Journal of Data Science **10**(2012), 19-36

# The Role of Rotation Type used to Extract Dietary Patterns through Principal Component Analysis, on their Short-Term Repeatability

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*Abstract*: Principal components analysis (PCA) is a widely used technique in nutritional epidemiology, to extract dietary patterns. To improve the interpretation of the derived patterns, it has been suggested to rotate the axes defined by PCA. This study aimed to evaluate whether rotation influences the repeatability of these patterns. For this reason PCA was applied in nutrient data of 500 participants (37 ± 15 years, 38% male) who were voluntarily enrolled in the study and asked to complete a semi-quantitative food frequency questionnaire (FFQ), twice within 15 days. The varimax and the quartimax orthogonal rotation methods, as well as the non-orthogonal promax and the oblimin methods were applied. The degree of agreement between the similar extracted patterns by each rotation method was assessed using the Bland and Altman method and Kendall's tau-b coefficient. Good agreement was observed between the two administrations of the FFQ for the un-rotated components, while low-to-moderate agreement was observed for all rotation types (the quartimax and the oblimin method lead to more repeatable results). To conclude, when rotation is needed to improve food patterns' interpretation, the quartimax and the oblimin methods seems to produce more robust results.

*Key words*: Multivariate analysis, principal components analysis, repeatability, rotation type.

## 1. Introduction

The traditional approach in nutrition epidemiology of single food or nutrient effect on health status has been progressively modified to an approach that takes under consideration how foods and nutrients consumed in combination (Hu, 2002). The concept of studying dietary patterns, as a "holistic" approach in order to better evaluate diet-disease associations, has educed extensive interest

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during the past years (Hu *et al.*, 1999). Multivariate statistical techniques, such as principal component analysis (PCA) and factor analysis (FA) have been introduced and widely used to nutritional epidemiology as an attempt to capture diet's variability and reduce data complexity (Randall *et al.*, 1989; Randall *et al.*, 1990). These statistical exploratory methods have already been applied in many population-based studies in order to derive the dietary patterns that people actually follow, through the retrieved nutrient information (Whichelow and Prevost, 1996; Slattery *et al.*, 1998; Schulze *et al.*, 2001). Specifically, the aforementioned data reduction methods, like PCA and FA, aimed to reduce the amount of information (i.e., number of variables) considered in an analysis and to detect specific structure in the relationships between variables. In other words, food variables that are correlated to each other, but are independent of other subsets of variables are combined into new components (or factors).

In order to facilitate the interpretation of these components that are considered relevant, a rotation method is usually followed. Rotation has been defined as "performing arithmetic calculations to obtain a new set of components' loadings from a given set" and has been used in order to maximize the variance explained of the extracted components (McDonald, 1987). Rotation can be explained as a variety of methods used to further analyze initial components, aiming to make the pattern of loadings clearer, more well-defined and thus, reveal a simple structure of the initial information. There are two types of rotation, the orthogonal rotation, where the rotated components are orthogonal to each other and thus, the data believed to be uncorrelated and the non-orthogonal (oblique) rotation by which the components are not required to be orthogonal to each other and thus, the data are allowed to be correlated (Vogt, 1998). The rotating procedure has been suggested as it simplifies the component structure and therefore makes its interpretation easier and more reliable (i.e., easier to reproduce with different data) (Cattell, 1978).

Repeatability of a measurement is a cornerstone in achieving robust, stable results in health related studies, and in all research, as well. The role of rotation in extracting more interpretable dietary components as regards the repeatability of these patterns has never been evaluated before. Thus, the purpose of this methodological study was to evaluate whether the rotation type affects the sort-term repeatability (i.e., stability) of dietary patterns derived from the application of PCA on empirical data from a nutrition survey.

## 2. Materials and Methods

### 2.1 Participants

From February 2008 to February 2009, 500 participants ($37 \pm 15$ years, 38%

male) were enrolled to the study on a voluntary basis (participation rate 85%). The participants were interviewed by specialised personnel (i.e., dieticians) in order to complete a semi-quantitative food frequency questionnaire (FFQ), based on their dietary habits. The sample size was considered adequate in achieving statistical power equal to 99% for the evaluation of two-sided mean differences in the frequency of food's intake, equal to 0.1 times per week, at 0.05 type-I error. The rationale of the power analysis was to evaluate the degree of validity and repeatability of the questionnaire used, by permitting very slight differences in recording food intake.

The retrieved data were confidential and the study followed the ethical considerations provided by the World Medical Association (52nd WMA General Assembly, Edinburgh, Scotland, October 2000). Moreover, the Ethics Committee of Harokopio University approved the design, procedures and aims of the study (GA 23/14.05.2009). All participants were informed about the aims and procedures of the study and agreed to participate providing their consent.

## 2.2 Administration of FFQ

The participants were asked to complete twice, within 15 days interval, a valid and repeatable semi-quantitative FFQ that included 69 questions for food items usually consumed in westernized populations, as well as 7 questions with respect to dietary behaviors. This time period has been suggested by several investigators (Streiner and Norman, 1995). Particularly, respondents were requested to recall how often they consumed the predefined food quantity (in g, mL or other common measures) during the past month, according to a 6-grade scale (i.e., 1: rarely/ never, 2: 1-3 times per month, 3: 1-2 times per week, 4: 3-6 times per week, 5: 1 time per day, 6: $\geq$ 2 times per day). All main food groups (dairy products, cereals, fruits, vegetables, meat, fish, legumes, added fats, alcoholic beverages, stimulants, sweets) were included in this questionnaire. Details related to food items included in the FFQ can be found elsewhere (Bountziouka *et al.*, 2010).

## 2.3 Food Grouping

To reduce the complexity of the data, food items were further grouped according to their similarity of nutrient profiles. Some individual food items were kept separately because they were assumed to represent distinct dietary patterns (i.e., wine, beer, spirits). Thus, 24 food groups were used in analyses to derive dietary patterns (see Appendix Table).

## 2.4 Statistical Analysis

PCA was used as the data driven technique to extract dietary patterns (components) on the basis of the correlation of the 24 food groups mentioned above. The Kaiser-Mayer-Olkin measure (KMO) was calculated to evaluate the level of intra-correlation between the food variables (values $> 0.6$ indicate good intra-correlation and, therefore, PCA could give interpretable results). Both orthogonal and non-orthogonal rotation has been further performed to assess the structure of the derived patterns. The components were first orthogonally rotated by the varimax and the quartimax method, leading to independent components which were considered easier to interpret. According to Kaiser's criterion (Kaiser, 1958), let $\Lambda$ be a $p \times k$ matrix, and $R$ an orthogonal $m \times m$ rotation matrix such as $R^T R = I$:

$$R_{\text{orthogonal}} = \arg\max_R \left( \sum_{j=1}^{k} \sum_{i=1}^{p} (\Lambda R)_{ij}^4 - \frac{\gamma}{p} \sum_{j=1}^{k} \left( \sum_{i=1}^{p} (\Lambda R)_{ij}^2 \right)^2 \right),$$

where $\gamma = 1$ for the varimax method, that maximizes the squared component loadings in each component, and $\gamma = 0$ for the quartimax method, that maximizes the variance of the squared component loadings in each variable (Stegmann *et al.*, 2006). In addition, non-orthogonal rotation by the promax and the oblimin methods was applied, since in many circumstances the dietary patterns cannot be entirely considered uncorrelated. The starting point of rotation is a $p \times m$ matrix $\Lambda$ of component loadings with components $\lambda_{ir}$. The $\lambda_{ir}$ represent the covariances between the observed variables and the reference components. Generalizing the varimax and the quartimax criterion to the oblique case, Caroll (1957) introduced the oblimin family:

$$\text{OBMIN} = \sum_{r \neq s} \left( n \sum_i \lambda_{ir}^2 \lambda_{is}^2 - \gamma \sum_i \lambda_{ir}^2 \sum_s \lambda_{is}^2 \right).$$

The direct oblimin method is actually a function that minimizes the primary-component-pattern coefficients:

$$\min F(\Lambda) = \sum_{r \neq s} \left( \sum_i \lambda_{ir}^2 \lambda_{is}^2 - \frac{\gamma}{n} \sum_i \lambda_{ir}^2 \sum_s \lambda_{is}^2 \right),$$

where $\Lambda = A(T')^{-1}$, with $A$ the initial loading matrix and $T$ a transformation matrix $T$ that will minimize $F(A(T') - 1)$, under the condition that $Diag(T'T) = I$ (Caroll, 1957; Jennrich and Sampson, 1966). Principal components (PCs) with eigenvalues of $\geq 1$ were retained. Each rotated PC was interpreted ("named") based on the foods that have loadings of $\geq |\, 0.3 \,|$, which were considered as significantly contributing to the specific component (pattern). Within a component, a positive score indicates a direct association, while a negative score indicates that foods were inversely associated with the component. The larger the score of a given food item or group, the greater the contribution to the specific component (Joliffe and Morgan, 1992). The extracted PCs, derived from the two FFQ administrations, were compared on the basis of their nutritional interpretation ("subjective" approach). For assessing the agreement of the dietary patterns as derived from PCA by the application of different rotation types, the Kendall's tau-b correlation coefficient was used between the respective components that subjectively described the same pattern. Values $> 0.3$ suggest moderate agreement, while values $> 0.6$ suggest good agreement (Kendall, 1938). To further confirm the agreement of patterns derived, the Bland and Altman method was applied. Specifically, the limits of agreement (i.e., mean(difference) $\pm$ $1.96X$ standard deviation(difference)) were used to quantify the degree of agreement for the repeatability process of the dietary patterns (Bland and Altman, 1986). The significance level for hypotheses tested was considered at 0.05. All statistical analyses were performed using the SPSS version 14 (SPSS Inc., Chicago, Il, USA).

## 3. Results

According to PCA, 8 components (that had eigenvalue $\geq 1$) were extracted from the 1st recording of the FFQ, explaining 57% of the total variance in consumption, while 7 components were extracted from the 2nd recording of the FFQ, explaining 55% of the total variance in consumption. In addition, the KMO was found 0.72 for the 1st recording and 0.77 for the 2nd recording indicating moderate to good level of inter-correlation among the initial food variables. However, 4 were the main components that were better reflecting a specific dietary pattern and were easy to interpret, from both recordings, explaining 38% and 40% of the total variance respectively.

### 3.1 Unrotated Components

The four main components that were derived when no rotation was applied were found similar in both recordings, in terms of nutritional information. Specifically, the 1st component was heavily loaded by white starchy products, eggs, potato, red meat, poultry, full fat delicatessens, bakery, sweets and sodas, describing a "Western dietary pattern". The 2nd component was consisted by a variety of foods reflecting a "Mediterranean dietary pattern" (i.e., low-fat dairy products, whole meal products, fish, legumes, fruit and vegetables). A "Drinking pattern" has been revealed, as regards to the 3rd component, mainly characterized by wine, beer, spirits and stimulants intake. Finally, the 4th component was heavily loaded by "light products" intake (i.e., low-fat dairy products, low-fat delicatessens, light sodas) (Table 1). Kendall's tau coefficients were $> 0.50$ (all $p < 0.0001$) suggesting a moderate-to-good agreement between the components derived from both recordings. Based on the Bland and Altman method it has been revealed acceptable limits of agreement for the mean difference between the patterns, with the narrowest limits to be noticed for the "Mediterranean/ healthy" pattern (Table 4).

Table 1: Components' scores for four major dietary patterns derived using Principal Components Analysis (no rotation), form the two records of a semi-quantitative Food Frequency Qustionnaire

| | FFQ1 | | | | FFQ2 | | | |
|---|---|---|---|---|---|---|---|---|
| | PC1 | PC2 | PC3 | PC4 | PC1 | PC2 | PC3 | PC4 |
| **Food group, (g-mL/d)** | | | | | | | | |
| *Full fat dairy* | 0.08 | -0.05 | -0.03 | -0.03 | 0.12 | -0.05 | -0.12 | -0.17 |
| *Low fat dairy* | -0.04 | 0.54 | 0.07 | 0.40 | -0.07 | 0.55 | 0.01 | 0.44 |
| *White starchy* | 0.58 | -0.10 | -0.02 | -0.16 | 0.58 | -0.06 | 0.08 | -0.17 |
| *Wholemeal starchy* | 0.43 | 0.47 | -0.11 | 0.19 | 0.49 | 0.46 | -0.09 | 0.11 |
| *Egg* | 0.43 | -0.04 | 0.03 | -0.18 | 0.31 | -0.06 | 0.08 | -0.03 |
| *Potato* | 0.51 | -0.08 | -0.09 | -0.44 | 0.61 | -0.11 | -0.01 | -0.37 |
| *Red meat* | 0.69 | -0.11 | -0.30 | -0.14 | 0.75 | -0.08 | -0.08 | -0.11 |
| *Poultry* | 0.53 | 0.20 | -0.22 | 0.05 | 0.54 | 0.10 | -0.11 | 0.05 |
| *Full fat delicatessens* | 0.58 | -0.27 | -0.10 | 0.30 | 0.61 | -0.27 | -0.16 | 0.16 |
| *Low fat delicatessens* | 0.35 | 0.22 | -0.01 | 0.53 | 0.37 | 0.20 | -0.05 | 0.52 |
| *Fish* | 0.43 | 0.45 | 0.09 | -0.35 | 0.53 | 0.47 | 0.10 | -0.34 |
| *Legumes* | 0.28 | 0.37 | 0.11 | -0.40 | 0.24 | 0.46 | 0.04 | -0.30 |
| *Vegetables* | 0.18 | 0.66 | 0.30 | -0.13 | 0.05 | 0.69 | 0.21 | -0.07 |
| *Fruit* | 0.09 | 0.53 | 0.22 | -0.03 | 0.06 | 0.62 | 0.16 | -0.07 |
| *Bakery* | 0.53 | -0.05 | 0.02 | 0.32 | 0.53 | -0.04 | -0.07 | 0.38 |
| *Sweets* | 0.42 | -0.16 | -0.04 | 0.03 | 0.56 | -0.11 | -0.15 | 0.12 |
| *Wine* | 0.11 | -0.24 | 0.71 | -0.01 | 0.09 | -0.13 | 0.75 | 0.00 |
| *Beer* | 0.23 | -0.36 | 0.50 | -0.16 | 0.23 | -0.29 | 0.60 | -0.08 |
| *Spirits* | 0.31 | -0.38 | 0.45 | 0.11 | 0.36 | -0.27 | 0.46 | 0.11 |
| *Stimulants* | 0.12 | 0.04 | 0.49 | 0.03 | 0.01 | 0.01 | 0.46 | 0.25 |
| *Sodas* | 0.40 | -0.34 | 0.00 | 0.06 | 0.52 | -0.30 | -0.02 | 0.06 |
| *Light sodas* | 0.31 | 0.01 | 0.14 | 0.50 | 0.40 | 0.08 | 0.03 | 0.34 |
| *Olive oil* | -0.07 | 0.20 | 0.42 | -0.04 | -0.13 | 0.14 | 0.46 | -0.04 |
| *Other oils & fats* | 0.23 | -0.05 | -0.23 | -0.17 | 0.34 | 0.04 | -0.16 | -0.33 |
| % of variance explained | **14.4** | **9.6** | **7.4** | **6.6** | **17.2** | **9.4** | **7.4** | **5.8** |

1st administration FFQ: PC1 "Western pattern", PC2 "Mediterranean pattern", PC3 "Drinking pattern", PC4 "Low fat pattern". 2nd administration FFQ: PC1 "Western pattern", PC2 "Mediterranean pattern", PC3 "Drinking pattern", PC4 "Low fat pattern".

### 3.2 Orthogonal Rotation

Afterwards the orthogonal rotation method was applied to the components using the varimax and the quartimax type of rotation. With respect to the varimax rotation, four were the main components that were reflecting a specific dietary scheme and were found repeatable in both recordings, although explained different percentage of variability each time. Regarding the components derived from the 1st recording, the 1st component was characterized as the "Western pattern", the 2nd as the "High protein pattern", the 3rd as the "Drinking pattern" and the 4th as the "Healthy pattern". Regarding the components derived from the 2nd recording, the 1st component was reflecting the "Western dietary pattern", the 2nd the "Healthy pattern", the 3rd the "High protein pattern" and the 4th the "Drinking pattern". Component loadings for each pattern are shown in Table 2.

As regards the components derived after the application of the quartimax rotation type, four were the main patterns that seemed to better reflect the participants' dietary habits and were easy to identify. Specifically, the dietary patterns derived from the 1st recording described the "Western pattern" (1st component), the "Drinking pattern" (2nd component), the "High protein pattern" (3rd component) and the "Healthy pattern" (4th component). In addition, the "Western pattern" (1st component), the "Healthy pattern" (2nd pattern) and the "Drinking pattern" (3rd pattern) were also revealed from the 2nd recording, while the 4th component was mainly characterized by a "Low calorie intake pattern" (Table 2). Hence, three were the major patterns that showed some similarities, and were further used for comparison purposes.

Based on Kendall's tau it was observed very low-to-moderate strength of agreement between the same patterns derived from both administrations using the varimax rotation (tau = 0.15 for the "High protein", tau = 0.18 for the "Western", tau = 0.24 for the "Healthy" and tau = 0.44 for the "Drinking" pattern; all $p < 0.0001$). In addition, according to the Bland and Altman method, although the mean difference of each two patterns loadings was equal to zero, the limits of agreement were wider as compared with the "un-rotated" results; a fact that also reflects the moderate level of agreement. With respect to the quartimax rotation type, the strength of the agreement between respective patterns was higher as compared with previous method. In particular, low-to-moderate agreement was found according to Kendall's tau (0.46 for the "Western", 0.28 for the "Healthy" and 0.45 for the "Drinking" pattern; all $p < 0.0001$), while the limits of agreement according to the Bland and Altman method were now closer to the mean difference as compared with the varimax rotation (Table 4); also confirming the aforementioned finding of moderate concordance.

Table 2: Components' scores for four major dietary patterns derived using Principal Components Analysis (orthogonal rotation), form the two records of a semi-quantitative Food Frequency Questionnaire

| | Varimax rotation | | | | | | | | Quartimax rotation | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | FFQ1 | | | | FFQ2 | | | | FFQ1 | | | | FFQ2 | | | |
| | PC1 | PC2 | PC3 | PC4 | PC1 | PC2 | PC3 | PC4 | PC1 | PC2 | PC3 | PC4 | PC1 | PC2 | PC3 | PC4 |
| **Food group, (g-mL/d)** | | | | | | | | | | | | | | | | |
| *Full fat dairy* | 0.30 | 0.12 | -0.12 | -0.22 | -0.13 | 0.13 | -0.21 | -0.01 | 0.30 | -0.12 | 0.12 | -0.23 | 0.10 | 0.10 | -0.03 | -0.20 |
| *Low fat dairy* | -0.14 | -0.01 | -0.18 | 0.06 | -0.33 | 0.39 | 0.49 | -0.08 | -0.15 | -0.18 | -0.01 | 0.06 | -0.23 | 0.31 | -0.06 | 0.63 |
| *White starchy* | 0.65 | 0.18 | 0.10 | 0.11 | 0.49 | 0.06 | 0.12 | 0.12 | 0.66 | 0.10 | 0.17 | 0.10 | 0.62 | 0.12 | 0.08 | -0.09 |
| *Wholemeal starchy* | 0.04 | 0.56 | -0.10 | 0.19 | 0.21 | 0.46 | 0.43 | 0.05 | 0.06 | -0.10 | 0.57 | 0.20 | 0.32 | 0.44 | 0.04 | 0.38 |
| *Egg* | 0.49 | -0.01 | 0.07 | 0.16 | 0.17 | -0.04 | 0.26 | 0.19 | 0.50 | 0.07 | -0.02 | 0.15 | 0.36 | -0.03 | 0.16 | 0.15 |
| *Potato* | 0.35 | 0.11 | 0.05 | 0.52 | 0.71 | 0.00 | -0.01 | 0.09 | 0.37 | 0.05 | 0.10 | 0.51 | 0.68 | 0.10 | 0.05 | -0.26 |
| *Red meat* | 0.34 | 0.61 | 0.03 | 0.26 | 0.64 | -0.03 | 0.35 | 0.22 | 0.37 | 0.02 | 0.60 | 0.26 | 0.74 | 0.03 | 0.18 | 0.10 |
| *Poultry* | 0.03 | 0.83 | 0.00 | 0.10 | 0.40 | 0.07 | 0.39 | 0.07 | 0.06 | 0.00 | 0.83 | 0.10 | 0.49 | 0.10 | 0.04 | 0.24 |
| *Full fat delicatessens* | 0.49 | 0.45 | 0.20 | -0.09 | 0.38 | -0.24 | 0.33 | -0.03 | 0.50 | 0.19 | 0.43 | -0.10 | 0.66 | -0.21 | -0.07 | 0.11 |
| *Low fat delicatessens* | 0.32 | 0.18 | 0.00 | -0.06 | 0.07 | 0.04 | 0.73 | -0.02 | 0.31 | -0.01 | 0.17 | -0.06 | 0.29 | 0.01 | -0.03 | 0.66 |
| *Fish* | 0.02 | 0.21 | 0.02 | 0.72 | 0.51 | 0.59 | 0.07 | 0.14 | 0.04 | 0.02 | 0.21 | 0.72 | 0.42 | 0.65 | 0.12 | -0.04 |
| *Legumes* | 0.04 | 0.03 | 0.00 | 0.72 | 0.39 | 0.47 | 0.01 | -0.14 | 0.05 | 0.00 | 0.03 | 0.72 | 0.24 | 0.53 | -0.14 | -0.07 |
| *Vegetables* | -0.08 | 0.17 | 0.03 | 0.38 | -0.07 | 0.77 | -0.02 | -0.03 | -0.08 | 0.03 | 0.18 | 0.38 | -0.12 | 0.75 | -0.01 | 0.08 |
| *Fruit* | 0.05 | -0.05 | -0.12 | 0.19 | -0.06 | 0.67 | 0.03 | -0.04 | 0.04 | -0.12 | -0.04 | 0.19 | -0.07 | 0.65 | -0.03 | 0.11 |
| *Bakery* | 0.65 | 0.05 | 0.04 | 0.01 | 0.16 | -0.08 | 0.58 | 0.03 | 0.65 | 0.04 | 0.03 | 0.00 | 0.51 | -0.10 | 0.00 | 0.44 |
| *Sweets* | 0.57 | 0.01 | -0.02 | 0.03 | 0.17 | 0.00 | 0.25 | 0.00 | 0.58 | -0.03 | -0.01 | 0.02 | 0.54 | -0.01 | -0.04 | 0.11 |
| *Wine* | -0.02 | 0.00 | 0.79 | -0.07 | -0.04 | 0.08 | -0.06 | 0.76 | -0.02 | 0.79 | 0.00 | -0.07 | -0.05 | 0.08 | 0.76 | -0.03 |
| *Beer* | 0.18 | -0.12 | 0.61 | 0.15 | 0.08 | -0.06 | -0.06 | 0.72 | 0.18 | 0.61 | -0.13 | 0.15 | 0.14 | -0.05 | 0.71 | -0.11 |
| *Spirits* | 0.05 | 0.20 | 0.68 | -0.04 | 0.11 | -0.10 | 0.16 | 0.70 | 0.07 | 0.68 | 0.20 | -0.04 | 0.21 | -0.11 | 0.69 | 0.10 |
| *Stimulants* | -0.04 | -0.16 | 0.42 | 0.09 | -0.03 | 0.03 | 0.09 | 0.14 | -0.03 | 0.42 | -0.16 | 0.09 | -0.01 | 0.03 | 0.14 | 0.08 |
| *Sodas* | 0.25 | -0.02 | 0.11 | 0.12 | 0.28 | -0.13 | -0.01 | 0.14 | 0.28 | 0.11 | -0.03 | 0.12 | 0.45 | -0.10 | 0.12 | -0.16 |
| *Light sodas* | 0.00 | 0.16 | 0.12 | -0.13 | 0.04 | 0.16 | 0.21 | 0.10 | 0.03 | 0.12 | 0.16 | -0.12 | 0.19 | 0.14 | 0.10 | 0.18 |
| *Olive oil* | 0.03 | -0.07 | 0.23 | -0.14 | -0.07 | 0.17 | -0.03 | 0.10 | 0.02 | 0.23 | -0.07 | -0.14 | -0.06 | 0.17 | 0.10 | -0.01 |
| *Other oils & fats* | 0.06 | 0.18 | -0.14 | -0.06 | 0.62 | 0.00 | 0.03 | -0.08 | 0.09 | -0.13 | 0.19 | -0.06 | 0.42 | 0.10 | -0.09 | -0.15 |
| % of variance explained by each factor | **9.3** | **7.9** | **7.8** | **7.5** | **11** | **8.9** | **8.1** | **7.6** | **9.7** | **7.8** | **7.8** | **7.5** | **16** | **9.0** | **7.3** | **6.4** |

Varimax: 1st administration FFQ: PC1 "Western pattern", PC2 "High protein pattern", PC3 "Drinking pattern", PC4 "Healthy pattern".
2nd administration FFQ: PC1 "Western pattern", PC2 "Healthy pattern", PC3 "High protein pattern", PC4 "Drinking pattern".
Quartimax: 1st administration FFQ: PC1 "Western pattern", PC2 "Drinking pattern", PC3 "High protein pattern", PC4 "Healthy pattern".
2nd administration FFQ: PC1 "Western pattern", PC2 "Healthy pattern", PC3 "Drinking pattern", PC4 "Low calorie".

### 3.3 Non-Orthogonal Rotation

Three major patterns that could be defined as similar (i.e., the "Unfavourable dietary habits", the "Healthy" and the "Drinking" pattern) were better reflecting the participants' dietary habits according to both non-orthogonal rotation types applied (i.e., the promax and the oblimin method) (Table 3). However, based on Kendall's tau coefficients very low level of agreement (the majority of the values were $< 0.6$) was observed, while better strength of agreement it was found between the "Healthy" pattern derived from both recordings according the oblimin method, as compared with the promax method (i.e., tau = 0.33 and tau = 0.21 respectively) and the "Drinking" pattern as well (i.e., tau = 0.46 and tau = 0.41 respectively). In addition to the aforementioned consideration of low agreement, the limits of agreement according to the Bland and Altman method were relatively wide, although showed acceptable mean differences (Table 4). Regarding the "unfavourable" dietary patterns observed using the oblimin and promax methods in the first component for the two administrations, although they are heavily loaded by different food items, these items reflect in general "unhealthy" dietary habits (i.e., high meat consumption, unrefined bakery products) and therefore they could be similarly named as "unfavourable". The agreement coefficient in this case also indicates the low agreement of participants' scores within the two components.

## 4. Discussion

The influence of the rotation of components derived through PCA on the short-term repeatability of the extracted food patterns was examined based on empirical data from a nutrition survey. The comparisons between dietary patterns extracted from two administrations of a FFQ, were performed for similar components, according to their nutritional meaning. Data analysis revealed a moderate-to-good repeatability of the extracted food patterns through the aforementioned multivariate analysis, for the un-rotated components, whilst the strength of the agreement was much lower for the rotated components and irrespective of the rotation type used.

Multivariate techniques, like PCA or factor analysis, have been extensively used to extract food patterns in nutrition epidemiology. It has been suggested that rotation of the components may allow for better interpretation of the extracted patterns (components). To better understand the nature of the problem tested here let's denote $Y_i$ the extracted components from the 1$^{\text{st}}$ administration of the FFQ and $Y'_i$ the extracted components from the 2$^{\text{nd}}$ administration of the FFQ, where $i = 1, 2, \cdots, k$ ($k$ is the number of food variables used). Moreover, $a_{ij}, a'_{ij}$ represent the corresponding loadings of the $k$ food variables, i.e., $X_i$, $X'_i$

Table 3: Components' scores for four major dietary patterns derived using Principal Components Analysis (non-orthogonal rotation), form the two records of a semi-quantitative Food Frequency Questionnaire

| | Promax rotation | | | | | | | | Oblimin rotation | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | FFQ1 | | | | FFQ2 | | | | FFQ1 | | | | FFQ2 | | | |
| | PC1 | PC2 | PC3 | PC4 | PC1 | PC2 | PC3 | PC4 | PC1 | PC2 | PC3 | PC4 | PC1 | PC2 | PC3 | PC4 |
| **Food group, (g-mL/d)** | | | | | | | | | | | | | | | | |
| *Full fat dairy* | 0.30 | 0.11 | -0.07 | -0.19 | -0.28 | 0.22 | -0.30 | -0.02 | 0.19 | -0.21 | -0.10 | -0.41 | -0.16 | 0.15 | -0.02 | -0.21 |
| *Low fat dairy* | -0.06 | -0.04 | -0.18 | 0.06 | -0.40 | 0.32 | 0.58 | -0.04 | -0.16 | 0.10 | -0.17 | 0.59 | -0.39 | 0.37 | -0.06 | 0.50 |
| *White starchy* | 0.70 | 0.09 | 0.04 | 0.03 | 0.45 | 0.09 | 0.03 | 0.02 | 0.68 | 0.05 | 0.06 | -0.05 | 0.45 | 0.05 | 0.08 | 0.12 |
| *Wholemeal starchy* | -0.02 | 0.57 | -0.08 | 0.13 | 0.12 | 0.40 | 0.36 | 0.04 | -0.03 | 0.17 | -0.08 | 0.35 | 0.10 | 0.44 | 0.07 | 0.38 |
| *Egg* | 0.58 | -0.11 | -0.01 | 0.06 | 0.11 | -0.08 | 0.26 | 0.16 | 0.59 | 0.09 | 0.02 | 0.05 | 0.12 | -0.06 | 0.18 | 0.29 |
| *Potato* | 0.29 | 0.02 | 0.00 | 0.50 | 0.76 | 0.02 | -0.13 | 0.00 | 0.34 | 0.47 | 0.01 | -0.23 | 0.70 | -0.01 | 0.07 | -0.04 |
| *Red meat* | 0.18 | 0.58 | 0.00 | 0.20 | 0.60 | -0.09 | 0.24 | 0.15 | 0.24 | 0.19 | 0.01 | -0.16 | 0.54 | -0.05 | 0.22 | 0.31 |
| *Poultry* | -0.15 | 0.89 | 0.04 | 0.01 | 0.36 | 0.02 | 0.34 | 0.02 | -0.09 | 0.05 | 0.03 | -0.03 | 0.32 | 0.05 | 0.06 | 0.37 |
| *Full fat delicatessens* | 0.41 | 0.37 | 0.16 | -0.13 | 0.25 | -0.22 | 0.28 | -0.14 | 0.36 | -0.15 | 0.18 | 0.15 | 0.29 | -0.25 | -0.07 | 0.35 |
| *Low fat delicatessens* | 0.40 | 0.09 | -0.06 | -0.11 | -0.03 | -0.05 | 0.79 | -0.06 | 0.30 | -0.08 | -0.02 | 0.72 | -0.04 | 0.00 | -0.03 | 0.75 |
| *Fish* | -0.04 | 0.17 | 0.02 | 0.72 | 0.54 | 0.59 | -0.07 | 0.11 | 0.00 | 0.72 | 0.02 | 0.06 | 0.47 | 0.59 | 0.15 | -0.01 |
| *Legumes* | 0.00 | -0.03 | 0.01 | 0.78 | 0.50 | 0.48 | -0.05 | -0.18 | 0.01 | 0.74 | 0.00 | -0.02 | 0.43 | 0.46 | -0.14 | -0.02 |
| *Vegetables* | -0.07 | 0.19 | 0.08 | 0.38 | -0.08 | 0.82 | -0.06 | -0.02 | -0.10 | 0.42 | 0.05 | 0.14 | -0.07 | 0.78 | -0.02 | -0.06 |
| *Fruit* | 0.13 | -0.08 | -0.10 | 0.19 | -0.07 | 0.70 | 0.01 | -0.03 | 0.03 | 0.23 | -0.11 | 0.11 | -0.06 | 0.68 | -0.03 | 0.01 |
| *Bakery* | 0.74 | -0.12 | -0.03 | -0.02 | -0.01 | -0.11 | 0.59 | -0.05 | 0.59 | -0.03 | 0.01 | 0.37 | 0.04 | -0.11 | -0.01 | 0.61 |
| *Sweets* | 0.61 | -0.12 | -0.07 | 0.02 | -0.03 | 0.04 | 0.17 | -0.08 | 0.51 | 0.00 | -0.05 | -0.06 | 0.07 | -0.01 | -0.04 | 0.26 |
| *Wine* | -0.06 | 0.03 | 0.83 | -0.08 | -0.09 | 0.09 | -0.08 | 0.78 | -0.04 | -0.06 | 0.80 | -0.02 | -0.09 | 0.11 | 0.77 | -0.10 |
| *Beer* | 0.13 | -0.17 | 0.61 | 0.19 | 0.02 | -0.05 | -0.13 | 0.73 | 0.13 | 0.15 | 0.60 | -0.15 | 0.02 | -0.04 | 0.73 | -0.10 |
| *Spirits* | -0.08 | 0.21 | 0.70 | -0.03 | 0.00 | -0.13 | 0.09 | 0.71 | -0.08 | -0.05 | 0.69 | -0.05 | 0.00 | -0.09 | 0.71 | 0.10 |
| *Stimulants* | 0.01 | -0.18 | 0.40 | 0.03 | -0.04 | 0.08 | 0.15 | 0.09 | 0.02 | 0.08 | 0.40 | 0.24 | -0.02 | 0.04 | 0.11 | 0.11 |
| *Sodas* | 0.16 | -0.12 | 0.06 | 0.14 | 0.15 | -0.05 | -0.13 | 0.06 | 0.10 | 0.10 | 0.08 | -0.16 | 0.20 | -0.10 | 0.11 | -0.05 |
| *Light sodas* | -0.06 | 0.11 | 0.11 | -0.16 | -0.11 | 0.21 | 0.14 | 0.06 | -0.16 | -0.13 | 0.11 | 0.28 | -0.07 | 0.18 | 0.08 | 0.15 |
| *Olive oil* | 0.12 | -0.03 | 0.27 | -0.17 | -0.03 | 0.21 | 0.05 | 0.08 | 0.09 | -0.12 | 0.24 | 0.01 | -0.01 | 0.16 | 0.08 | 0.03 |
| *Other oils & fats* | 0.04 | 0.21 | -0.18 | -0.21 | 0.77 | -0.04 | -0.04 | -0.12 | 0.14 | -0.13 | -0.17 | -0.20 | 0.65 | -0.01 | -0.07 | -0.01 |

* The sums of squared loadings cannot be added to obtain the percentage of total variance, under correlated factors.
Promax: 1st administration FFQ: PC1 "Unfavourable dietary habits", PC2 "High protein pattern", PC3 "Drinking pattern", PC4 "Healthy pattern".
2nd administration FFQ: PC1 "Unfavourable dietary habits", PC2 "Healthy pattern", PC3 "Low calorie pattern", PC4 "Drinking pattern".
Oblimin: 1st administration FFQ: PC1 "Unfavourable dietary habits", PC2 "Healthy pattern", PC3 "Drinking pattern", PC4 "Low calorie pattern".
2nd administration FFQ: PC1 "Unfavourable dietary habits", PC2 "Healthy pattern", PC3 "Drinking pattern", PC4 "High protein pattern".

Table 4: Results of the degree of agreement between the extracted components of the two administrations of the Food Frequency Questionnaire, according to type of rotation. Results presented according to Kendall's tau coefficient and Bland & Altman Limits of Agreement (LoA)

| | Type of rotation | |
|---|---|---|
| | None | |
| | Kendall's tau-b | Mean Difference (LoA)† |
| **Dietary pattern** | | |
| *Western/ Unfavorable* | 0.58* | 0 (-1.44, 1.44) |
| *Mediterranean/ Healthy* | 0.63* | 0 (-1.19, 1.19) |
| *Drinking* | 0.57* | 0 (-1.29, 1.29) |
| *Wholemeal starchy* | 0.50* | 0 (-1.52, 1.52) |
| *Egg* | - | - |

| | Orthogonal | | | |
|---|---|---|---|---|
| | *Varimax* | | *Quartimax* | |
| | Kendall's tau-b | Mean Difference (LoA)† | Kendall's tau-b | Mean Difference (LoA)† |
| **Dietary pattern** | | | | |
| *Western/ Unfavorable* | 0.18* | 0 (-2.42, 2,42) | 0.46* | 0 (-1.77, 1.77) |
| *Mediterranean/ Healthy* | 0.24* | 0 (-2.04, 2.04) | 0.28* | 0 (-1.92, 1.92) |
| *Drinking* | 0.44* | 0 (-1.42, 1.42) | 0.45* | 0 (-1.42, 1.42) |
| *Wholemeal starchy* | - | - | - | - |
| *Egg* | 0.15* | 0 (-2.33, 2.33) | - | - |

| | Non Orthogonal | | | |
|---|---|---|---|---|
| | *Promax* | | *Oblimin* | |
| | Kendall's tau-b | Mean Difference (LoA)† | Kendall's tau-b | Mean Difference (LoA)† |
| **Dietary pattern** | | | | |
| *Western/ Unfavorable* | 0.37* | 0 (-1.93, 1.93) | 0.31* | 0 (-2.12, 2.12) |
| *Mediterranean/ Healthy* | 0.21* | 0 (-2.12, 2.12) | 0.33* | 0 (-1.87, 1.87) |
| *Drinking* | 0.41* | 0 (-1.48, 1.48) | 0.46* | 0 (-1.40, 1.40) |
| *Wholemeal starchy* | - | - | - | - |
| *Egg* | - | - | - | - |

* $p < 0.0001$; †Limits of Agreement

of the two administrations, respectively.

Thus, based on the common formation of the PCA we have:

$$\begin{aligned} Y_1 &= a_{11}X_1 + a_{12}X_2 + \cdots + a_{1k}X_k, \\ Y_2 &= a_{21}X_1 + a_{22}X_2 + \cdots + a_{2k}X_k, \\ &\cdots \\ Y_k &= a_{k1}X_1 + a_{k2}X_2 + \cdots + a_{kk}X_k, \end{aligned}$$

and for the 2nd administration of the FFQ

$$\begin{aligned} Y_1' &= a_{11}'X_1' + a_{12}'X_2' + \cdots + a_{1k}'X_k', \\ Y_2' &= a_{21}'X_1' + a_{22}'X_2' + \cdots + a_{2k}'X_k', \\ &\cdots \\ Y_k' &= a_{k1}'X_1' + a_{k2}'X_2' + \cdots + a_{kk}'X_k'. \end{aligned}$$

Therefore, for the un-rotated components the tested null hypothesis as regards the repeatability of the extracted $k$ components and for $m$ cases (i.e., representing the subjects of each survey) takes the form:

$$\mathrm{H}_0 : [Y_i]_{m\times k} = [Y'_i]_{m\times k}, \quad \text{for} \quad i = 1, 2, \cdots, k.$$

The aforementioned analysis did not reject the null hypothesis, although differences between the two administrations of the FFQ were observed as regards the values of the loadings (i.e., $\alpha_{ij}$ and $\alpha'_{ij}$), as well as the reported frequencies in consumption (i.e., $\mathrm{X}_i$ and $\mathrm{X'}_i$).

As regards the rotated components (either orthogonal or non orthogonal rotation type), let's $R$ and $R$' denote the rotation matrices of the 1st and the 2nd administration of the FFQ. The matrices are different since they are dependent from the dietary information retrieved (i.e., the $X$ and $X$' data matrices). Thus, the tested null hypothesis of the repeatability of the extracted components can be expressed as:

$$\mathrm{H}_0 : R * [Y_i]_{m\times k} = R' * [Y'_i]_{m\times k}, \quad \text{for} \quad i = 1, 2, \cdots, k.$$

In the presented analysis, the level of the repeatability between similar extracted food patterns was low and irrespective of the type of rotation used, i.e., orthogonal or non-orthogonal (oblique). Moreover, it should be noted here that as compared with the rotated, the un-rotated PCA revealed more repeatable results. It seems that the use of an additional source of bias, i.e., the rotation matrix $R$, increases the level of disagreement between the two recordings as regards the nutrient information retrieved. Moreover, when rotation was applied, the quartimax and the oblimin rotation methods lead to more repeatable results regarding the orthogonal and the non-orthogonal rotation respectively. Four different orthogonal methods have been listed, while for the oblique rotation 15 different types have been listed (Gorsuch, 1983). In this study, varimax and quartimax method has been selected as the orthogonal types, while promax and direct oblimin method has been selected as the oblique types. In general, the varimax method leads to a number of components that each one has a small number of large loadings and a large number of small (or zero) loadings. This simplifies the interpretation because each original variable tends to be correlated with one component, and each component represents only a small number of variables (Kaiser, 1958). In contrast, the quartimax rotation minimizes the number of components needed to explain each variable. The generated component is usually loaded to a medium or high degree by the most variables (Neuhaus and Wrigley, 1954). The promax rotation necessitates two steps. The first step defines the target matrix, based on the original solutions and almost always obtained as the result of a varimax rotation. The second step is obtained by computing a least square fit from the varimax solution to the target matrix (Abdi, 2003). Direct oblimin rotation allows the components to be correlated and thus result in higher eigenvalues. In other words, *oblimin* rotation tends to produce oblique "varimax" looking components (Garson, 2008[1]). The varimax and the promax method were the most common methods, of the orthogonal and non-orthogonal rotation respectively, to derive dietary patterns (Hu, 2002; Togo *et al.*, 2003; Panagiotakos *et al.*, 2007). For studies that no rotation has been applied, it could be speculated that the rotation has been tested and did not improve the results. The varimax rotation, simplifies the columns of the component loading matrix, thus, in each component the large loadings are increased and the small ones are decreased so that each component only has a few variables with large loadings. In contrast, the quartimax rotation, simplifies the rows of the component loading matrix. Thus, in each variable the large loadings are increased and the small ones are decreased so that each variable tends to place large loadings on one component (Harman, 1960). In addition, the researcher faces decision problems regarding the application of promax and oblimin methods. In these methods a certain parameter need to be specified (delta in oblimin and the power parameter kappa in promax) that may influence the component structure/pattern as well as the component intercorrelations and may, thus, affect the solution considerably. Promax method has the advantage of being quicker and simpler as compared to the oblimin method, hence its use tends to be preferable (Hendrickson and White, 1964). In this study, the default delta (i.e., 0) and kappa (i.e., 4) were used for the promax and oblimin

[1]Garson, G. D. (2008). *Factor Analysis.* From Statnotes: Topics in Multivariate Analysis. Retrieved 06/29/2010 from http://faculty.chass.ncsu.edu/garson/pa765/statnote.htm.

rotation type to avoid unnecessary complexity for interpretation of results that may occur by manipulating delta or kappa. The use of orthogonal rotation is generally suggested because it produces more easily interpretable results. However, in the biomedical and nutritional sciences a correlation among components is expected. Therefore an oblique rotation should theoretically render a more accurate solution, while orthogonal rotation results in a loss of valuable information if the components are correlated. Nevertheless, if the components are truly uncorrelated orthogonal and oblique rotation produce similar results (Costello and Osborne, 2005).

Although rotation aims to simplify and clarify the data structure, it cannot improve the basic aspects of the analysis, such as the amount of variance extracted from the variables included. Thurstone (1931) suggested five criteria to identify a simple structure: 1) each row contains at least one zero, 2) for each column, there are at least as many zeros as there are columns (i.e., number of components kept), 3) for any pair of components, there are some variables with zero loadings on one component and large loadings on the other component, 4) for any pair of components, there is a sizable proportion of zero loadings, 5) for any pair of components, there is only a small number of large loadings. If the above criteria are fulfilled, the matrix of loadings is considered simple and thus, there is no need to proceed to a rotation method (Thurstone, 1931). The present study revealed that the un-rotated method results to easily identified, interpreted and repeatable patterns and much of the aforementioned criteria seemed to be fulfilled.

## 5. Conclusion

The present analysis revealed that un-rotated food patters were more repeatable as compared with the rotated; a fact that may lead to the conclusion that when patterns are easily identified from the un-rotated analysis, rotation does not necessarily improve the reliability of the dietary patterns derived. However, when a rotation type is needed to improve the patterns interpretation, the quartimax method of the orthogonal rotation type and the oblimin method of the non-orthogonal rotation type lead to more repeatable patterns and thus, more robust results. Even though orthogonal rotations are much popular than oblique rotation methods, it should be taken under consideration whether an independent component analysis as derived through orthogonal rotation is what the investigators need, especially in nutrition assessment. However, further analyses with simulation data sets of various multivariate structures are necessary to test the stability on the multivariate method that consistently retrieves the simulated structure.

## Appendix Table

Food groups used in dietary pattern analysis

| Food groups | Food items |
|---|---|
| fat dairy products | Full fat milk/ yogurt, yellow cheese, white cheese |
| Low fat dairy products | Low fat milk/ yogurt, low fat cheese (i.e., light/ cottage cheese) |
| Refined grains | White bread/ toast, burger bread, white rice, pasta, pearl barley |
| Whole-wheat grains | Whole-wheat bread/ toast, crisp breads, cereals, brown rice, whole-wheat pasta |
| Eggs | Eggs |
| Potato | Potato baked/ mashed/ fried |
| Red meat | Pork, beef, lamp, minced meat |
| Poultry | Chicken, turkey |
| Full fat delicatessens | Cold, sliced meat, sausages, bacon, processed meat products |
| Low fat delicatessens | Light/ no fat cold sliced meat, processed meat products |
| Fish & seafood | Fish(small, large), seafood |
| Legumes | Lentils, beans, fava beans |
| Vegetables | Tomato, cucumber, carrots, fresh green vegetables, cabbage, broccoli |
| Fruit | Fresh fruit(orange, apple, pear, banana, cherries, strawberries etc), fresh fruit juice |
| Bakery | Pies(spinach pie, cheese pie, meat pie etc), sandwiches |
| Sweet | Jelly, sugar, marmalade, croissant, cake, gofer, biscuits, chocolate, tartes, ice-cream |
| Wine | Red wine, white wine |
| Beer | Beer |
| Spirits | Whiskey, vodka, gin, liqueurs |
| Stimulants | Coffee, tea |
| Soft drinks | Cola type sodas |
| Light soft drinks | Light cola type sodas |
| Olive oil | Olive oil |
| Other oils & fats | Seed oil, butter, margarine |

## Acknowledgements

We are, particularly, grateful to the men and women from the residence of Athens, who participated in and collaborated on this research. We also wish to express our gratitude to: Dr. E. Bathrellou for her valuable contribution in the development of the questionnaire and to E. Serpanou, T. Rabbah, E. Pagourtzi, K. Tsoutsoulopoulou, A. Mitsopoulou (field investigators from Harokopio University), for their substantial assistance in the enrolment of the participants, as well as to the anonymous Reviewer that helped us to better interpret our findings.

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Received March 29, 2011; accepted July 18, 2011.

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