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ORIGINAL CONTRIBUTION

A comparison of principal component analysis, partial least-squares and reduced-rank regressions in the identification of dietary patterns associated with bone mass in ageing Australians

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Abstract

Purpose The relative advantages of dietary analysis methods, particularly in identifying dietary patterns associated with bone mass, have not been investigated. We evaluated principal component analysis (PCA), partial least-squares (PLS) and reduced-rank regressions (RRR) in determining dietary patterns associated with bone mass.

Methods Data from 1182 study participants (45.9% males; aged 50 years and above) from the North West Adelaide Health Study (NWAHS) were used. Dietary data were collected using a food frequency questionnaire (FFQ). Dietary patterns were constructed using PCA, PLS and RRR and compared based on the performance to identify plausible patterns associated with bone mineral density (BMD) and content (BMC).

Results PCA, PLS and RRR identified two, four and four dietary patterns, respectively. All methods identified similar patterns for the first two factors (factor 1, "prudent" and factor 2, "western" patterns). Three, one and none of the patterns derived by RRR, PLS and PCA were significantly associated with bone mass, respectively. The "prudent" and dairy (factor 3) patterns determined by RRR were positively and significantly associated with BMD and BMC. Vegetables and fruit pattern (factor 4) of PLS and RRR was negatively and significantly associated with BMD and BMC, respectively.

Conclusions RRR was found to be more appropriate in identifying more (plausible) dietary patterns that are associated with bone mass than PCA and PLS. Nevertheless, the advantage of RRR over the other two methods (PCA and PLS) should be confirmed in future studies.

Keywords Dietary analysis methods · Principal component analysis · Partial least-squares regression · Reduced-rank regression · Bone mass · Ageing population

Abbreviations

AIC	Akaike's information criterion
BMC	Bone mineral content
BMD	Bone mineral density
BMI	Body mass index
CATI	Computer assisted telephone interview
DQES	Dietary Questionnaire for Epidemiological Studies
DXA	Dual energy X-ray absorptiometry
EFA	Explanatory factor analyses
FFQ	Food frequency questionnaire
KMO	Kaiser–Mayer–Olkin
NHS	National Health Survey
NWAHS	North West Adelaide Health Study
PLS	Partial least-squares
PAL	Physical activity level
PCA	Principal component analysis
RRR	Reduced-rank regression
sTOFHLA	Short test of functional health literacy in adults
WHO	World Health Organization

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Introduction

Assessment of food habits and nutrients and their associations with a specific disease outcome can be determined based on pre-existing evidence, that is, a priori methods. This is usually done by constructing scores and indices based on food guidelines and nutritional recommendations [1]. This method is useful to evaluate adherence and the magnitude of the effect of dietary recommendations on disease outcomes [2]. However, because it is only based on a prior selection of foods and nutrients, it does not consider and describe the overall dietary patterns of the population group under the study [2, 3]. Therefore, methods to explore the association between overall diet intake and disease outcomes through a systematic consideration of the correlations between components are increasingly used [4]. Such methods are referred to as a posteriori—a method based on collected data (data driven) in a specific group of population.

There are two main approaches to a posteriori methods [4]. In the first approach, the dietary variables are combined into fewer variables (or factors) based on their correlation, and the latent variables are virtually constructed to represent the original dietary variables [5]. Principal component analysis (PCA) and explanatory factor analysis (EFA) are examples of these approaches [4]. The second approach is cluster analysis, where unlike PCA and EFA approaches, non-overlapping clusters of individuals are constructed [6].

Another approach in dietary data analysis is a "hybrid" method of the a priori and a posteriori methods. In this approach, response variables that mediate dietary risks and outcomes are determined based on a "priori" knowledge. These variables can be biomarkers, nutrient intakes or an overall dietary quality that are known to have association with the outcome of interest [3]. These methods mathematically work by creating a linear combination of the predictors (food groups) and response variables [3, 7]. The two most common examples of these methods are partial least-squares (PLS) and reduced-rank regressions (RRR). The two methods are considered as alternatives for PCA [3].

Studies have reported different recommendations in terms of the utility of the methods [3, 8]. When investigating the association between dietary patterns and bone mass, most studies have used a posteriori methods, although hybrid methods are being increasingly used in recent years [9, 10]. However, the relative advantages and a thorough evaluation of the methods used to identify dietary patterns associated with bone mass have not been investigated. Thus, for the first time, we evaluated the three dietary analysis methods (PCA, PLS and RRR), in this study, to determine dietary patterns associated with bone mass among ageing Australian population.

Methods

Detailed methods are presented previously [11]; however, some of the important issues in this specific study are highlighted below.

Study design and population

The study population was selected from participants of the North West Adelaide Health Study (NWAHS), which is a community-based cohort study. Three major stages of data collection have been conducted between 1999 and 2003, 2004 and 2006 and 2008 and 2010. In the cohort, data were collected using self-complete questionnaire, Computer-Assisted Telephone Interview (CATI) and clinical assessments. Adults (both sexes and aged 18 years and above; $n = 4056$) from randomly selected households were recruited at the inception of the study [12]. The focus of this specific study is the bone mass data [bone mineral density (BMD) and bone mineral content (BMC)] collected at Stage 2 from those aged 50 years and over (2004–2006, $n = 1,588$). Data related to both BMD/C were provided in a total of 1182 adults (545 males, 45.9%) aged 50 years and above. Dietary data were collected at Stage 3 (2008–2010, $n = 2500$) (Fig. 1).

Diet and other covariates assessment

Dietary intake was assessed using the Dietary Questionnaire for Epidemiological Studies (DQES-V3.1) from Cancer Council of Victoria [13]. The questionnaire assesses intake of foods and beverages over the previous 12 months. Analyses of total daily intake of food items and nutrients were performed using the Australian NUTTAB 95 (Food Standards Australia New Zealand, Canberra, 1995) food composition database. For each study participant, the amount of food items consumed per day was calculated in grams and aggregated into 39 food groups [14].

At Stage 2 of the NWAHS, sex, age and family history of osteoporosis were assessed. Annual household income was determined and categorized as up to \$20,000, \$20,001–\$40,000, \$40,001–\$60,000, and more than \$60,000. Marital status was classified as married or living together with partner (in union), separated/divorced, widowed or never married. Alcohol risk was assessed using frequency and number of standard drinks [15]. Smoking was defined as non-smokers, ex-smokers and current smokers. Height and weight of the study participants were measured during the clinic assessment. Body mass index (BMI) was calculated and classified based on the World Health Organization (WHO) standard [16].

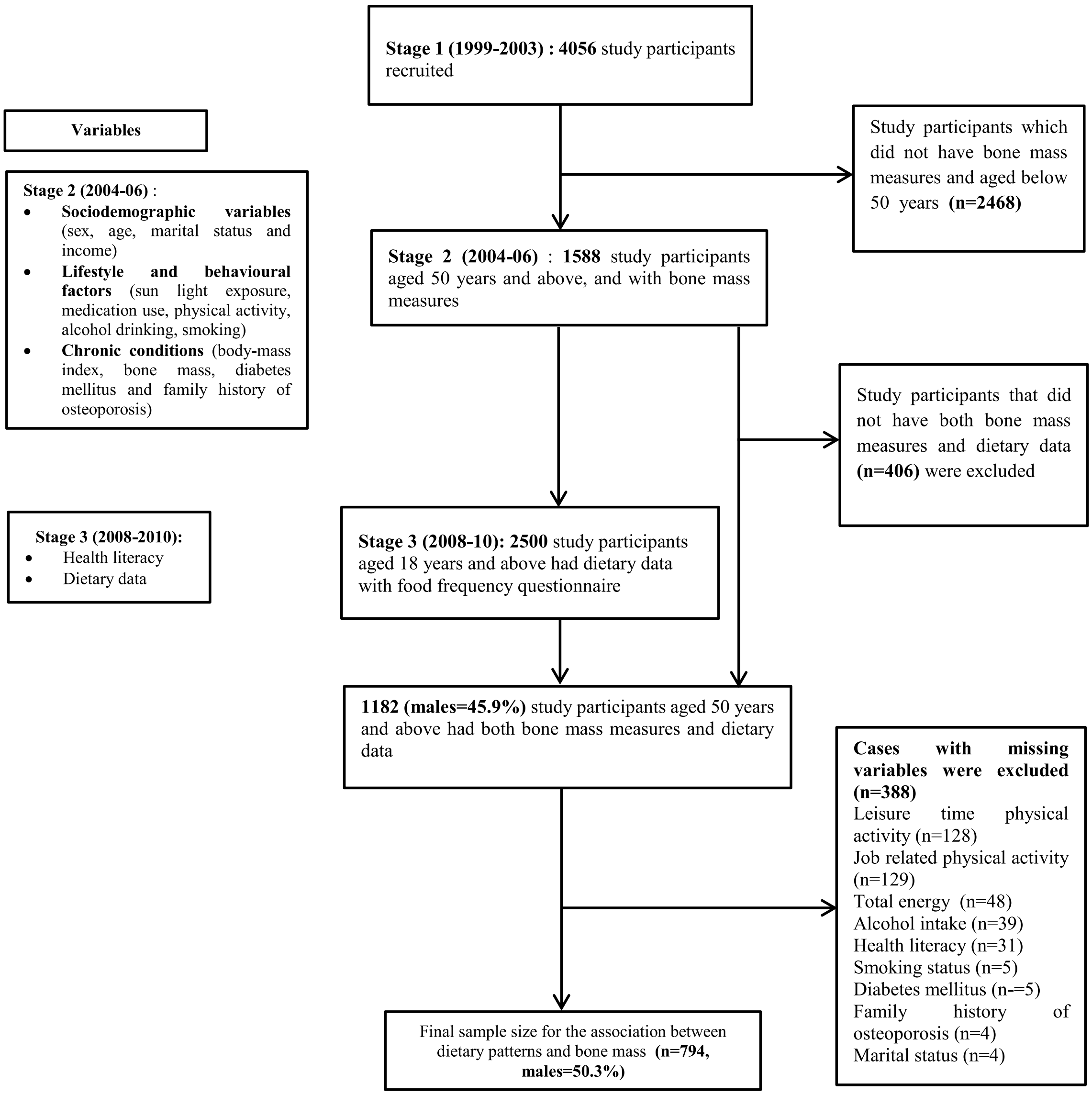

Fig. 1 Sampling description of study participants with dietary intake and bone mass records, the North West Adelaide Health Study, South Australia

Participants with diabetes were identified by either self-report or laboratory diagnosis using blood samples collected at the clinic visit.

Assessment of leisure time physical activity levels (PAL) was undertaken using the Australian National Health Survey (NHS) questions [17], considering the number of times a person exercised in the last two weeks and the total amount of time spent walking or doing moderate or vigorous exercise at Stage 2. Job-related PAL was also assessed based on the type of profession. Detailed methods of both forms of PAL are published elsewhere [18]. Medication use (for hypertension, high cholesterol, mental health problems and asthma) and sun light exposure were also assessed at this stage.

At Stage 3, health literacy was assessed using the Newest Vital Sign test tool [19]. For 31 cases with missing values, we used data collected from the short Test of Functional Health Literacy in Adults (sTOFHLA) tool [20], which was also collected at this stage. Health literacy was classified as limited or adequate.

The number of missing values for each variable includes smoking status ($n = 5$ cases), alcohol risk ($n = 39$), diabetes ($n = 5$), family history of osteoporosis ($n = 4$), marital status (4), leisure time PAL ($n = 128$), job-related

PAL ($n = 129$), total energy ($n = 48$) and health literacy ($n = 31$). We excluded all cases which had at least one missing value of these variables from the analysis ($n = 388$, 32.8%).

Prodigy and DPX + Dual Energy X-ray Absorptiometry (DXA) (GE Lunar, Madison, WI) was used to assess whole body BMD/C as part of the clinic visit at Stage 2. Details of the DXA measurement procedures can be found elsewhere [21]. BMD and BMC were reported as grams/cm^2 and grams, respectively. T-scores for BMD were also reported for each study participant. Study participants who were osteopenic or osteoporotic (T-scores of less than −1) [22] were classified as having low BMD.

Response variables for PLS and RRR analyses

To identify potential response variables, we reviewed previously published studies and chose the dietary intake of four nutrients (protein, calcium, potassium and vitamin D). These nutrients have been strongly linked with bone mass [23–27]. Diet was also found to be a considerable source of vitamin D in the study population [mean intake = 3.5 mcg/day (140 international unit/day)]. We calculated the percentage of energy from total protein intake, calcium, potassium and vitamin D densities and used these values as response variables. The percentage of energy from total protein intake was calculated as follows: total energy intake from protein (kJ) divided by total energy intake, multiplied by 100. Calcium, potassium and vitamin D densities were expressed as absolute intakes of calcium (mg/day), potassium (mg/day) and vitamin D (ng/day), respectively, divided by total daily energy intake (kJ/day) [10].

Statistical analysis

Dietary analysis

To reflect the larger population dietary intake, factor scores and dietary patterns were calculated and constructed for 2453 study participants after excluding 47 participants who had a significant amount of missing dietary data. Data reduction techniques using PCA, PLS and RRR were used to identify dietary patterns out of 39 food groups. Using PCA, a similar number of factors (39 factors) to food groups were produced; however, we retained four factors, of which the first two were chosen based on scree plot, eigenvalues (>1) and interpretability. These two factors were used to investigate the association between dietary patterns and bone mass as only these gave meaningful interpretations of the dietary groups [11]. Varimax rotation was applied, and sample adequacy was checked using the Kaiser–Mayer–Olkin (KMO) test. Linear regression analysis of the factor scores and response variables described above (percentage of energy from total protein intake, calcium, potassium and vitamin D densities) was used to obtain the variance of the response variables explained by the two factors of PCA. An explained variance measures the proportion of variation of a dietary pattern that can be attributable to the food groups or response variables (in this case, nutrients).

The *PROC PLS* statement in SAS (SAS Institute Inc., Cary, NC, USA) was used to conduct both PLS and RRR analysis, defining each in turn in the "method=" [3]. In the analysis, we used a dietary data file containing the 39 food groups coded as *fg1, fg2…fg39* and the four response variables. Four factors were specified and retained in each method.

Different algorisms are applied to construct the scores in each of the three methods. For each method, we calculated the continuous factor scores [the linear functions of food groups (predictors)] and response scores were used in the subsequent statistical analyses and interpretations.

In PCA, the factors explain as much variation as possible of the food groups [7]. Unlike PCA, RRR uses a covariance matrix of responses and predictors (food groups) in calculating the scores. PLS combines the two methods and produces scores considering both the predictor (food group) and response matrixes simultaneously [3]. In this case, the explained variance of both the response variables and food groups is expected to be between the other two methods. Tertiles [T1 (lowest intake), T2 and T3 (highest intake)] of each of the factor scores were constructed. Factor loadings of each food group on the factors were also calculated. Factor loadings are the correlation between the factors and food groups. The proportion of factor-specific and all factor variances across all three methods that explain the response variables and food groups was also determined. Correlations (response scores) between the factors of each method and the response variables were computed. Pearson correlation coefficients for the response variables were also calculated.

Descriptive analysis and modelling

Mean and standard deviation (for continuous normally distributed variables), median and interquartile ranges (for continuous non-normally distributed variables) and proportions (for categorical variables) were calculated. The tertiles of factor scores produced by PCA, PLS, and RRR analyses were used to assess the association of dietary patterns with bone mass. We applied linear regression models to evaluate the associations between tertiles of each factor scores, and BMD and BMC. The initial models (model 1) were adjusted for sex and age. Model 2 was additionally adjusted for socio-economic and lifestyle factors (income, marital status, smoking, alcohol intake, health literacy, leisure time and job-related PAL), chronic conditions (diabetes mellitus, family history of osteoporosis and BMI) and height (BMC). The last models (model 3) were additionally adjusted for total energy intake to assess the potential confounding effect of energy intake in the associations. To compare the relative quality of the models, Akaike's information criterion (AIC) was determined for each model.

Trend of associations across tertiles of each factor was assessed by entering the tertiles of factor scores as continuous variables in the models. Additional adjustments for medications, season of DXA measurement, sunlight exposure and dietary supplements did not materially affect estimates and were not retained in the final models. PLS and RRR analyses were performed using SAS version 9.4 (SAS Institute Inc., Cary, North Carolina). All other statistical analyses were conducted with Stata/SE version 14.1 (StataCorp, College Station, TX, USA).

Comparison of methods

Previous studies have used different approaches to evaluate and compare dietary assessment methods [3, 8]. In this study, we compared PCA, PLS and RRR methods mainly based on the relative loading of food groups within each dietary pattern and its association with bone mass [28]. We additionally evaluated the methods based on the magnitude of variances of each method that explained the response variables and food groups.

Ethical considerations

Ethics approval for the NWAHS was provided by The Queen Elizabeth Hospital, Ethics of Human Research Committee. Participants provided written informed consent.

Results

A total of 1182 (45.9%, males) study participants provided dietary and BMD data. In the multivariable analysis, we excluded those who had missing data from covariates, leaving a total of 794 (67.2%) of participants. The median age of the participants was 62 years (interquartile range = 56.0, 69.0). One-fifth (19.2%) of the participants reported a family history of osteoporosis (Table 1).

Dietary patterns

Food groups are provided in the supplementary material. Factor loadings (standardized correlations of the food groups with the dietary patterns) derived by PCA, PLS and RRR methods are shown in Fig. 2. The first factor (dairy, vegetables and fruit pattern—"prudent" pattern) was similar across the three methods and was characterized primarily by high intakes of medium fat dairy, vegetables and fish and, low intake of soft drinks, processed meat and take away foods. Factor 2 of each of the three methods was also similar in terms of the constituents of the food groups. Factor 2 ("western" pattern) of the PCA method was characterized by high intake of processed meat, take away foods, white bread, red meat and soft drinks and low intake of dairy products and nuts. Factor 2 ("western" pattern) of the other two methods was characterized by high consumption of animal foods (poultry, eggs, red and processed meat, fish and high fat dairy) and low intakes of medium fat dairy, fruit and nuts.

Factor 3 (dairy pattern) was generally characterised by high intake of dairy products; however, a slight difference in food groups was identified using PLS and RRR. Factor 4 (vegetables and fruit pattern) was primarily characterized by low intake of dairy products and high consumption of vegetables (Fig. 2). The intake of major foods and nutrients across tertiles of dietary patterns is provided in the Supplementary material.

Explained variations in response variables and food groups

The two factors of PCA explained 37.1% of the response variable variation (proportion of energy from protein, calcium, potassium and vitamin D densities). Both PLS (75.5%) and RRR (70.6%) explained a larger amount of variation in the response variables. In PLS and RRR, the largest explained variations of responses were observed in vitamin D (65.2%) and calcium (80.0%) densities, respectively. Potassium density was the most explained response in the other two methods (22.7% in PCA and 43.4% in PLS) in the "prudent" pattern; however, calcium density was the most explained (56.5%) response in RRR (Table 2).

Using PLS, 21.1% of variation in predictors (food groups) was found, compared to 16.7% of PCA and 14.0% of RRR. Whereas factor 1 explained 10.3% of variation of predictors in PCA, only 3.4 and 7.3% variations were explained by this factor for RRR and PLS, respectively (Table 2).

The correlation (response scores) between factors and response variables estimated using PCA, PLS and RRR methods are depicted in Fig. 3. Factor 1 of the PCA was positively correlated with protein energy, calcium and potassium densities. Using PLS, the proportion of energy from protein was positively correlated with all factors. RRR analysis estimated a positive correlation between calcium density and factors 1 and 3. We also found that the correlation among proportion of energy from protein, calcium and potassium densities was positive and high (Supplementary material).

Table 1 Participants' characteristics of adults aged 50 years and above, the North West Adelaide Health Study, South Australia ($n = 1182$)

Characteristics	Category	Value
N		1182
Sex	Male	543 (45.9%)
Age category (years)	50–59 years	513 (43.4%)
	60–69 years	400 (33.8%)
	70 and above	269 (22.8%)
Age in years, median (IQR)		62.0 (56.0, 69.0)
Monthly income	Up to $20,000	352 (29.8%)
	$20,001-$40,000	361 (30.5%)
	$40,001-$60,000	203 (17.2%)
	More than $60,000	206 (17.4%)
	Missing	60 (5.1%)
Marital status	Married or living with a partner	779 (65.9%)
	Separated/divorced	196 (16.6%)
	Widowed	154 (13.0%)
	Never married	45 (3.8%)
	Missing	8 (0.7%)
Smoking status	Non-smoker	581 (49.2%)
	Ex-smoker	476 (40.3%)
	Current smoker	120 (10.2%)
	Missing	5 (0.4%)
Alcohol risk level	Non-drinkers (no risk)	609 (51.5%)
	Low risk	474 (40.1%)
	Intermediate to very high risk	60 (5.1%)
	Missing	39 (3.3%)
Leisure time PAL	Sedentary/low	667 (56.4%)
	Moderate/high	387 (32.7%)
	Missing	128 (10.8%)
Job-related PAL	Sedentary/light	581 (49.2%)
	Medium/heavy	472 (39.9%)
	Missing	129 (10.9%)
Health literacy	Limited	402 (34.0%)
	Adequate	715 (60.5%)
	Missing	65 (5.5%)
Diabetes mellitus	Yes	137 (11.6%)
	No	1040 (88.0%)
	Missing	5 (0.4%)
Family history of osteoporosis	Yes	227 (19.2%)
	No	951 (80.5%)
	Missing	4 (0.3%)
Body mass index category	Normal	299 (25.3%)
	Pre-obese (overweight)	524 (44.3%)
	Obese	359 (30.4%)
Body mass index, mean (SD) (kg/m^2)		28.2 (4.7)
Total energy, mean (SD) (kJ/day)		8665.4 (2611.3)
Percent of energy from protein, mean (SD)		18.6 (3.3)
Protein (g/d), mean (SD)		94.5 (34.0)
Calcium density, mean (SD) (mg/kJ/day)		0.4 (0.1)
Calcium (mg/d), mean (SD)		878.6 (329.1)
Potassium density, mean (SD) (mg/kJ/day)		1.9 (0.4)
Potassium (mg/d), mean (SD)		3919.9 (1452.4)

Table 1 continued

Characteristics	Category	Value
Vitamin D density, mean (SD) (ng/kJ/day)		1.7 (0.9)
Vitamin D (μg/d), mean (SD)		3.5 (2.0)
Bone mineral density, mean (SD) (mg/cm^2)		1195.6 (118.4)
DXA T-score, mean (SD)		0.34 (1.32)
Bone mineral content, mean (SD) (g)		2755.4 (550.8)
Low bone mineral density		188 (15.9%)
Height, mean (SD) (cm)		166.67 (9.5)

IQR interquartile range, *PAL* physical activity level, *SD* standard deviation, *DXA* dual-energy X-ray absorptiometry

Dietary patterns and bone mass

Table 3 provides the different associations of factors identified by PCA, PLS and RRR with BMD and BMC. In the more fully adjusted models, none of the factors of PCA was significantly associated with bone mass; and more dietary factors determined by RRR compared to PLS were found to be associated with BMD and BMC. However, in all methods, the coefficients increased across tertiles of the "prudent" and dairy patterns, and decreased across the tertiles of vegetables and fruit pattern. Participants in T3 of vegetables and fruit pattern determined by PLS had a 17.3 mg/cm^2 ($\beta = -17.29$; 95% CI -34.0, -0.58) decrease in BMD compared to those in T1 of model 3. No significant association of this dietary pattern determined by PLS with BMC was observed.

In model 3, the "prudent" and dairy patterns of RRR were significantly and positively associated with BMD and BMC. Participants in T2 and T3 of "prudent" pattern had a 21.4 mg/cm^2 ($\beta = 21.36$; 95% CI 5.70, 37.02) and 27.0 mg/cm^2 ($\beta = 26.99$; 95% CI 10.94, 43.04) increased BMD than those in T1, respectively. Those in T3 of dairy pattern had a 24.6 mg/cm^2 ($\beta = 24.58$; 95% CI 8.44, 40.72) higher BMD than those in T1. Compared to those in T1 of "prudent" and dairy patterns, a 69.7 g ($\beta = 69.65$; 95% CI 16.67, 122.63) and a 55.5 g ($\beta = 55.49$; 95% CI 2.26, 108.73) increase in BMC was found among participants in T3, respectively. Vegetables and fruit pattern was negatively and significantly associated with BMC. Participants in T2 of vegetables and fruit pattern had a 52.8 g ($\beta = -52.79$; 95% CI -104.10, -1.47) decrease in BMC compared to those in T1. The AIC was comparable across the corresponding dietary patterns of each of the dietary analysis methods (Table 3).

Discussion

We identified and compared dietary patterns (PCA = 2; PLS = 4; RRR = 4 patterns) using three analysis methods. The first pattern ("prudent" pattern) of all methods was characterized by high intake of dairy products, vegetables and fruit. The second pattern ("western" pattern) was characterized by high intake of fish, poultry, high fat dairy, processed and red meat and low intake of medium fat dairy, vegetables and fruit. In assessing the association between factors and bone mass, RRR identified more (plausible) factors which were significantly associated with bone mass than the other two methods.

Whereas the "prudent" pattern of RRR was significantly and positively associated with bone mass, the one computed by PCA and PLS was not. This dietary pattern was characterized by high intake of vegetables, fruit and dairy products. In numerous studies, intake of these food groups has been linked with a decreased risk of reduced bone mass [27, 29–31]. However, despite the similarity in contents of the food groups, only the "prudent" pattern determined by RRR was significantly and positively associated with bone mass. In line with this finding, an absence of association between Mediterranean dietary pattern derived by PCA and indices of bone mass was reported [32]. Furthermore, in the RRR analysis, the correlation of factor scores of "prudent" pattern with calcium desnity—which has an indispensable role as a component of bone mass—was the highest (0.71) compared to the other two methods (PCA = 0.19 and PLS = 0.50). As there was a low correlation between the "prudent" pattern with protein in the PCA and PLS, this may also be an explanation for the absence of significant positive association, as evidence suggests that the role of calcium on bone mass is enhanced when there is an adequate intake of protein and vice versa [33]. In addition, RRR extracts dietary patterns that combine eating behaviours and the pathway to the outcome (through the response variables) taking into account the physiological importance.

Our findings show that the dairy pattern of RRR was positively associated with bone mass. However, there was a non-significant positive association across the tertiles of the dairy pattern and bone mass with PLS. This could be due to the following reasons. First, a careful observation of

Food groups	Principal component analysis		Partial least-squares				Reduced-rank regression			
	"Prudent" pattern	"Western" pattern	"Prudent" pattern	"Western" pattern	Dairy pattern	Vegetables and fruit pattern	"Prudent" pattern	"Western" pattern	Dairy pattern	Vegetables and fruit pattern
Medium fat dairy	0.39	-0.05	0.33	-0.19	0.35	0.03	0.57	-0.39	0.04	-0.3
Fruity vegetables	0.75	0.07	0.33	0.01	-0.31	0.21	0.18	-0.16	-0.09	0.35
Stalk vegetables	0.58	-0.05	0.28	0.07	-0.27	0.11	0.14	-0.07	-0.06	0.23
Leafy vegetables	0.61	-0.01	0.27	0.10	-0.26	0.14	0.17	-0.07	-0.08	0.28
Cabbages	0.53	0.12	0.27	0.04	-0.22	0.10	0.20	-0.09	-0.08	0.28
Root vegetables	0.54	0.16	0.26	-0.06	-0.25	0.12	0.13	-0.14	-0.05	0.26
Other fruits	0.55	0.06	0.23	-0.15	-0.27	0.08	0.05	-0.15	0.05	0.29
Potato without fat	0.28	0.18	0.15	-0.07	-0.13	0.03	0.08	-0.08	-0.01	0.15
Tea and water	0.37	0.42	0.13	-0.10	-0.14	0.05	0.12	-0.11	0.09	0.16
Citrus fruit	0.28	-0.08	0.13	-0.09	-0.15	0.03	0.05	-0.08	0.02	0.15
Nuts dairy	0.39	-0.13	0.12	-0.16	-0.15	0.14	-0.05	-0.14	0.03	0.06
Fish	0.36	0.14	0.12	0.34	-0.18	0.03	0.18	0.39	-0.17	0.15
Legumes	0.31	0.02	0.10	-0.01	-0.14	0.09	0.05	-0.05	-0.03	0.13
High fibre cereal	0.09	-0.04	0.08	0.03	0.02	-0.02	0.08	-0.03	0.00	0.03
Sugar	0.46	0.54	0.07	-0.33	-0.17	0.12	-0.01	-0.17	0.27	0.01
Tomato sauce	0.28	0.28	0.07	0.09	-0.17	0.17	0.04	-0.01	-0.08	0.15
High fibre bread	0.24	0.16	0.06	-0.16	-0.15	0.04	-0.08	-0.02	0.10	-0.06
Other cereal	0.17	0.18	0.06	-0.14	-0.06	-0.01	0.00	-0.06	0.07	-0.03
Coffee	-0.02	0.17	0.05	0.08	0.01	-0.11	0.18	-0.02	0.01	0.25
Poultry	0.18	0.28	0.04	0.37	0.10	0.33	0.11	0.1	-0.48	-0.10
Wine	0.00	0.01	0.01	0.11	-0.04	0.14	-0.03	0	-0.10	0.06
Juice	0.18	0.25	0.00	-0.11	-0.12	0.11	-0.05	-0.06	0.00	0.11
Eggs	0.08	0.19	-0.02	0.14	-0.13	0.02	-0.01	0.16	-0.05	0.00
Flavoured milk	0.01	0.06	-0.03	-0.15	0.15	-0.06	0.07	-0.1	0.15	-0.24
Saturated spread	0.01	0.14	-0.04	-0.12	-0.08	0.06	-0.12	-0.06	0.06	-0.05
Jam and vegemite	0.13	0.49	-0.04	-0.18	-0.18	0.18	-0.13	-0.04	0.02	0.05
Potato with fat	-0.06	0.24	-0.04	-0.07	-0.05	0.05	-0.07	-0.03	0.02	0.04
Red meat	0.09	0.44	-0.04	0.38	0.04	0.39	0.02	0.17	-0.57	-0.11
Pasta and rice	0.13	0.01	-0.04	-0.04	-0.10	0.18	-0.16	-0.02	-0.04	-0.06
peanut butter	0.13	0.20	-0.05	-0.15	-0.10	0.18	-0.15	-0.04	-0.01	-0.06
Spirits	-0.09	0.04	-0.07	0.07	0.04	-0.02	0.00	0.07	-0.02	-0.04
Snacks	0.02	0.54	-0.13	-0.28	-0.05	0.28	-0.29	-0.11	0.08	-0.17
Beer	-0.13	0.34	-0.16	0.07	-0.06	0.07	-0.15	0.1	-0.02	-0.04
Unsaturated spread	-0.09	0.43	-0.16	-0.10	-0.12	0.05	-0.20	0.13	0.11	-0.09
Soft drinks	-0.15	0.32	-0.17	-0.13	0.03	0.11	-0.21	-0.01	0.02	-0.14
Processed meat	-0.06	0.59	-0.18	0.14	-0.01	0.31	-0.14	0.15	-0.22	-0.14
Take away foods	-0.13	0.51	-0.22	-0.04	-0.03	0.23	-0.22	0.08	-0.08	-0.14
High fat dairy	-0.23	0.19	-0.22	0.19	-0.29	-0.40	-0.01	0.6	0.40	0.05
White bread	-0.31	0.31	-0.25	-0.04	-0.05	0.05	-0.27	0.11	0.05	-0.12

Fig. 2 Factor loadings of food groups in dietary patterns identified using principal component analysis, partial least-squares and reduced-rank regressions, the North West Adelaide Health Study, South Australia ($n = 2453$) (The *colour* gradation denotes the strength and direction of the correlation between the food groups and the dietary patterns. *Deep green colour* represents a relatively higher correlation (a higher intake) of the food groups with the corresponding dietary patterns. *Deep red* represents relatively a lower correlation (a lower intake) of the food groups with the corresponding patterns.)

the factor loadings of vegetables and fruit showed that the intake of vegetables and fruit in the RRR analysis was not as low as those in PLS. Second, we also found an inverse correlation between potassium and vitamin D densities, and dairy pattern of PLS. With regard to this, evidence has shown a significant positive role of vegetables and fruit [30] as well as potassium [34] and vitamin D on bone mass. Third, despite these two methods use existing knowledge of the association between nutrients and diseases, the fact that RRR mainly focuses on explaining variation in the response nutrients [3] rather than the food groups can partly explain why dairy pattern of RRR analysis is significantly associated with bone mass.

Dairy products are the most important food groups which assist in the prevention of osteoporosis [29]. In line with this, our finding also supports the importance of dairy

Table 2 Explained variation in responses and food groups by dietary patterns identified using principal component analysis, partial least-squares and reduced-rank regressions, the North West Adelaide Health Study, South Australia

Factors	Proportion (%) of explained variation in responses															Proportion (%) of explained variation in food groups		
	Principal component analysis					Partial least-squares					Reduced-rank regression							
	Energy from protein	Calcium density	Potassium density	Vitamin D density	Total	Energy from protein	Calcium density	Potassium density	Vitamin D density	Total	Energy from protein	Calcium density	Potassium density	Vitamin D density	Total	Partial least-squares	Reduced-rank regression	Principal component analysis
"Prudent" pattern	2.1	3.8	22.7	3.3	24.9	7.0	18.6	43.4	6.0	18.8	26.2	56.5	29.0	1.4	28.3	7.3	3.4	10.3
"Western" pattern	0.0	7.8	7.2	0.4	12.2	41.6	1.0	0.6	21.9	16.3	5.5	1.4	5.6	65.5	19.5	3.9	3.4	6.7
Dairy pattern (Factor 3[a])	(3.8)[a]	(2.2)[a]	(0.0)[a]	(0.0)[a]	(8.1)[a]	9.5	16.1	0.3	12.6	9.6	36.2	13.8	0.0	5.3	13.8	5.4	3.3	(5.0)[a]
Vegetables and fruit pattern (Factor 4[a])	(8.6)[a]	(2.6)[a]	(0.0)[a]	(3.1)[a]	(17.2)[a]	3.1	21.1	2.8	24.6	12.9	1.5	8.4	24.1	1.9	9.0	4.5	4.0	(4.4)[a]
Total	2.1 (14.5)[a]	11.6 (16.4)[a]	29.9 (29.9)[a]	3.7(6.8)[a]	37.1 (62.4)[a]	61.1	56.8	47.1	65.2	57.5	69.5	80.0	58.6	74.1	70.6	21.1	14.0	16.7 (26.3)[a]

[a] These are results (proportions of explained variations) from factors 3 and 4 of principal component analysis. Factors 3 and 4 of principal component analysis were neither interpretable nor considered in the analysis that assesses the association between dietary patterns and bone mass. We present the explained variations due to these factors for comparison purpose

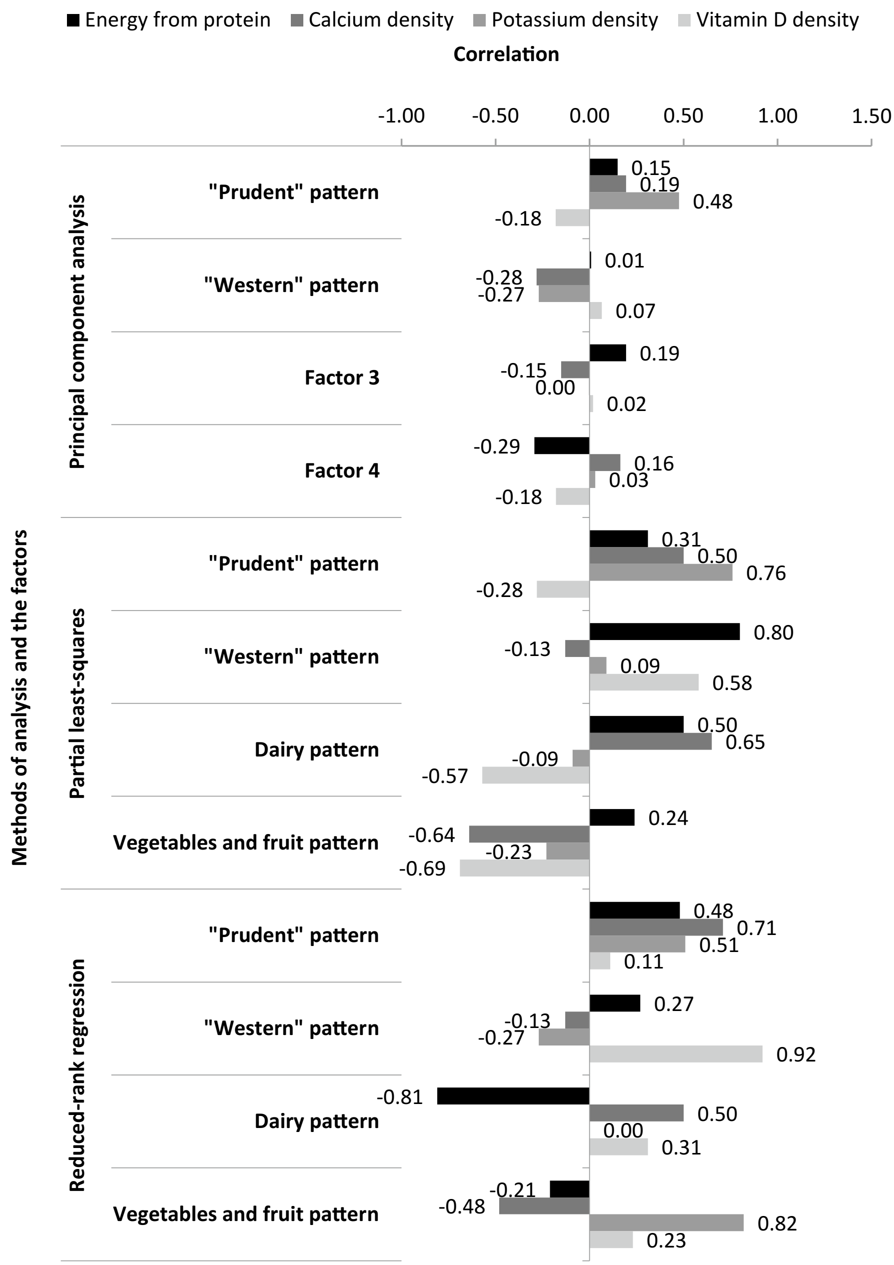

Fig. 3 Correlation (response scores) between factors and response variables obtained from principal component analysis, partial least-squares and reduced-rank regressions, the North West Adelaide Health Study, South Australia

products in building bone mass. The vegetables and fruit pattern of RRR, which is characterized by low consumption of dairy products and high consumption of vegetables and fruit, was negatively and significantly associated with bone mass, highlighting the imperative role of dairy on bone mass. In our previous study, we have also highlighted the importance of dairy products as part of “prudent” dietary pattern [11].

Information obtained by PCA can give clearer understanding of dietary patterns within a specific population which helps in the formulation of tailored nutrition interventions [35, 36]. However, PCA does not necessarily explain the variation and amount of nutrient intake in the identified patterns, rather it explains the cultural and behavioural aspects of food [37]. The effects of diet could be also mediated through specific nutrients which cannot be captured by this method [28] and could create difficulty in providing a plausible interpretation of findings. In line with this, our results showed that although PCA explains the highest variation in food groups (considering all four factors), no factor was significantly associated with bone mass in the most adjusted models. This supports the view that PCA is unlikely to identify dietary patterns associated with bone mass. The selection of the dietary patterns in PCA is subjective, although aided by methods such as eigenvalues and scree plots. However, these subjective decisions

Table 3 Coefficients (β) and 95% confidence intervals for bone mineral density and content and tertiles of factor scores derived using principal component analysis, partial least-squares and reduced-rank regressions, the North West Adelaide Health Study, South Australia ($n = 794$)

	β (95% confidence interval), BMD (mg/cm^2)					β (95% confidence interval), BMC[#] (g)			
	T_1	T_2	T_3	*P for trend*	AIC	T_2	T_3	*P for trend*	AIC
Principal component analysis									
Model 1									
"Prudent" pattern	Ref.	3.94 (−13.73, 21.60)	9.68 (−7.78, 27.15)	0.276	9601	43.80 (−25.94, 113.55)	44.20 (−24.76, 113.16)	0.210	11,782
"Western" pattern	Ref.	−18.14 (−35.90, −0.39)*	0.19 (−18.10, 18.48)	0.962	9597	−71.00 (−140.98, −1.03)*	33.34 (−38.75, 105.43)	0.349	11,775
Model 2									
"Prudent" pattern	Ref.	−0.74 (−16.87, 15.39)	8.65 (−7.64, 24.94)	0.293	9438	−9.48 (−62.42, 43.46)	1.23 (−52.28, 54.73)	0.959	11,324
"Western" pattern	Ref.	−10.80 (−26.90, 5.30)	2.04 (−14.57, 18.66)	0.794	9437	−25.88 (−78.65, 26.89)	12.91 (−41.62, 67.44)	0.635	11,322
Model 3									
"Prudent" pattern	Ref.	−2.50 (−18.91, 13.92)	4.25 (−13.74, 22.24)	0.649	9439	−12.48 (−66.38, 41.41)	−6.30 (−65.40, 52.81)	0.831	11,326
"Western" pattern	Ref.	−15.33 (−32.35, 1.68)	−8.45 (−29.46, 12.56)	0.403	9436	−28.41 (−84.28, 27.46)	7.04 (−62.01, 76.10)	0.878	11,324
Partial least-squares									
Model 1									
"Prudent" pattern	Ref.	−0.32 (−17.75, 17.10)	15.76 (−2.11, 33.63)	0.087	9598	7.62 (−61.15, 76.39)	78.85 (8.33, 149.38)*	0.030	11,778
"Western" pattern	Ref.	−9.37 (−26.81, 8.06)	3.70 (−13.69, 21.10)	0.678	9600	−19.18 (−88.14, 49.77)	−5.59 (−74.41, 63.23)	0.873	11,784
Dairy pattern	Ref.	9.16 (−8.37, 26.69)	12.09 (−5.34, 29.53)	0.175	9600	17.37 (−51.92, 86.66)	41.49 (−27.42, 110.40)	0.237	11,782
Vegetables and fruit pattern	Ref.	8.40 (−9.03, 25.83)	−3.01 (−20.48, 14.47)	0.741	9600	22.17 (−46.68, 91.01)	−30.77 (−99.79, 38.24)	0.385	11,782
Model 2									
"Prudent" pattern	Ref.	−6.02 (−21.95, 9.91)	14.87 (−1.69, 31.42)	0.081	9433	−3.73 (−56.08, 48.61)	30.22 (−24.30, 84.74)	0.281	11,323
"Western" pattern	Ref.	−13.22 (−28.85, 2.41)	−2.96 (−18.75, 12.82)	0.699	9436	−8.17 (−59.49, 43.15)	11.80 (−40.05, 63.64)	0.660	11,324
Dairy pattern	Ref.	−0.19 (−16.08, 15.70)	4.28 (−11.58, 20.15)	0.592	9439	−18.52 (−70.51, 33.48)	16.75 (−35.16, 68.67)	0.515	11,323
Vegetables and fruit pattern	Ref.	−1.19 (−17.00, 14.62)	−12.25 (−28.31, 3.81)	0.135	9437	17.62 (−34.12, 69.36)	−41.84 (−94.37, 10.70)	0.119	11,319
Model 3									
"Prudent" pattern	Ref.	−6.02 (−21.94, 9.91)	13.71 (−2.95, 30.37)	0.113	9433	−3.73 (−56.11, 48.65)	28.95 (−25.96, 83.85)	0.308	11,324
"Western" pattern	Ref.	−11.07 (−27.05, 4.91)	−0.72 (−16.88, 15.44)	0.948	9437	−4.74 (−57.22, 47.74)	15.38 (−37.71, 68.48)	0.564	11,325
Dairy pattern	Ref.	4.77 (−12.04, 21.59)	9.47 (−7.40, 26.33)	0.269	9438	−12.65 (−67.78, 42.48)	22.88 (−32.44, 78.20)	0.369	11,324
Vegetables and fruit pattern	Ref.	−2.47 (−18.30, 13.36)	−17.29 (−34.00, −0.58)*	0.045	9434	15.12 (−36.76, 67.00)	−51.53 (−106.33, 3.27)	0.073	11,319
Reduced-rank regression									
Model 1									
"Prudent" pattern	Ref.	28.02 (10.84, 45.19)**	30.58 (13.07, 48.08)**	0.001	9587	88.92 (20.99, 156.84)*	122.00 (52.78, 191.22)**	0.001	11,771
"Western" pattern	Ref.	−12.37 (−29.59, 4.85)	−10.97 (−28.62, 6.67)	0.217	9600	−25.91 (−94.02, 42.20)	−16.01 (−85.80, 53.78)	0.645	11,783
Dairy pattern	Ref.	2.66 (−14.95, 20.26)	12.71 (−5.02, 30.45)	0.155	9600	29.12 (−40.38, 98.63)	61.13 (−8.89, 131.16)	0.086	11,781
Vegetables and fruit pattern	Ref.	−15.14 (−32.42, 2.13)	−16.36 (−34.11, 1.39)	0.070	9598	−85.92 (−154.08, −17.75)*	−47.21 (−117.25, 22.83)	0.186	11,778

Table 3 continued

	β (95% confidence interval), BMD (mg/cm^2)					β (95% confidence interval), BMC$^{\#}$ (g)			
	T_1	T_2	T_3	*P for trend*	AIC	T_2	T_3	*P for trend*	AIC
Model 2									
"Prudent" pattern	Ref.	20.26 (4.64, 35.88)*	26.84 (10.77, 42.91)**	0.001	9427	45.66 (−5.70, 97.02)	69.40 (16.44, 122.35)*	0.010	11,317
"Western" pattern	Ref.	−9.50 (−25.08, 6.09)	−8.96 (−24.98, 7.07)	0.268	9438	8.79 (−42.37, 59.95)	14.95 (−37.63, 67.54)	0.576	11,324
Dairy pattern	Ref.	6.67 (−9.13, 22.47)	25.46 (9.39, 41.54)**	0.002	9429	14.88 (−37.11, 66.87)	56.34 (3.35, 109.33)*	0.035	11,320
Vegetables and fruit pattern	Ref.	−9.00 (−24.61, 6.61)	−10.14 (−26.27, 5.98)	0.218	9438	−53.71 (−104.79, −2.62)*	−27.89 (−80.65, 24.86)	0.302	11,320
Model 3									
"Prudent" pattern	Ref.	21.36 (5.70, 37.02)**	26.99 (10.94, 43.04)**	0.001	9427	47.14 (−4.42, 98.70)	69.65 (16.67, 122.63)*	0.009	11,319
"Western" pattern	Ref.	−7.55 (−23.39, 8.29)	−8.26 (−24.31, 7.78)	0.312	9438	11.82 (−40.21, 63.86)	16.03 (−36.68, 68.74)	0.550	11,326
Dairy pattern	Ref.	6.76 (−9.04, 22.56)	24.58 (8.44, 40.72)**	0.003	9429	14.97 (−37.05, 66.99)	55.49 (2.26, 108.73)*	0.040	11,321
Vegetables and fruit pattern	Ref.	−7.96 (−23.62, 7.71)	−10.19 (−26.31, 5.92)	0.215	9437	−52.79 (−104.10, −1.47)*	−27.95 (−80.73, 24.84)	0.301	11,322

Model 1 was adjusted for sex and age

Model 2 was additionally adjusted for socio-economic and lifestyle factors (income, marital status, smoking, alcohol risk, health literacy, leisure time and job related physical activity levels), chronic conditions (diabetes mellitus, family history of osteoporosis and body mass index)

Model 3 was additionally adjusted for total energy intake

P for trend was calculated by including the tertiles of the factor scores as continuous variables in the models

AIC Akaike's information criterion, *BMD* bone mineral density, *BMC* bone mineral content

* $P < 0.05$; ** $P < 0.01$

\# Models 2 and 3 of bone mineral content (BMC) were additionally adjusted for height (cm) could introduce a bias in identifying the optimal number of dietary patterns. Without due consideration of selecting the optimal number of factors, investigators could also miss disease-related dietary patterns. Thus, it is important to note that critical evaluation is required when selecting the number of patterns using this method.

PLS, a method mathematically thought to be between PCA and RRR, is an alternative method for deriving dietary patterns. In this method, the covariance matrixes of both response (nutrients) and predictors (food groups) are explained in the latent variables [3]. In the current study, none of the factors identified by PLS was significantly associated with BMD and BMC. Although no study has evaluated dietary analysis methods in association with bone mass, some studies have used these types of analyses for different outcomes. For instance, DiBello et al. claimed that PCA and PLS were found to be more appropriate in identifying dietary patterns associated with cardiovascular diseases [8]. However, it may be that the differences in the findings of our study and this study could be impacted by the disease outcome used and the types of response variables.

In the current study, we found more dietary patterns associated with bone mass using RRR which are plausible in the context of existing evidence. In line with our findings, a study by Hoffmann et al. compared PCA, PLS and RRR in identifying dietary patterns associated with diabetes and concluded that RRR is the most appropriate method in extracting more dietary patterns that are significantly associated with diabetes [3]. RRR is also the most commonly used hybrid method in nutritional epidemiology [9, 10]. The method is better to explain the dietary patterns in the responses [8] and dietary patterns can be evaluated based on the response variables for their plausibility in their association with disease outcomes. Although most of the previous studies used a posteriori methods [38, 39], in recent years, RRR is being increasingly used in identifying plausible dietary patterns associated with bone mass [9, 10, 27, 40].

Some limitations should be acknowledged when interpreting the findings. First, dietary information was collected between 2008 and 2010 while bone mass was determined between 2004 and 2006 with a 4.3-year median difference (minimum = 2.8 and maximum = 6.1 years). Although habits of elderly people in relation to the choice of the food groups have been found to be stable over years [41], eating behaviours of the study participants, particularly change of behaviours towards a healthy pattern among participants diagnosed with chronic diseases, could exist. In addition, since study participants were told the result of DXA measurements, those who knew they had low BMD could also change their behaviour towards a favourable diet. Thus, the association between dietary pattern and bone mass in our study may be underestimated. To investigate the effect, we did a sensitivity analysis by dividing study participants into two groups based on the median gap of time (i.e. early and late measures of dietary data after bone mass measurement). The estimates of associations for the early measures were either consistent or stronger compared with the whole sample. On the other hand, estimates of participants with late measures were attenuated, further highlighting the underestimated associations between dietary patterns and bone mass.

Although food frequency questionnaires (FFQs) have limitations in providing valid dietary information, they are commonly used to measure usual dietary habits [42]. In this regard, measurement error for every diet component will tend to underestimate the effects in the statistical analysis [43]. However, in the presence of correlation between dietary variables, the direction of bias associated with measurement error is unknown [44, 45]. Furthermore, in ranking intake levels of dietary components, FFQ is relatively robust [37]. Recall bias is also another potential limitation associated with FFQ.

In conclusion, although PCA, PLS and RRR are similar in terms of their mathematical foundations (use of covariance matrix to reduce dimensionality) and extraction of factors that are not correlated, studies have reported different recommendations regarding their utility. In this particular study, RRR was found to be more appropriate in identifying dietary patterns that are associated with bone mass than the other two methods. Nevertheless, the advantage of RRR over the other two methods (PCA and PLS) should be confirmed in future studies in different settings, population groups, response variables and disease outcomes.

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Authors' contribution YAM, TKG, RA and ZS conceived the study. YAM conducted all analyses and wrote all drafts of the paper. ZS assisted with analysis and reviewed and provided comment on all drafts. TKG, AWT and RA reviewed and commented on all drafts. All authors read and approved the final manuscript.

Compliance with ethical standards

Conflict of interest The authors have no financial or personal conflicts of interest to declare.

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