

1 **Dietary patterns obtained through principal components analysis:**
2 **the effect of input variable quantification**

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1 **Abstract**

2 Principal components analysis (PCA) is a popular method for deriving dietary patterns. A
3 number of decisions must be made throughout the analytic process, including how to quantify
4 the input variables of the PCA. This study aims to compare the effect of using different input
5 variables on the patterns extracted using PCA on three-day diet diary data collected from
6 7,473 children, aged 10 years, in the Avon Longitudinal Study of Parents and Children
7 (ALSPAC). Four options were examined: weight consumed of each food group (g/d), energy
8 adjusted weight, percent contribution to energy of each food group, and binary intake
9 (consumed / not consumed). Four separate PCAs were performed, one for each intake
10 measurement. Three or four dietary patterns were obtained from each analysis, with at least
11 one component that described ‘more healthy’ and ‘less healthy’ diets, and one component
12 that described a diet with high consumption of meat, potatoes and vegetables. There were no
13 obvious differences between the patterns derived using percentage energy as a measurement,
14 or adjusting weight for total energy intake, compared to those derived using gram weights.
15 Using binary input variables yielded a component that loaded positively on reduced-fat,
16 reduced-sugar foods. Our results suggest that food intakes quantified by gram weights or as
17 binary variables both resulted in meaningful dietary patterns, and each method has distinct
18 advantages: weight takes into account the amount of each food consumed and binary intake
19 appears to describe general food preferences, which are potentially easier to modify and
20 useful in public health settings.

21

1 **Introduction**

2 The use of dietary patterns to explore the effects of diet on a variety of health outcomes is
3 now well established as a method that complements examining individual foods and
4 nutrients. Dietary patterns allow the assessment of the whole diet, accounting for the fact that
5 foods/nutrients are consumed in combination and are therefore highly correlated. Principal
6 components analysis (PCA), a form of factor analysis, is a popular method for deriving
7 dietary patterns. It makes use of the correlations between food intakes to identify underlying
8 patterns in the data. There are several subjective decisions that must be made when using
9 PCA. A particularly important one, which is often overlooked, is how to quantify the input
10 variables. Depending on the source of dietary data a number of different variables could be
11 considered. For example, data from diet diaries can be quantified continuously as gram
12 weights or percent energy from food groups or dichotomously (i.e., whether each food group
13 was consumed or not).

14 The input variables used in PCA vary across studies⁽¹⁾ and include frequency of consumption,
15 gram weights, energy-adjusted weight, daily percent energy contribution, and binary
16 variables. Many studies based on diet diaries use weight of foods consumed as the input
17 variable⁽²⁻⁵⁾. Energy adjustment using the residual method⁽⁶⁾ is often applied in studies based
18 on diet diaries and diet recalls⁽⁷⁻⁹⁾ as well as studies based on FFQ data⁽¹⁰⁻¹²⁾. Percent energy
19 is another potential input variable⁽¹³⁾ and a few studies⁽¹⁴⁻¹⁵⁾ have dichotomized intakes into
20 binary variables. Most studies select one strategy, for dietary patterns analyses, but seldom
21 justify the decision and only a few studies have made comparisons between the different
22 input variables but with no formal conclusions^(14, 16, 17). There are no studies to our
23 knowledge that have compared all four strategies and no studies have made comparisons in
24 children.

1 In order to facilitate comparisons across studies, it is vital that researchers are as informed as
2 possible about the decisions that they need to make and use the best evidence available.
3 Therefore, the aim of the current study is to derive dietary patterns using PCA using four
4 different input variables – weight (g/d), energy-adjusted weight, percent energy contribution,
5 and binary (consume or not consume) – and compare the interpretability of the patterns
6 among children participating in the Avon Longitudinal Study of Parents and Children.

7

1 **Methods**

2 **Participants**

3 The Avon Longitudinal Study of Parents and Children (ALSPAC) is an ongoing longitudinal
4 cohort study designed to investigate determinants of development, health and disease during
5 and after childhood. Eligible participants were pregnant women resident in the former Avon
6 Health Authority, in South West England, due to deliver between 1 April 1991 and 31
7 December 1992. Further details are given elsewhere⁽¹⁸⁾ and can be found on the website
8 www.bris.ac.uk/alspac. The study includes children from the core ALSPAC sample,
9 consisting of 14,541 pregnancies, and an additional 542 eligible pregnancies not in the core
10 sample, invited to participate at a later date. This study was conducted according to the
11 guidelines laid down in the Declaration of Helsinki and all procedures involving human
12 subjects/patients were approved by the ALSPAC Law and Ethics Committee and the Local
13 Research Ethics Committees. Written informed consent was obtained from all
14 subjects/patients.

15 **Dietary assessment**

16 The study children were invited to attend a clinic when they were 10 years old, and a diet
17 diary was sent with their confirmation to be completed prior to their visit. Children and their
18 care-givers recorded, in household measures, all food and drink consumed by the child over
19 two (not necessarily consecutive) weekdays and one weekend day. During clinic attendance
20 the children were interviewed to ensure the quality of the diary (e.g., clarifying portion size or
21 omitted details on the types of food and drinks consumed). If the child did not bring a diary to
22 the clinic, the fieldworker conducted a 24-hour recall to record all food and drink consumed
23 by the child in the previous day. Further details are given elsewhere⁽¹⁹⁾. The completed diaries

1 were entered into the DIDO (Diet In Data Out) computer program⁽²⁰⁾, which, generated the
2 weight and energy contribution of every food consumed by each child. For the purposes of
3 this study the average daily intake of food weight and energy were used.

4 Each food consumed was initially allocated to one of 95 food groups that were based on those
5 used in FFQ that had previously been administered to the ALSPAC cohort⁽²¹⁾. Sugar-free
6 confectionery, alcohol, herbs and spices were removed from the analysis, as very few
7 children consumed these foods and thus they did not contribute meaningfully to any dietary
8 patterns. The remaining food items were combined into 62 groups, based on similarities
9 between foods (for example nuts, peanuts and peanut butter were combined), to reduce the
10 number of input variables and prevent infrequently consumed foods from diluting the dietary
11 patterns. The appendix describes the food groups in detail.

12 **Statistical methods**

13 Dietary patterns were derived using PCA. Principal components are linear combinations of
14 the input variables and explain as much of the variation in the data as possible. Each
15 component describes a dietary pattern and the linear combination allows the calculation of a
16 component score for each child, the higher the score the more likely this pattern is present in
17 an individual's diet. The patterns described by each component may be interpreted by its
18 factor loadings, which are the correlations between the component and each input variable.
19 Large positive or negative factor loadings indicate the foods that are important in that
20 component; loadings with magnitude of at least 0.2 were considered when describing dietary
21 patterns. Scree plots⁽²²⁾ and the interpretability of each component, were also used to
22 determine the appropriate number of components to select. Varimax rotation⁽²³⁾ was
23 employed to aid the interpretation of components. The purpose of this study was to compare

1 the different dietary patterns obtained using each of the input variables, therefore the patterns
2 were given alphanumeric labels rather than descriptive names to aid reporting.

3 Four separate analyses were carried out, using four different input variables. The first used
4 the weight (g/d) of each food consumed. The variables were standardized prior to entry into
5 the PCA to prevent components being dominated by the foods that are consumed in the
6 highest quantities, such as water. The second analysis adjusted the mean weight for total
7 energy intake, using the residuals method⁽⁶⁾. Specifically, the PCA input variables were the
8 standardized residuals from a linear regression of mean weight on mean daily energy intake.
9 Regression was only performed on non-zero values, and both weight and energy were log-
10 transformed before regression and transformed back before standardization. The third
11 analysis used the percent contribution of each food to the daily energy intake as input
12 variables. These percent energy input variables were also standardized prior to entry into the
13 PCA to prevent components being dominated by the foods that provide the highest percent
14 energy. In the fourth analysis the input variables were dichotomized into binary variables
15 (consumed or not consumed), as food intake variables were highly skewed and many children
16 did not consume some of the food groups. PCA was performed directly on their covariance
17 matrix for this fourth method (as opposed to the correlation matrix for the previous three
18 methods), as standardization is not appropriate for binary variables. For each of the four
19 PCA, scores were calculated for each subject for each pattern derived by summing the
20 products of each standardized input variable and their corresponding coefficient in the
21 component (or dichotomized in the case of binary variables).

22 Agreement between the derived patterns was assessed in two ways. Agreement between
23 component scores was assessed by calculating Pearson's sample correlation coefficients.

24 Congruence coefficients⁽²⁴⁾ were also calculated for pairs of matrices of component

- 1 coefficients in order to assess the difference between the coefficients assigned to individual
- 2 foods by each component.
- 3

1 **Results**

2 Of the 11,868 children eligible to attend the clinic, a total of 7,557 (63.7%) attended and
3 7,473 of these (98.9%) provided dietary information. Of these 5,769 (77.2%) provided 3 days
4 of dietary records. Girls, white children, children with older, more educated, non-smoking
5 mothers, and children from homes that were owned or mortgaged were more likely to provide
6 data (all $p < 0.001$; data not shown).

7 When gram weights were used as input variables, three principal components were retained
8 and explained 10.4% of the variation in the sample. Factor loadings are shown in Table 1.

9 The first component (W1) had high positive loadings on non-white bread, fruit and
10 vegetables, cooked pasta, tuna and oily fish, cheese, yoghurt, high energy density sauce (e.g.
11 mayonnaise), fruit juice, and water. There were high negative loadings on processed meat,
12 coated poultry, tinned pasta/baked beans, chips (French fries), crisps (potato chips), and
13 carbonated sweet drinks (non-diet soda). The second component (W2) had high positive
14 loadings on meat, roast potatoes, batter/pastry products, vegetables, puddings and low energy
15 density sauce (e.g. gravy, ketchup), and a high negative loading on chips. The third
16 component (W3) had high positive loadings on white bread, margarine, cheese, cold meats,
17 salty flavourings, crisps, biscuits (cookies), and diet squash/cordial.

18 As can be seen in Table 2, energy adjustment did not have a discernible effect on the dietary
19 patterns when compared with those using unadjusted weights: the factor loadings were almost
20 identical, differing by no more than 0.084.

21 Four components were obtained when percent energy contribution was used as the input
22 variable, explaining 12.3% of the variation in the sample. Factor loadings are shown in Table
23 3. The first three components, labelled P1, P2 and P3, had high loadings on the same foods

1 that loaded highly on components W1, W2 and W3, with the exception that water loaded
2 highly on W1 but not P1, vegetarian products, legumes and nuts loaded highly on P1 but not
3 W1, and diet squash/cordial loaded highly on W3 but not P3. The fourth component (P4) had
4 high positive loadings on reduced fat milk, yoghurt, breakfast cereal and biscuits, and high
5 negative loadings on rice, other breads (e.g. pitta), poultry, eggs, butter, salad, legumes and
6 carbonated sweet drinks.

7 When PCA was performed on binary variables, four components were obtained, explaining
8 17.3% of the variation in the sample. Table 4 shows factor loadings for these four
9 components. The first component (B1) had high loadings on meat, roast potatoes,
10 batter/pastry products, vegetables, and low energy density sauces. The second component
11 (B2) had high positive loadings on non-white bread, fruit, nuts, salad, vegetarian foods and
12 vegetable dishes, potatoes, pasta, tuna and oily fish, cheese, yoghurt, eggs, butter, high
13 energy density sauce, sweet spreads (e.g. jam), dairy puddings, cakes, chocolate, fruit juice,
14 regular squash/cordial, and water. There were high negative loadings on diet squash/cordial,
15 and roast potatoes. The third component (B3) had high loadings on processed meat, coated
16 poultry, tinned pasta/baked beans, white bread, margarine, vegetable oil, chips, crisps,
17 chocolate, sweets (candy), sweet spreads (jams), sugar, cakes, dairy puddings, biscuits,
18 carbonated sweet drinks, and diet squash/cordial. The fourth component (B4) had high
19 positive loadings on reduced fat milk, margarine, diet carbonated drinks, and diet
20 squash/cordial. It also had high negative loadings on their alternatives: full fat milk, butter,
21 carbonated sweet drinks, and regular squash/cordial. It also had a high positive loading on
22 breakfast cereals.

23 Table 5 shows the correlations between the component scores, and Table 6 shows congruence
24 coefficients between components. The components generated from gram weights and energy-

1 adjusted weight input variables are very similar, as assessed by correlations between
2 component scores and the congruence coefficient between these components. The first three
3 components from the analysis with percent energy input variables were also similar to those
4 generated from gram weights: the correlations between P1, P2, P3, and W1, W2, W3 were at
5 least 0.907. The components generated by binary input variables share partial similarities
6 with the other components. In terms of component scores, B1 was positively correlated with
7 W2, B2 with W1 and B3 was negatively correlated with W1.
8

1 **Discussion**

2 This study of dietary diary data from ten-year-old children compared dietary patterns derived
3 from PCA using four strategies for quantifying input variables. When continuous variables
4 were used (gram weights, energy adjusted weight and percent energy contribution), the first
5 three components extracted had similar loadings and described similar dietary patterns: one
6 contrasting 'more healthy' foods with 'less healthy' foods, one with high loadings on meat,
7 potatoes and vegetables, and one with high loadings on lunch and snack foods. The fourth
8 component, present only when intake was measured as percent energy, was difficult to
9 interpret. When binary variables were used, the four components extracted described slightly
10 different dietary patterns: the component with high loadings on meat, potatoes and vegetables
11 was still present, but the component with positive loadings on 'more healthy' foods and
12 negative loadings on 'less healthy' foods was replaced by two components: one with high
13 loadings on the 'more healthy' foods and the other with high loadings on the 'less healthy'
14 foods. The fourth component had positive loadings for reduced-fat, reduced-sugar foods and
15 negative loadings on their alternatives.

16 There are strong similarities between patterns in the presence and absence of energy
17 adjustment, the main differences being in the relative loadings of high- and low-fibre bread,
18 and full- and low-fat milk. In a comparison of energy-adjusted and unadjusted analyses of
19 data from FFQ administered to the ALSPAC mothers⁽¹⁶⁾, five components appear in the
20 unadjusted analysis but four components suffice under energy adjustment; the missing
21 component described a 'processed' dietary pattern. A study⁽¹⁷⁾ comparing gram weights and
22 percent energy as input variables, in PCA of FFQ data from Irish adults, concludes that gram
23 weights give more interpretable patterns than percent energy.

1 In our study, the patterns obtained when gram weights were used as the input variables were
2 the most interpretable. Weight is a clear, quantitative way to measure food consumption and
3 can be easily linked to portion sizes. A drawback of using gram weights (unadjusted and
4 adjusted for energy) and percent energy was that they potentially led to skewed input
5 variables, with many zeroes for foods that weren't frequently consumed. This resulted in
6 component scores with skewed distributions. Adjusting the weight for energy intake did not
7 alter the dietary patterns, agreeing with research in adults⁽¹⁴⁾. These results suggest that
8 energy-adjusting the input variables does not offer any specific benefit when determining
9 dietary patterns, using PCA, from diet diaries administered to children. It may be more
10 appropriate to perform energy adjustment later in the analytic process as this allows for more
11 accurate assessment of the effect of energy itself. A similar conclusion was reached when
12 obtaining dietary patterns using PCA in the ALSPAC mothers, although this was based on
13 FFQ data⁽¹⁶⁾.

14 In agreement with other research [in adults]⁽¹⁷⁾, using percent energy as an input variable led
15 to patterns that were harder to interpret than those derived from gram weights. In this study,
16 the percent energy strategy led to components in which water did not load highly, as it does
17 not contribute to energy intake. This could be considered an inherent limitation of this
18 approach, given non-energy containing foods (e.g., water, coffee, tea, and diet soda) often
19 contribute meaningfully to dietary patterns. This is shown in the current study, in which water
20 loaded highly on the components obtained when gram weights were used as the input
21 variable strategy, whether energy-adjusted and unadjusted. These results indicate that
22 variation in water intake is an important part of childhood diet and is missed when using the
23 percent energy method. Percent energy is an attractive concept as it considers one's overall
24 dietary composition. However, it is harder to comprehend when dealing with individual food

1 groups, which provide relatively small contributions to total energy intake when considered
2 on their own (i.e., in contrast to considering, say, the macronutrient composition of the diet).

3 Few studies have used binary input variables to derived dietary patterns using PCA. Using
4 this method overcame the issues of skewness and the sometimes large numbers of non-
5 consumers of food groups and led to interpretable dietary patterns. A study of data from an
6 FFQ administered to adults in four European cohorts⁽¹⁴⁾ showed no effect of dichotomization
7 of input variables on dietary patterns. However, in our study the patterns were different from
8 those obtained from continuous variables, Binary (consumed/not consumed) variables are
9 easy to understand and conceptually represent choices and/or preferences of food rather than
10 quantities consumed. This was evident in component B4, which seemed to differentiate
11 between individuals who chose reduced fat, reduced sugar foods, and those who chose the
12 regular (full fat, full sugar) options for those foods. Food choices are potentially easier to
13 modify, but it must be recognized that people consume food in different quantities and
14 dichotomizing food intakes does not capture the complexity of eating behaviour.

15 The findings of this study are strengthened by the large sample size. However, the sample is
16 biased towards higher socioeconomic status. As well, this study has not assessed the effect of
17 different input variables on a specific diet-disease association, As the patterns obtained with
18 different strategies were similar, the effect of input variables on a given diet-disease
19 association may be similar, although this is an important next step to further this literature
20 and needs to be examined. Another input variable that could be considered is the number of
21 servings per day, which is commonly used in studies that assess diet using an FFQ. However,
22 as this study made use of diet diaries, considered a gold standard method of self-reported
23 dietary assessment, we elected not to consider this semi-quantitative approach commonly
24 used in FFQS given the level of detail we have in the diet diaries.

1 In conclusion, this study is the first to comprehensively compare different input variables
2 used in dietary pattern analysis obtained using PCA. Our results indicate that there appears to
3 be no benefit associated with energy adjustment, given results were similar to those when
4 unadjusted. We also showed that patterns based on percent energy did not capture meaningful
5 dietary intakes, completely missing some items consumed such as water, and were also
6 harder to interpret. Thus, while the final choice of input variable treatment may depend on the
7 purpose of a particular analysis the use of food weights and binary variables appeared to be
8 the best approaches to quantify input variables in this study among children. More research is
9 needed to see whether input variable treatment impacts diet-disease associations, as
10 understanding the role of diet on health outcomes is the ultimate objective of nutritional
11 epidemiologic studies. However, for the purposes of describing the underlying patterns of
12 diet in a population we would recommend using weights of foods; binary input variables
13 would be a complementary approach to this in which specific dietary choices can be
14 identified.

15

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Table 1: Factor loadings from PCA of diet diary data on 7473 children aged 10 years, where input variables are weights (g/d). Factor loadings with magnitude greater than 0.2 are shown in bold.

Factor	W1	W2	W3
(variance explained)	(3.8%)	(3.6%)	(3.1%)
Full fat milk	-0.056	0.004	-0.055
Reduced fat milk	0.158	0.023	-0.012
Cheese	0.309	-0.123	0.261
Yoghurt and fromage frais	0.208	-0.030	0.157
Butter and animal fat	0.162	-0.081	-0.099
Margarine	0.061	0.035	0.712
Vegetable oil	-0.083	-0.058	-0.057
High fibre bread	0.334	-0.099	-0.063
Low fibre bread	-0.012	-0.040	0.707
Other bread (e.g. pitta)	0.223	-0.077	-0.101
Batter and pastry products	0.032	0.277	0.081
Breakfast cereal	0.098	-0.036	-0.175
Rice	0.164	-0.016	-0.156
Pasta	0.249	-0.045	-0.086
Baked beans and tinned pasta	-0.210	-0.117	-0.099
Pizza	-0.036	-0.176	-0.090
Eggs	0.089	-0.074	-0.030
Coated and fried chicken	-0.310	-0.132	-0.104
Poultry	0.052	0.223	-0.047
Ham and bacon	-0.008	0.006	0.235
Red meat	0.023	0.233	-0.056
Meat pies and pasties	-0.142	0.059	-0.037
Processed meat	-0.295	-0.042	-0.015
Coated and fried white fish	-0.087	-0.087	-0.100
White fish and shellfish	0.095	-0.026	-0.098
Tuna and oily fish	0.276	-0.099	-0.042
Vegetarian products	0.190	-0.069	-0.036
Chips (French fries)	-0.512	-0.224	-0.176
Roast potatoes	-0.149	0.678	0.013
Other potatoes	0.152	0.159	-0.027
Root vegetables	0.114	0.251	-0.025
Carrots	0.104	0.610	0.002
Green leafy vegetables	0.124	0.527	-0.032
Peas, broad beans and sweetcorn	0.031	0.249	-0.096
Other cooked vegetables and dishes	0.234	0.179	-0.069
Salad and tomatoes	0.443	-0.149	-0.035
Legumes	0.235	-0.086	-0.068
Soup	0.134	-0.081	-0.012
Nuts, seeds and peanut butter	0.193	-0.039	0.041
Fresh fruit	0.427	-0.007	0.048

Tinned and dried fruit	0.143	0.007	-0.026
Puddings	0.012	0.240	-0.169
Dairy puddings	-0.098	0.218	-0.180
Cakes	0.095	0.041	-0.053
Chocolate	-0.133	-0.023	0.015
Sweets (candy)	-0.149	-0.012	0.028
Sugar	-0.093	0.053	-0.008
Sweet spreads (e.g. jam)	0.105	0.042	0.174
Biscuits (cookies)	-0.116	0.040	0.245
Crackers and crispbreads	0.145	-0.038	0.106
Crisps (potato chips)	-0.207	-0.035	0.333
Low energy density sauce (e.g. gravy, ketchup)	0.014	0.599	-0.008
High energy density sauce (e.g. mayonnaise)	0.302	-0.138	-0.010
Salty flavouring (e.g. yeast extract)	0.110	-0.035	0.345
Water and flavoured water	0.304	-0.016	-0.128
Carbonated sweet drinks (soda)	-0.246	-0.076	-0.090
Carbonated diet drinks (diet soda)	-0.226	0.050	0.079
Regular squash and cordial	0.046	-0.065	0.002
Diet squash and cordial	-0.184	0.083	0.289
Fruit juice	0.263	-0.055	-0.029
Flavoured milk drinks	-0.034	-0.003	0.006
Tea and coffee	-0.034	0.093	0.079

Table 2: Factor loadings from PCA of diet diary data on 7473 children aged 10 years, where input variables are weights (g/d) adjusted for total energy intake using the residual method. Factor loadings with magnitude greater than 0.2 are shown in bold.

Factor	A1	A2	A3
(variance explained)	(3.8%)	(3.6%)	(3.1%)
Full fat milk	-0.062	-0.014	-0.126
Reduced fat milk	0.154	0.022	-0.034
Cheese	0.309	-0.131	0.211
Yoghurt and fromage frais	0.202	-0.038	0.108
Butter and animal fat	0.155	-0.104	-0.133
Margarine	0.058	0.037	0.713
Vegetable oil	-0.079	-0.072	-0.085
High fibre bread	0.333	-0.104	-0.096
Low fibre bread	-0.020	-0.047	0.718
Other bread (e.g. pitta)	0.224	-0.083	-0.093
Batter and pastry products	0.024	0.271	0.048
Breakfast cereal	0.101	-0.047	-0.220
Rice	0.172	-0.020	-0.121
Pasta	0.251	-0.041	-0.082
Baked beans and tinned pasta	-0.212	-0.121	-0.111
Pizza	-0.039	-0.183	-0.100
Eggs	0.091	-0.082	-0.051
Coated and fried chicken	-0.308	-0.143	-0.105
Poultry	0.058	0.223	-0.025
Ham and bacon	-0.006	0.003	0.224
Red meat	0.020	0.230	-0.072
Meat pies and pasties	-0.142	0.054	-0.064
Processed meat	-0.297	-0.048	-0.046
Coated and fried white fish	-0.092	-0.095	-0.103
White fish and shellfish	0.098	-0.029	-0.095
Tuna and oily fish	0.269	-0.101	-0.032
Vegetarian products	0.187	-0.068	-0.026
Chips (French fries)	-0.515	-0.241	-0.194
Roast potatoes	-0.148	0.676	0.008
Other potatoes	0.149	0.157	-0.044
Root vegetables	0.112	0.249	-0.009
Carrots	0.105	0.606	-0.004
Green leafy vegetables	0.125	0.521	-0.036
Peas, broad beans and sweetcorn	0.029	0.245	-0.101
Other cooked vegetables and dishes	0.240	0.176	-0.060
Salad and tomatoes	0.442	-0.152	-0.039
Legumes	0.241	-0.087	-0.054
Soup	0.136	-0.081	-0.011
Nuts, seeds and peanut butter	0.191	-0.047	0.024
Fresh fruit	0.422	-0.014	0.012
Tinned and dried fruit	0.130	0.001	-0.057
Puddings	0.010	0.228	-0.180

Dairy puddings	-0.099	0.198	-0.264
Cakes	0.093	0.030	-0.129
Chocolate	-0.142	-0.040	-0.052
Sweets (candy)	-0.155	-0.022	-0.016
Sugar	-0.096	0.044	-0.083
Sweet spreads (e.g. jam)	0.098	0.026	0.132
Biscuits (cookies)	-0.130	0.023	0.177
Crackers and crispbreads	0.138	-0.042	0.079
Crisps (potato chips)	-0.217	-0.048	0.295
Low energy density sauce (e.g. gravy, ketchup)	0.017	0.597	-0.016
High energy density sauce (e.g. mayonnaise)	0.304	-0.150	-0.012
Salty flavouring (e.g. yeast extract)	0.106	-0.027	0.353
Water and flavoured water	0.307	-0.019	-0.109
Carbonated sweet drinks (soda)	-0.255	-0.095	-0.132
Carbonated diet drinks (diet soda)	-0.223	0.055	0.080
Regular squash and cordial	0.038	-0.083	-0.023
Diet squash and cordial	-0.193	0.091	0.262
Fruit juice	0.266	-0.079	-0.066
Flavoured milk drinks	-0.035	-0.011	-0.042
Tea and coffee	-0.037	0.089	0.048

Table 3: Factor loadings from PCA of diet diary data on 7473 children aged 10 years, where input variables are percent contribution of each food to total energy intake. Factor loadings with magnitude greater than 0.2 are shown in bold.

Factor	P1	P2	P3	P4
(variance explained)	(3.5%)	(3.2%)	(3.0%)	(2.6%)
Full fat milk	-0.054	-0.041	-0.134	-0.004
Reduced fat milk	0.151	0.007	-0.082	0.492
Cheese	0.306	-0.137	0.184	0.062
Yoghurt and fromage frais	0.203	-0.075	0.054	0.258
Butter and animal fat	0.143	-0.099	-0.118	-0.230
Margarine	0.066	0.014	0.720	0.078
Vegetable oil	-0.076	-0.086	-0.086	-0.038
High fibre bread	0.331	-0.123	-0.106	0.163
Low fibre bread	-0.019	-0.025	0.740	-0.174
Other bread (e.g. pitta)	0.235	-0.097	-0.117	-0.340
Batter and pastry products	0.060	0.207	0.013	-0.136
Breakfast cereal	0.099	-0.043	-0.263	0.556
Rice	0.183	-0.003	-0.114	-0.312
Pasta	0.255	-0.013	-0.096	0.060
Baked beans and tinned pasta	-0.172	-0.136	-0.071	0.057
Pizza	-0.071	-0.174	-0.095	0.074
Eggs	0.084	-0.078	-0.049	-0.214
Coated and fried chicken	-0.315	-0.129	-0.079	-0.037
Poultry	0.063	0.246	-0.035	-0.302
Ham and bacon	-0.039	0.064	0.153	-0.150
Red meat	-0.013	0.363	-0.069	0.032
Meat pies and pasties	-0.163	0.032	-0.064	0.065
Processed meat	-0.323	-0.029	-0.046	-0.071
Coated and fried white fish	-0.115	-0.093	-0.073	0.144
White fish and shellfish	0.076	-0.048	-0.096	-0.047
Tuna and oily fish	0.263	-0.109	-0.061	-0.050
Vegetarian products	0.271	-0.125	-0.008	-0.004
Chips (French fries)	-0.558	-0.210	-0.154	-0.089
Roast potatoes	-0.121	0.679	0.009	-0.052
Other potatoes	0.146	0.091	-0.045	0.098
Root vegetables	0.192	0.175	-0.011	-0.148
Carrots	0.134	0.588	-0.006	0.047
Green leafy vegetables	0.138	0.534	-0.020	0.037
Peas, broad beans and sweetcorn	0.024	0.204	-0.111	0.034
Other cooked vegetables and dishes	0.160	-0.046	-0.073	-0.140
Salad and tomatoes	0.203	-0.111	-0.065	-0.208
Legumes	0.272	-0.110	-0.075	-0.234
Soup	0.130	-0.097	-0.015	-0.061
Nuts, seeds and peanut butter	0.204	-0.062	0.048	0.009
Fresh fruit	0.389	0.001	-0.004	0.088
Tinned and dried fruit	0.205	-0.066	-0.037	0.054
Puddings	0.017	0.189	-0.171	-0.050

Dairy puddings	-0.082	0.147	-0.249	-0.033
Cakes	0.084	0.021	-0.145	-0.080
Chocolate	-0.145	-0.049	-0.047	-0.120
Sweets (candy)	-0.162	-0.015	-0.018	-0.066
Sugar	-0.078	0.017	-0.108	0.112
Sweet spreads (e.g. jam)	0.086	-0.004	0.130	0.027
Biscuits (cookies)	-0.120	0.004	0.159	0.259
Crackers and crispbreads	0.147	-0.077	0.065	0.054
Crisps (potato chips)	-0.208	-0.021	0.301	0.043
Low energy density sauce (e.g. gravy, ketchup)	0.082	0.407	-0.047	-0.043
High energy density sauce (e.g. mayonnaise)	0.279	-0.163	-0.020	-0.141
Salty flavouring (e.g. yeast extract)	0.105	-0.009	0.394	-0.013
Water and flavoured water	0.005	0.029	-0.043	-0.050
Carbonated sweet drinks (soda)	-0.280	-0.098	-0.087	-0.255
Carbonated diet drinks (diet soda)	-0.220	0.138	0.074	-0.062
Regular squash and cordial	0.012	-0.065	0.024	-0.036
Diet squash and cordial	-0.071	0.033	0.068	0.165
Fruit juice	0.271	-0.088	-0.052	-0.091
Flavoured milk drinks	-0.022	-0.022	-0.057	-0.011
Tea and coffee	0.012	-0.010	-0.043	-0.052

Table 4: Factor loadings from PCA of diet diary data on 7473 children aged 10 years, where intakes are expressed as binary (consumed/not consumed) variables. Factor loadings with magnitude greater than 0.2 are shown in bold.

Factor	B1	B2	B3	B4
(variance explained)	(5.2%)	(5.0%)	(3.9%)	(3.2%)
Full fat milk	0.065	0.043	0.106	-0.654
Reduced fat milk	-0.032	0.077	-0.002	0.773
Cheese	-0.091	0.424	0.025	0.089
Yoghurt and fromage frais	-0.019	0.264	0.057	0.200
Butter and animal fat	-0.030	0.298	-0.069	-0.282
Margarine	0.086	-0.080	0.230	0.320
Vegetable oil	-0.088	0.171	0.313	-0.009
High fibre bread	-0.068	0.341	-0.109	0.112
Low fibre bread	0.045	0.042	0.230	0.040
Other bread (e.g. pitta)	-0.001	0.171	-0.060	-0.020
Batter and pastry products	0.392	-0.003	0.132	-0.029
Breakfast cereal	0.015	0.164	0.089	0.204
Rice	0.050	0.173	-0.120	-0.014
Pasta	-0.052	0.348	-0.147	0.075
Baked beans and tinned pasta	-0.053	-0.064	0.386	-0.047
Pizza	-0.151	0.101	0.154	0.029
Eggs	-0.035	0.249	0.078	-0.017
Coated and fried chicken	-0.070	-0.099	0.386	-0.043
Poultry	0.369	0.032	0.029	0.024
Ham and bacon	0.084	0.097	0.128	0.094
Red meat	0.425	0.032	-0.056	0.023
Meat pies and pasties	0.083	-0.066	0.080	0.006
Processed meat	0.039	-0.092	0.368	-0.030
Coated and fried white fish	-0.027	-0.013	0.147	-0.018
White fish and shellfish	-0.012	0.146	-0.044	-0.014
Tuna and oily fish	-0.047	0.306	-0.079	0.040
Vegetarian products	-0.080	0.203	-0.069	-0.019
Chips (French fries)	-0.096	-0.187	0.551	-0.091
Roast potatoes	0.761	-0.210	0.040	-0.053
Other potatoes	0.166	0.238	0.028	0.022
Root vegetables	0.233	0.181	-0.078	-0.011
Carrots	0.700	0.062	-0.074	-0.022
Green leafy vegetables	0.579	0.078	-0.113	-0.025
Peas, broad beans and sweetcorn	0.368	0.098	0.057	0.013
Other cooked vegetables and dishes	0.343	0.266	-0.135	0.034
Salad and tomatoes	-0.069	0.594	-0.086	-0.001
Legumes	-0.031	0.190	-0.090	-0.034
Soup	-0.017	0.137	-0.048	-0.025
Nuts, seeds and peanut butter	-0.043	0.236	-0.023	0.012
Fresh fruit	0.041	0.459	0.010	0.082
Tinned and dried fruit	0.011	0.298	0.021	0.003
Puddings	0.193	0.123	0.064	-0.040

Dairy puddings	0.157	0.227	0.292	-0.045
Cakes	0.054	0.267	0.243	-0.020
Chocolate	-0.021	0.210	0.349	-0.031
Sweets (candy)	0.011	0.137	0.367	-0.054
Sugar	-0.013	0.129	0.342	0.051
Sweet spreads (e.g. jam)	-0.044	0.299	0.254	-0.022
Biscuits (cookies)	0.062	0.127	0.222	0.067
Crackers and crispbreads	-0.016	0.170	0.043	0.021
Crisps (potato chips)	0.048	-0.015	0.216	0.063
Low energy density sauce (e.g. gravy, ketchup)	0.507	0.040	0.085	0.011
High energy density sauce (e.g. mayonnaise)	-0.082	0.362	-0.058	0.037
Salty flavouring (e.g. yeast extract)	0.010	0.123	0.000	0.017
Water and flavoured water	0.015	0.336	-0.140	-0.053
Carbonated sweet drinks (soda)	-0.020	0.050	0.213	-0.321
Carbonated diet drinks (diet soda)	0.036	-0.127	0.252	0.241
Regular squash and cordial	-0.070	0.241	0.123	-0.258
Diet squash and cordial	0.123	-0.244	0.296	0.346
Fruit juice	-0.043	0.410	0.049	0.007
Flavoured milk drinks	0.030	0.122	0.129	0.017
Tea and coffee	0.074	-0.031	0.121	0.067

Table 5: Correlations between component scores obtained from different input variables*.

	W1	W2	W3		B1	B2	B3	B4
A1	0.995	0.105	-0.066		0.143	0.652	-0.430	0.159
A2	0.101	0.996	-0.040		0.765	0.058	-0.052	0.075
A3	-0.051	-0.059	0.962		-0.043	-0.151	0.050	0.241
P1	0.931	0.142	-0.023		0.159	0.599	-0.413	0.199
P2	0.061	0.918	-0.050		0.708	0.010	-0.086	0.068
P3	-0.056	-0.084	0.907		-0.069	-0.154	0.029	0.160
P4	0.003	-0.010	-0.076		0.044	0.043	-0.006	-0.392
B1	0.145	0.767	-0.026		P1	P2	P3	P4
B2	0.653	0.074	-0.102	A1	0.942	0.065	-0.063	0.004
B3	-0.420	-0.037	0.119	A2	0.144	0.937	-0.078	-0.018
B4	0.156	0.061	0.219	A3	-0.011	-0.034	0.962	-0.045

*W: components derived from Weights (g/d); A: components derived from weights (g/d)

Adjusted for total energy intake using the residual method; P: components derived from Percent contribution of each food to total energy intake; B: components derived from binary variables

Table 6: Congruence coefficients between components obtained from different input variables.*

First set	Second set	Congruence
W1, W2, W3	A1, A2, A3	0.994
W1, W2, W3	P1, P2, P3	0.954
W1, W2, W3	B2, B1, B3	0.624
A1, A2, A3	P1, P2, P3	0.964
A1, A2, A3	B2, B1, B3	0.579
P1, P2, P3, P4	B2, B1, B3, B4	0.505

*W: components derived from Weights (g/d); A: components derived from weights (g/d) Adjusted for total energy intake using the residual method; P: components derived from Percent contribution of each food to total energy intake; B: components derived from binary variables

1 **Appendix:** food groups and their components

2

Full fat milk	Full fat cow's, sheep's or goat's milk
Reduced fat milk	Skimmed or semi-skimmed cow's milk
Cheese	Hard, soft, cream or cottage cheese
Yoghurt and fromage frais	Plain or fruit yoghurt, fromage frais
Butter and animal fat	Butter, dripping, ghee, lard, suet
Margarine	Hard or soft margarine or spread
Vegetable oil	Canola/rapeseed, coconut, cod liver, corn, olive, peanut, safflower, sesame, soya or sunflower oil
High fibre bread	White bread, hamburger buns , bagels
Low fibre bread	Brown, wholemeal, granary or rye bread
Other bread	Pitta or naan bread, ciabatta, chapattis, papadums, tortillas
Batter and pastry products	Breadcrumbs, brioche, croissants, pancakes, pastry, scones, stuffing, Yorkshire pudding
Breakfast cereal	Bran, corn, rice or oat-based cereal or sweetened cereal
Rice	Brown, white, risotto or pilau rice
Pasta	Pasta, spaghetti, macaroni, lasagna, noodles, couscous
Baked beans and tinned pasta	Baked beans, canned spaghetti or ravioli, macaroni cheese, pasta salad, gnocchi, cannelloni, pot snacks
Pizza	Pizza, lunchbox snacks
Eggs	Hen's, duck's or quail's eggs, quiche, omelette, Scotch eggs
Coated and fried chicken	Chicken or turkey burgers, fingers, Kiev, nuggets or in crumbs
Poultry	Chicken, turkey, duck, rabbit, grouse, pheasant
Ham and bacon	Ham, gammon, bacon
Red meat	Beef, lamb, pork, veal, venison, haggis, liver, kidney
Meat pies and pasties	Beef, chicken or pork pie, sausage rolls
Processed meat	Sausages, burgers, luncheon meat
Coated and fried white fish	Cod, haddock, plaice, skate all in batter or breadcrumbs
White fish and shellfish	Cod, coley, haddock, hake, halibut, monkfish, plaice, sea bass, snapper, sole, clams, crab, cockles, mussels, scallops, scampi, squid, prawns
Tuna and oily fish	Tuna, anchovies, herring, kipper, mackerel, pilchards, salmon, sardines, swordfish, trout
Vegetarian products	Vegetable or bean burgers/sausages, Quorn, soya
Chips (French fries)	Chips, fried potatoes, potato waffles or croquettes
Roast potatoes	Old potatoes, roasted in fat
Other potatoes	New and old potatoes, boiled or baked
Root vegetables	Artichoke, beetroot, garlic, onion, parsnip, swede, turnip, yam
Carrots	Carrots
Green leafy vegetables	Broccoli, Brussels sprouts, cabbage, kale, spinach,
Peas, broad beans and sweetcorn	Peas, broad beans, sweetcorn, mange-tout
Other cooked vegetables and dishes	Asparagus, cauliflower, celery, courgette, green or French beans, leek, marrow, peppers, pumpkin, squash, vegetable flans or pastries, cauliflower cheese
Salad and tomatoes	Raw vegetables, tomatoes
Legumes	Beans, lentils
Soup	Soup
Nuts, seeds and peanut butter	Nuts, peanuts, seeds, peanut butter
Fresh fruit	Citrus or other fruit
Tinned and dried fruit	Tinned or dried fruit

Puddings	Cheesecake, Christmas pudding, crumble, flan, fruit pie, jelly, Pavlova, sponge, trifle
Dairy puddings	Blancmange, bread and butter pudding, cream, custard, ice cream, mousse, rice pudding
Cakes	Buns, cakes, pastries
Chocolate	Chocolate confectionary
Sweets (candy)	Sugar confectionary
Sugar	Sugar, icing
Sweet spreads	Jam, honey, chocolate spread, lemon curd, marmalade
Biscuits (cookies)	Biscuits, fully-coated chocolate biscuits
Crackers and crispbreads	Crackers, oatcakes, water biscuits, cheese biscuits, rice cakes
Crisps (potato chips)	Potato crisps, corn snacks, pretzels
Low energy density sauce	Bread/ cheese/ tomato sauces, gravy, mustard, vinegar.
High energy density sauce	Energy density below 2kcal/g
Salty flavouring	Mayonnaise, salad cream, chutney. Energy density above 2kcal/g
Water and flavoured water	
Carbonated sweet drinks (soda)	Yeast extract, stock cubes, table salt
Carbonated diet drinks (diet soda)	Water, flavoured water
Regular squash and cordial	Cola, lemonade, ginger ale, tonic water, energy drinks
Diet squash and cordial	Diet cola, lemonade or energy drinks
Fruit juice	Fruit squash or cordial ¹
Flavoured milk drinks	Low sugar fruit squash or cordial ¹
Tea and coffee	Fruit juice Flavoured milk Tea, coffee ² , herbal tea
Foods not included³	Sugar-free sweets/ jelly/ mints/ chewing gum, artificial sweetener, black treacle, instant dessert powder, diabetic jam/ chocolate Alcoholic drinks Herbs, spices

¹ Weight of undiluted squash was multiplied by 5 to obtain equivalent diluted weight.

² Weight of coffee granules was multiplied by 190 to obtain equivalent liquid weight.

³ Due to infrequency of consumption and lack of importance in any extracted component.