, where $\tilde{A}$ is a $J \times (K - 1)$-matrix, $W$ contains a
vector of singular values, and $V$ is an orthogonal matrix, then the result for
conditional expectations is

$$g_{\ell k} = \sum_{k'=1}^{K-1} \frac{V_{kk'}}{W_{kk'}} \tilde{A}_{jj'} \left( \frac{f_{\ell j}}{f_{\ell j}} - \lambda_{j\ell_j}^K \right)$$ \hspace{1cm} (29)

for $k = 1, \ldots, K - 1$ and $g_{\ell K} = 1 - \sum_{k=1}^{K-1} g_{\ell k}$.

### 3.6 Mixing distribution

The mixing distribution for an analyzed set of data is approximated by empirical
distribution, where an individual gives a unit contribution to the histogram
of the distribution. A support of this distribution is a set of $I$ points. Probabilities of the joint distribution (4) are estimated as the sum over sample
individuals or to the sum over possible outcome patterns,

$$p_{\ell}^* = \sum_i \prod_{j: j \neq 0} \beta_{j\ell_j}^i = \sum_{e'} \sum_{j: j \neq 0} \sum_k g_{e'k} \lambda_{j\ell_j}^k.$$  \hspace{1cm} (30)

### 3.7 Quadratic programming problem.

The quadratic programming problem is used by the algorithm in the comple-
tion procedure, in calculation of individual LLS scores, and in basis construc-
tion. Corresponding expressions for Lagrangians are given in eqs. (22), (27),
and (31). In all cases, the function minimized is quadratic, and equality and inequality conditions are linear functions of the sought parameters. The matrix of quadratic form is positive definite in all cases. The solution is based on Kuhn-Tucker conditions which become sufficient in these cases. The method of antigradient projection is used in searching for the optimal point (Attetkov et al., 2001). The antigradient direction is defined by the direction opposite to the gradient in a current point. Then the antigradient is projected to a subspace defined by so-called active conditions: all equality conditions and those inequality conditions which are strictly satisfied (i.e., the current point belongs to the corresponding plane). If the absolute value of the projection is not zero then the current point is moved in this direction up to the intersection with the closest boundary, or to the minimum of the quadratic function, whichever is closer. If the absolute value of the projection is zero, then the sign of Lagrange multipliers corresponding to active inequality restrictions is checked. If they all are positive, the current point is the minimum; otherwise a restriction corresponding to the negative Lagrange multiplier is removed and a new antigradient projection is calculated.

3.8 Clustering

Clustering LLS scores is not a necessary component for finding the subspace or calculation of LLS scores; however, it is helpful in selecting a basis and in cross-checking in simulation studies. Two types of clustering procedures (Manton et al., 2003) are implemented in the algorithm. The first is the k-means algorithm for the situation where the number of clusters is fixed a priori. The second is a hierarchical procedure, which sequentially joins clusters with minimal distance between them. Several distance definitions are possible: distance between centers of mass in clusters, between closest and the most outlying cluster members. Numerical comparison shows that the most reliable results are obtained for the center-of-mass scheme.

3.9 Missing data

Missing data are often difficult problems in statistical analyses. Missing data are generated by the absence of responses for an individual to specific questions. The properties of LLS analysis make this kind of missing data relatively easy to handle. Two main sources of missing answers could be considered: first, when the failure to answer the question is random; and second, when the failure to answer the question correlates with answers to other questions. In the first case (missing data are random), the solution is provided by the fact that the input of the LLS algorithm consists of frequencies of partial response pat-
terns (like the frequency of giving response C to the 2nd question and response A to the 5th question). With missing data, such frequencies can be calculated by relating the number of individuals with a particular response pattern to the number of individuals who gave answers to the questions covered by the response pattern (rather than to the total number of individuals). The only drawback of this method is decreased precision of frequency estimators. As LLS scores are expectations of latent variables conditional on the arbitrary part of the response pattern for an individual, the available part of the response pattern can be used to estimate the value of the latent variable. In the second case (missing data are not random), the absence of an answer can be considered an additional alternative for answering a multi-choice question; in this case, standard LLS analysis can be applied.

4 Applications

Below we i) perform a series of simulation experiments to test the predictive power of LLS model and its ability to reveal and to quantitatively reconstruct a hidden latent structure and ii) demonstrate how the model performs when applied to a real dataset considering as an example a demographic survey with 57 questions about disability and health status in 5,161 individuals (Manton and Gu, 2001).

4.1 Simulation studies

We perform three types of simulation experiments which demonstrate the quality of the reconstruction of i) linear subspace, ii) LLS score distribution, and iii) clusters in LLS score space. At the first stage of each simulation study, the dimensionality of the latent structure (strictly, dimensionality of the linear space supporting the structure in the space of individual probabilities) is chosen. Then, assuming a specific structure of questions and numbers of outcomes to each question (i.e., set of indexes $j\ell_j$), basis vectors $\lambda^1, \ldots, \lambda^K$ and mixing distribution $G$ are constructed from some arguments or simulated randomly. Then using individual probabilities calculated as in Eq. (5), outcomes of the specified number of individuals are simulated. The database generated is used as an input for LLS analysis to extract the supporting linear $K$-dimensional subspace and to estimate the mixing distribution via estimation of individual conditional expectations. The comparison of original and extracted linear subspace and mixing distribution provides information about the quality of LLS analysis in conditions defined by $K$, $I$, $J$, and $L_j$. 

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4.1.1 Linear subspace

We started with investigation of the quality of reconstruction of linear subspace. Choosing initial 2-, 3-, and 5-dimensional subspaces with 60, 120, and 240 dichotomous questions and assuming uniform distribution of LLS scores, we simulated 1,430 and 14,300 sets of individual responses. Then we reconstructed a linear subspace and compared it with the initial linear subspace. For such comparisons, we needed a procedure for the quantitative comparison of closeness of multidimensional subspaces, i.e., a measure of a distance or angle between the linear subspaces. Such measure \( d \) is constructed on the basis of the theory of orthogonal projector operators (see Golub and Van Loan, 1989), by which it is possible to define a distance between linear subspaces. By using CS-decomposition, it was proved that the distance may be interpreted as the sine of the generalized angle between subspaces. Technically, \( d = \sqrt{1 - \sigma_{\text{min}}^2} \), where \( \sigma_{\text{min}} \) is the minimal singular value obtained by SVD of \( K \)-dimensional matrix \( Q = P_1^T P_2 \), and \( P_1 \) and \( P_2 \) are \( |L| \times K \)-orthogonal projectors onto comparing subspaces. We will use \( d \) as a measure of the quality reconstruction.

Specifically, original vectors \( \lambda^1, \ldots, \lambda^K \) are constructed as follows: i) vectors \( \lambda^1, \ldots, \lambda^K \) can only take values 0 or 1, ii) \( \lambda_{j1}^j = 1 \) for all \( j \), iii) for \( k \geq 2 \), \( \lambda_{j1}^k = 0 \) if \( j \leq J/(K - 1) \) and \( \lambda_{j1}^k = 1 \) otherwise. In all cases \( \lambda_{j2}^k = 1 - \lambda_{j1}^k \).

The distribution of \( G \) was chosen to the concentrated in a set of discrete points uniformly covering the \( K \)-dimensional simplex. Then a set of probabilities \( \beta_{j1}^i \) is calculated for all individuals and \( J \) outcomes per individual are simulated according to these probabilities. To get stable results we performed a sufficient number of experiments (on the order of 100) and obtained \( d \) presented in the Table 1.

Table 1
Distances between simulated and reconstructed subspaces

| \( K \) | \( N=1,430 \) | \( \text{J=60} \) | \( \text{J=120} \) | \( \text{J=240} \) | \( N=14,300 \) | \( \text{J=60} \) | \( \text{J=120} \) | \( \text{J=240} \) |
|------|---------|---------|---------|---------|---------|---------|---------|---------|
| 2    |         | 0.023   | 0.023   | 0.022   |         | 0.008   | 0.007   | 0.007   |
| 3    |         | 0.075   | 0.072   | 0.070   |         | 0.023   | 0.023   | 0.023   |
| 5    |         | 0.222   | 0.190   | 0.176   |         | 0.073   | 0.059   | 0.057   |

4.1.2 LLS score distribution

We designed the experiments to have statistical stability and to analyze a large number of questions (\( J = 1,500 \)). The position of the supporting plane was chosen randomly. LLS scores are distributed over a union of intervals \([0.10, 0.25]\) and \([0.50, 0.75]\). Specific values of LLS scores are chosen determin-
istically but not simulated as in Kovtun et al. (2005b): 5,000 from 0.10 to 0.25 and 5,000 from 0.50 to 0.75. In total, a sample of 10,000 individuals was generated. First, a mixing distribution was restored from the sample data using the original basis used for outcome simulation. Figure 1a demonstrates reconstructed and true distributions. The latter is shown as a solid line. The figure demonstrates an excellent quality of restoration of the mixing distribution when for reconstruction of mixing distribution we used a simulated, but not reconstructed, basis. Using original vectors $\lambda^1$ and $\lambda^2$ in this comparison allows us to test the procedure of reconstruction of LLS scores separately. These results together with results of a separate test of quality of supporting subspace reconstruction in Table 1 complete the test of the two main components of the LLS algorithm.

However, it is still not clear how overall reconstruction is good, i.e. how uncertainties of the subspace reconstruction could impact the reconstruction of the mixing distribution. To perform this test we used reconstructed vectors $\lambda^1$ and $\lambda^2$ instead of original in the example. The results are given in Figure 1b.

![Fig. 1. Reconstructed mixing distribution using simulated (left) and reconstructed (right) basis. Lines show simulated mixing distribution](image)

In addition, to analyze the performance of the algorithm we conducted this experiment for different numbers of individuals $I$ and variables $J$. The time spent on the algorithm almost does not depend on the size of the sample, as the most time-consuming part of the algorithm is SVD of moment matrix, which has to be performed 6 times (for rank estimation and for 5 iterations of supporting subspace finding). Size of moment matrix depends on the number of measurements $J$. In the table below we give the time spent by the algorithm for different values of $J$ using a computer with an AthlonXP 2500 (2.5GHz) processor and 512MB DDR RAM. In all cases sample size is 8100.
4.1.3 Clusters in LLS score space

We checked the ability of the LLS analysis to identify clusters of LLS scores. We assumed the LLS score distribution was concentrated at five points with equal weights. Then setting $K = 3$ and $I = 1,000$ we simulated individual responses for $J=100, 200$ and $500$. Then we applied a complete-linkage hierarchical clustering procedure (Section 3.8) both to the reconstructed LLS scores and to the original vector of response to combine individuals in 5 classes. As a measure of quality, we used the fraction of individuals assigned to the correct class. We performed 10 simulations to make the calculation statistically stable. The average number of misclassified individuals is given in Table 3.

Table 3
The average number of misclassified individuals for different $J$

| $J$  | 100   | 200   | 500   |
|------|-------|-------|-------|
| Original responses | 22.7% | 17.3% | 14.9% |
| LLS scores       | 4.8%  | 0.2%  | 0.0%  |

This example demonstrates that the individual conditional expectations are better suited for the purpose of classification than the original vectors of responses.

4.2 Application to the NLTCS data

The National Long Term Care Survey is a longitudinal survey designed to study changes in the health and functional status of older Americans (aged 65+). It also tracks health expenditures, Medicare service use, and the availability of personal, family, and community resources for caregiving. The survey began in 1982, with follow-up surveys done in 1982, 1984, 1989, 1994, and 1999. A sixth follow-up survey was conducted in 2004-2005. A detailed description of the NLTCS may be found at [http://nltcs.cds.duke.edu/](http://nltcs.cds.duke.edu/).

We analyzed a sample of 5,161 individuals from the 1999 NLTCS, and selected 57 questions. 27 variables characterize disability level with respect to activities of daily living, instrumental activities of daily living, and physical impairment. 30 variables describe self-reports of chronic diseases. Details about these questions may be found in Manton and Gu (2001). Then we excluded 370 individuals with at least one missing outcome. Thus, 4,791 remaining in-
individuals are subject to 57 questions, 49 of which have 2 possible answers, and 8 have 4 possible answers. In total, we have $|L| = 130$.

The first task is to define the dimensionality of the LLS problem, $K$. As mentioned above, $K$ is the rank of the moment matrix, and thus it could be estimated as the rank of the frequency matrix. We used the SVD to estimate the rank of the frequency matrix. As the frequency matrix is incomplete, we decompose not the whole matrix, but its bottom left corner of size 64. The singular values obtained were compared to total statistical error found as a quadratic sum of cell errors. This ratio was 0.292. Individual cell standard errors were estimated using Wilson’s approach (19). The first 10 singular values are given in Table 4.

The computations show that the hypothesis $K = 4$ has to be accepted with confidence level 95%; that corresponds approximately to the double standard error interval (0.584). For comparison, we will also consider the case of $K = 3$. Note that there is no significant gap between the 4th and 5th singular numbers. This suggests that the support of the distribution is an ellipsoid of full dimensionality which is thinner in higher dimensions, and choosing a particular value for $K$ approximates this ellipsoid by a lower-dimensional ellipsoid obtained from the true one by collapsing a number of smaller axis.

Table 4
First 10 singular values of frequency matrix of NLTCS

| $\sigma_1$ | $\sigma_2$ | $\sigma_3$ | $\sigma_4$ | $\sigma_5$ | $\sigma_6$ | $\sigma_7$ | $\sigma_8$ | $\sigma_9$ | $\sigma_{10}$ |
|------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|
| 39.112     | 3.217      | 1.464      | 0.652      | 0.363      | 0.310      | 0.243      | 0.220      | 0.198      | 0.148       |

When the dimensionality of the LLS-problem is fixed, we can complete the moment matrix using the algorithm described in Section 3.3. The sub-matrix corresponding to the first four dichotomous variables is,

\[
\begin{pmatrix}
0.094 & 0.513 & 0.051 & 0.328 & 0.011 & 0.258 & 0.012 & 0.518 & 0.014 \\
0.906 & 0.487 & 0.949 & 0.672 & 0.989 & 0.742 & 0.988 & 0.482 & 0.986 \\
0.264 & 0.918 & 0.196 & 0.633 & 0.128 & 0.688 & 0.051 & 0.846 & 0.153 \\
0.736 & 0.082 & 0.804 & 0.367 & 0.872 & 0.312 & 0.949 & 0.154 & 0.847 \\
0.335 & 0.916 & 0.275 & 0.872 & 0.142 & 0.664 & 0.164 & 0.888 & 0.230 \\
0.665 & 0.084 & 0.725 & 0.128 & 0.858 & 0.336 & 0.836 & 0.112 & 0.770 \\
0.160 & 0.879 & 0.085 & 0.514 & 0.034 & 0.424 & 0.027 & 0.640 & 0.069 \\
0.840 & 0.121 & 0.915 & 0.486 & 0.966 & 0.576 & 0.973 & 0.360 & 0.931 \\
\end{pmatrix}
\]

Completed values are marked in bold style. Renormalization of the frequency matrix is performed (see Section 3.1). Recall that columns of the frequency ma-
atrix are approximately in the sought linear subspace. The procedure described in Section 3.3 provides an unambiguous definition of the sought subspace and some basis vectors $\lambda_{jl}^k$. The basis cannot be defined uniquely, and any convex combination keeping LLS restrictions (3) can be considered an alternative. In this example, we apply a combination of the methods discussed in Section 3.4. Specifically, in the beginning we estimated LLS scores in some prior basis. Since subsequent conclusions are made on the basis of clusterization and analysis of probability vectors, which are independent of initial basis choice, the initial basis is taken as it was obtained from subspace construction, i.e., it is arbitrary. Then LLS scores are assigned to 7-8 clusters (i.e., for slightly larger numbers of clusters than $K$) using methods of cluster analysis. By analyzing outcomes of typical representative respondents (with LLS scores closest to centers of clusters) and of probabilities $\beta_{jl}^k$ calculated as means over each cluster, we can identify the cluster structure of the analyzed population. Based on this analysis, we chose $K = 4$ clusters corresponding to i) healthy individuals ($k = 1$), ii) partly disabled individuals ($k = 4$), iii) strongly disabled individuals ($k = 2$), and iv) individuals with chronic diseases but without evidence of disability ($k = 3$). For each such group, we created a “typical” vector of probabilities $\beta_{jl}^k$ by hand. Specifically, for the first group we chose unit probabilities for all answers corresponding to healthy states. For the second group, mean frequencies over the sample are chosen. For the third group, unit probabilities are assigned to answers corresponding to strongly disabled states and means over samples for chronic disease questions. For the fourth group, unit probabilities correspond to non-disabled states and to all disease diagnoses. The final basis is constructed by projection of all four vectors to the simplex. Technically, finding vectors $g_k$ minimizes the Lagrangian (27), which for this task has the form:

$$L_{g_k'} = \sum_{jl} \left( \sum_k \lambda_{jl}^k \cdot g_k - \beta_{jl}^k \right)^2 + \sum_{jl} \rho_{jl} \sum_k \lambda_{jl}^k \cdot g_k + \rho \left( \sum_k g_k - 1 \right), \quad (31)$$

and applying the algorithm sketched in Section 3.7. Then a similar analysis was performed for $K = 3$, where the basis component for partly disabled individuals was rejected. Figure 2 demonstrates the results. The plots on the left show 2d-polyhedron for $K = 3$ and two projections of 3d-polyhedron for $K = 4$. These polyhedrons are defined by LLS restrictions (3). In this case, LLS scores are restricted by 130 inequality and 1 equality. 2d-polyhedron is shown as it is in the plane normal to vector $g = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$. 3d-polyhedron is in the plane normal to $g = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. Basis vectors produced unit simplexes are labeled by numbers. Plots on the right demonstrate how the polyhedrons are filled by the considered population. For the filling we performed clustering to 1,000 clusters. Each point in the plots represents one cluster. The area of each point is proportional to the number of individuals assigned to the corresponding cluster. The exception is the point marked by open circles with a closed point inside. About half of the total population was assigned to this
Fig. 2. Polyhedrons defined by LLS constrains for $K=3$ (a) and $K=4$ (c,e) and their filling by LLS scores of NLTCS individuals (b,d,f). See text for further explanations.

cluster. We restrict consideration to this illustration.
5 Discussion and Conclusion

LLS is a model describing high-dimensional categorical data assuming existence of a latent structure described by $K$-dimensional random vectors. This vector is interpreted as explanatory variables which can shed light on mutual correlations observed in measured categorical variables. This vector plays the role of a random variable mixing independent distribution such that the observed joint distribution is maximally close to the data. Mathematically, LLS analysis considers the observed joint distribution of categorical variables as a mixture of individual joint distributions, which are assumed to be independent. This is the standard “local independence” assumption of latent structure analysis; the specific LLS assumption is that the mixing distribution is supported by a $K$-dimensional subspace $\Lambda$ of the space of all independent distributions or, equivalently, of the space of individual probabilities. The mixing distribution can be considered as a distribution of random vectors $G$, which take values in $\Lambda$. The vectors $g_i$ (LLS scores) are the hidden states of individuals in which we are interested. They can be estimated as conditional expectations of $G$, $g_\ell = E(G|X_1 = \ell_1, \ldots, X_J = \ell_J)$, where $\ell = (\ell_1, \ldots, \ell_J)$ is a response pattern. Support of this random vector is a $K$-dimensional space, the dimension of which is defined by the dataset. Linear support is a distinctive feature of LLS compared to other latent structure analyses. For example, LCM is characterized by mixing distribution concentrated in several isolated points.

Another important distinction is the existence of an algorithm capable of estimating a LLS model for large numbers of questions and individuals. When a basis $\lambda^1, \ldots, \lambda^K$ of linear subspace supported mixing distribution is known, conditional expectations $g_\ell$ can be calculated by solving a linear system of equations. A basis $\lambda^1, \ldots, \lambda^K$, in turn, can be identified by applying principal component analysis to the moment matrix. As the choice of a basis is not unique, one has to apply substantial knowledge derived from the applied domain to make the most appropriate choice. This algorithm, being a sequence of linear algebra methods, does not use maximum likelihood methods. This is an advantage of the method, because individual information is presented via nuisance parameters, which creates difficulties in the maximum likelihood approach. The LLS algorithm for parameter estimation is based on two theorems which became possible because of a linear assumption about the support of the mixing distribution. The first identifies properties of the moment matrix. The second presents the main system of equations. Just the existence of the system of equations that describes parameters of the model is a significant advantage of the LLS method, as it allows us to avoid using maximum likelihood estimators, which may not be consistent in the presence of nuisance parameters.

Construction of LLS analysis on the basis of the theory of mixed distributions
provides clear and simple proof of basic statistical properties of the estimator. Regarding consistency, note that parameter estimations of the LLS model are solutions of a quasilinear system of equations, whose coefficients are the observed frequencies. When true moments are substituted in the system instead of frequencies, its solution represents the true values of parameters. The consistency of LLS estimators follows from the fact that i) solutions of the system continuously depend on its coefficients, and ii) frequencies are consistent estimators for the moments. Regarding identifiability, it was shown in Kovtun et al. (2005b) that the LLS model is identifiable if the moment matrix is “sufficiently non-degenerated”. It was also shown in Kovtun et al. (2005b) that for almost all mixing distributions the moment matrix is non-degenerated. Thus, LLS models are almost surely identifiable.

We performed a series of simulation experiments to analyze the quality of reconstruction of: i) linear subspace; ii) LLS mixing distribution; and iii) clustering properties. The results demonstrated an acceptable quality of reconstruction. It is interesting to compare the results of the LLS model with the potential results of a latent class model. If mixing distribution is concentrated in several isolated points, LCM would restore the same picture as LLS, and thus, it could be an alternative for the LLS model. However, in cases like in Figure 2 LCM may only be used as an approximation, and it may be shown that LCM should involve approximately 1,000 latent classes (the number of classes in this case is approximately equal to number of different LLS scores obtained by the LLS model).

Analysis of demographic data on disability and chronic diseases demonstrated the potential of the LLS model to investigate the properties of populations with latent heterogeneity. Performing cluster analysis, we identified four basic population groups corresponding to healthy, disabled, strongly disabled individuals, and persons with chronic diseases. We found linear subspaces for $K = 3$ and $K = 4$. Empirical mixing distributions for these cases are presented as distributions on supportive polyhedrons (Figure 2) defined by LLS restrictions.

This analysis can be naturally generalized to the case of longitudinal data using a binomial quadratic hazard model (Manton et al, 1992) or stochastic process model (Yashin and Manton, 1997). This can provide the possibility of introducing mortality into the model. The basic advantages of these models are that they provide a biologically justified U- or J- shaped hazard function versus covariates (Witteman et al., 1994). In our case, LLS scores would play the role of covariates. LLS scores are constrained to have a sum of one. This is appropriate for interpretation and applications. Constraints of LLS scores (e.g., $\sum_k g_k = 1$) prevent the direct use of a stochastic process model for projection. One way to eliminate this restriction without losing the advantage in interpretation is to eliminate the component corresponding to the healthiest
pure type (due to the freedom in basis choice, a basis with healthy state can always be chosen), thereby solving the problem of dealing with this restriction and, moreover, allowing us to specify a model for the hazard function. For the hazard we will use a quadratic hazard model, where the quadratic form models dependence on the components of state vectors. Since the health component of the LLS score vector is eliminated, it is reasonable (and technically appropriate) to assume that the minimum of mortality is located in the origin over the remaining components (i.e., mortality is minimal for the healthiest people). This allows us to drop the linear component of the quadratic hazard function. After estimating the parameters, a scheme for the projection calculation has to be developed. In the general case, possibly including nonlinear relations in dynamic equations, the approach can be based on a microsimulation procedure; i.e., a method for simulating trajectories for each person in the cohort (Akushevich et al., 2005).

Furthermore, LLS opens its own possibilities for longitudinal analyses of repeated measurements using its inherent features. Supporting planes obtained for different waves may not coincide with each other. The first question to be analyzed is how different are supportive planes obtained from different waves and whether a plane obtained for combined dataset is a good fit or there is a trend in the plane movement over a state space. In the first case, a plane obtained for joint analysis would be taken for longitudinal analysis. Basis becomes time independent and chosen by taking specifics of the problem into account. If a trend of time movement of supportive plane is found, we should analyze the possible explanation of the trend in terms of time trends in the population measured in different waves of such experiments. Basis in this case would first be calculated for the joined plane, and then projections of basis vectors of a specific plane provide a time dependence of the basis. In all cases we can investigate the difference between results obtained for time dependent and approximate time independent bases.

This way a series of mathematical models to deal with the longitudinal analysis of biomedical data with repeated categorical measurements and event history data can be created. They will be oriented both for population and individual prognoses through analysis of individual trajectories in state space. For example, if the models are calibrated using NLTCS and Medicare data, the results could provide a better understanding of the biodemographic mechanisms responsible for aging and morbidity, and could be useful in forecasting health and population trends and in stochastic investigation in medical economics, including estimating the financial effectiveness of new medical technologies.

After such investigation of missing data, they can be filled by probabilities $\beta_{ij}$, which can be calculated using LLS scores of the known part of the outcome pattern and the found linear subspace $\Lambda$. This filling probability does not depend on basis choice and on prior information used for the basis selection.
procedure. The largely model independent imputation procedure could be very useful in filling categorical data in historical cohorts or in dataset where data collection is difficult or costly.

LLS can be used to analyze data where a high dimensional measurement vector represents a hidden structure affecting the results of measurements. An abundance of such data recently appeared in genetic studies of biological systems where the expression of thousands of genes in cells taken from different organs and tissues of humans or laboratory animals is measured. Such measurements are performed to find appropriate regularities in biological functioning of organs and tissues of respective organisms and to detect changes in hidden biological structure due to disease, exposure to external factors, aging related changes, etc. Such an analysis will help us to better understand mechanisms of genetic regulation, by suggesting genes playing key roles in organizing response to changes in internal or external milieu.

Forthcoming steps with LLS and the algorithms will include further investigation of algorithm properties and development of computer code in a form convenient for use by applied researchers. The most important property to be investigated is numerical stability of the algorithm. Different possibilities to perform subtasks should be investigated to avoid ill-posed problems. Several steps in algorithms are based on heuristic approaches, so they have to be theoretically investigated and improved. This will, on the one hand, provide a basis for selection of numerical methods used in the algorithm and, on the other hand, provide rigorous proofs of conditions of applicability of the algorithm and reliability of its results.

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Appendix

The mixing distribution (which is a distribution in Euclidean space $R^{|L|}$ carried by a polyhedron defined by (3)) can be given in form of either a probabilistic measure $\mu(\beta)$, or probability density function $\rho_\beta(\beta)$ (or cumulative distribution function $F(\beta)$) with respect to the standard Lebesque measure in $R^{|L|}$). In the last case one must allow $\rho_\beta(\beta)$ to be a generalized function to capture cases where $\mu_\beta$ has a singular component with respect to a Lebesque measure.

The permitted domain (3) of density function $\rho_\beta(\beta)$ in (7) can be reflected explicitly in terms of products of $\delta-$ and $\theta-$functions, so the density function
has a representation

\[ \rho_\beta(\beta) = \bar{\rho}(\beta) \left( \prod_{jl} \theta(\beta_{jl}) \right) \prod_j \delta \left( \sum_l \beta_{jl} - 1 \right) \]  

(32)

Recall that the generalized p.d.f. \( \delta(x) \) corresponds to a distribution concentrated at a single point \( x = 0 \) and is characterized by properties \( \delta(x) = 0 \) for \( x \neq 0 \) and \( \int_{-\infty}^{\infty} dx \delta(x) = 1 \); \( \theta(x) \) is a characteristic function of positive half-axis, i.e. \( \theta(x) = 0 \) if \( x < 0 \) and \( \theta(x) = 1 \) if \( x \geq 0 \). Product \( \prod_{jl} \theta \prod_j \delta \) is 0 outside the polyhedron \( P_\beta \) defined by conditions (3), thus values of \( \bar{\rho}(\beta) \) outside \( P_\beta \) are insignificant.

In transferring from the integration over \( \beta \) to the integration over \( g \), the integral dimension is reduced from \( |L| \) with \( J \) restrictions defined by \( \delta \)-functions to \( K \) with one restriction. Explicitly it can be obtained from (7) by i) orthogonal transformation of integration variables such that \( K \) new variables belong to \( \Lambda \); ii) using the fact (main LLS assumption) that the density function depends only on these \( K \) variables; iii) integration over remaining \( |L| - K \) variables. Formally such a procedure corresponds to representation of \( \bar{\rho}(\beta) \),

\[ \bar{\rho}(\beta) = \int dg \hat{\rho}(g) \prod_{jl} \delta \left( \beta_{jl} - \sum_k g_k \lambda^k_{jl} \right) \]  

(33)

and forthcoming integration over all \( \beta_{jl} \) using \( |L| \) delta functions in (33). \( \delta \)- and \( \theta \)-functions extracting permitted integration area (3) in integrals (7) and (32) are transformed such that permitted area in integration over \( g \) are given by (6). As a result we obtain unconditional moments \( M_\ell \) (and, therefore probabilities \( p_\ell \)) as integrals over \( g \) coordinates:

\[ M_\ell = p_\ell = \int dg \left[ \prod_{j,l,j \neq 0} \sum_k g_k \lambda^k_{jl} \right] \times \]  

\[ \times \hat{\rho}(g) \delta \left( \sum_k g_k - 1 \right) \prod_{jl} \theta \left( \sum_k g_k \lambda^k_{jl} \right) \]  

(34)

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