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Chemometric analysis of nutritional and bread-making quality attributes of wheat cultivars

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Abstract

The term of wheat grain quality can be interpreted in many ways, because there are different demands according to the needs of agriculture, processing industry, consumers, etc. Increasing attention is devoted to nutritional and health aspect of wheat quality. In this work, a set of 44 wheat cultivars was characterized by fourteen variables referring to: (1) nutritional and health-promoting quality of wheat grain, (2) technological quality of grain samples and (3) dough/ bread-making quality. Data were analyzed by means of several statistical/chemometrical tools.

Keywords: wheat cultivars, wheat quality, analysis of variance, linear discriminant analysis

Introduction

Bread wheat (*Triticum aestivum* L.) belongs to most grown cereals in the world. Wheat varieties with superior quality attributes are highly desired as they can better satisfy the requirements of the market. The term of wheat grain quality can be interpreted in many ways, because there are different demands according to the needs of agriculture, processing industry, consumers, etc. Recently, many research papers point out the nutritional and health aspect of wheat quality. Thus, the major objective of plant breeders is to develop varieties with improved agronomic as well as technological properties, containing increased amounts of compounds beneficial to our health and lower concentrations of anti-nutrients (Welch and Graham 2002, Welch 2005, Šramková et al. 2009a, Šramková et al. 2009b).

Among all the cereals, only the flour of bread wheat is able to form dough that exhibits the rheological properties required for the production of leavened bread. This property results from the ability of wheat storage proteins, gliadins and glutenins, to form special protein complex known as gluten. Amount of wheat storage proteins as well as their quality is one of the most important factors determining the end-uses of wheat grain. Parameters such as Zeleny sedimentation test, falling number, hardness, water binding capacity, as well as farinograph, extensograph and mixograph parameters, etc., are used to characterize dough properties and the baking quality (Belderok et al. 2000). Wheat starch does not only affect the processing quality of grain but this fraction is important also from nutritional point of view, especially when wheat is the main (or the only) source of energy and nutrients in human diet.

Numerous studies (McKee and Latner 2000, Weickert and Pfeiffer 2007, Rave et al. 2008) have demonstrated the beneficial effects of fiber consumption in protection against heart disease and cancer, normalization of blood lipids, regulation of glucose absorption and insulin secretion and prevention of constipation and diverticular disease. Mixed (1→3),(1→4)-β-D-glucan (referred to as β-glucan) is a component of wheat fiber, which attracts attention of many researchers due to its immuno-stimulating activity (Dalmo and Bøgwald 2008). Although wheat is not generally thought of as a β-glucan source, some studies revealed that β-glucan content in cereal grains is genotype-dependent and high level of variability was found among other cereal crop species such as oat and barley (Ehrenbergerová 2008).

In this work we measured fourteen variables of 44 wheat cultivars originated from 7 countries. The measurements are divided into three groups: analysis of nutrients and health-promoting compounds in grain samples, parameters of technological quality of grain samples and rheological properties of dough. These data were analyzed by means of several statistical/chemometrical tools.

Material and Methods

Wheat samples

Set of 44 wheat (*Triticum aestivum* L.) samples kept in the Genebank Piešťany was investigated. Wheat cultivars originated from seven countries: France, Great Britain, Italy, Russia, Slovakia, Ukraine, United States of America.

Description of the studied data

All investigated samples were characterized by the following variables: starch content (denominated as *StDM*, *StRM*, resp.), fiber content (*fiber*), (1→3),(1→4)-*β*-D-glucan content (*gluc*), protein content (*Prot*), wet gluten content (*glu*), Zeleny sedimentation index (*SedInd*), grain hardness (*Tvr*), farinographic water absorption (*VazVody*), dough development (*Vyv*), dough stability (*Stab*), degree of dough softening (*M10*, *M12*), farinograph quality number (*FQN*).

Categorical variables

Categorical variables representing four different classification criteria: (1) Country of origin, by which the samples are distributed to seven classes designated as 1- France (FRA, 11 samples), 2- Great Britain (GBR, 4 samples), 3- Italia (ITA, 5 samples), 4- Russia (RUS, 4 samples), 5-Slovakia (SVK, 9 samples), 6- Ukraine (UKR, 5 samples), 7- United States of America (USA, 7 samples); (2) Protein content- *Prot* (NIRS method) by which the samples are distributed to three classes designated as 1 (E-best, 20 samples), 2 (A, 21 samples), 3 (B-worst, 11 samples); (3) Wet gluten content- *Lep* (STN 46 1011-9) by which the samples are distributed to three classes designated as 1 (E-best, 42 samples), 2 (A, 7 samples), 3 (B-worst, 3 samples); (4) Dough development- *Vyv* (Farinograph-E: Brabender OhG, Duisburg, Germany, ICC standard 115/1) by which the samples are distributed to three classes designated as 1 (best, 16 samples), 2 (17 samples), 3 (B- worst, 19 samples).

Sample distribution into classes 1-3 for protein content and wet gluten content was performed according to data shown in standard STN (46 1100-2): E-elite class, A-good quality class, B-standard class; sample distribution into classes 1-3 by dough development was performed in accordance to data reported by Dodok and Szemes (1998): 1- strong flour, 2- medium flour, 3- weak flour.

Multidimensional data analysis

Statistical calculations were performed using following techniques: analysis of variance (ANOVA) and linear discriminant analysis (LDA). Commercial software package SPSS (ver. 15) were used for the performed calculations.

Results and Discussion

Analysis of variance (Anova)

Analysis of variance, ANOVA, determines which variables affect the response of the investigated problem and it is one of the predominant statistical methods used to interpret experimental data. It is a technique dividing total variations into their appropriate components (Cvijović et al. 2005).

According to ANOVA results, among the selected variables the largest influence to partitionate the wheat samples into seven groups according to country of origin have: *fiber*, *gluc*, *VazVody*, *Vyv*, *Stab*, *M10*, *M12* and *FQN*. All these effects are significant at the significance level (*p*) 0.05; the importance of the given factor is greater when the *p*- value is smaller. These two kinds of Post Hoc tests were evaluated: the least significant difference (LSD) test and Bonferroni test.

LSD test showed that variable *gluc* separates the class 7 (USA cultivars) from the other classes and the variable *Vyv* separates the class 3 (ITA) from all others. When using the Bonferroni test, only the variable *gluc* was shown to discriminate the class 7 from the other classes.

The following variables were shown to be significant for the categorical variable *Prot*: dry matter (*DM*), starch (*StRM*, *StDM*), fiber (*fiber*) and wet gluten content (*lepDM*), dough development (*Vyv*) and stability (*Stab*), farinograph quality number (*FQN*). According to LSD test, the variable *lepDM* differentiates all the three classes from each other. Class 1, which includes the best (elite) cultivars with the highest content of proteins, is separated from classes 2 and 3 only by variable *Vyv* (dough development), if the LSD test is used. However, if the Bonferroni test is used, the first class is differentiated from the others also by variable *lepDM*. Class 3 is differentiated from the other classes by variable *StDM* (starch) according to both tests. For categorical variable *Lep,* the variables *StDM*, *Tvr* and *Prot* are significant. Only the variable *Prot* can separate the first class (cultivars having the highest level of wet gluten) from the classes 2 and 3, using the LSD test.

Linear discriminant analysis

LDA is one of the most widely used classification procedures. The method maximizes the variance between categories and minimizes the variance within categories. It merely looks for a sensible rule to discriminate between them by forming linear functions of the data maximizing the ratio of the between-group sum of squares to the within-group sum of squares. The linear functions are constrained to be orthogonal. Once the linear functions have been found, an observation is classified by computing its Euclidean distance from the group centroids, projected onto the subspace defined by a subset of the linear functions. The observation is then assigned to the closest group. To assess the performance of this method, the group centroids are estimated using a 'leave one out' cross-validation method. Each observation is removed in turn from the data set and the group centroids calculated without reference to the missing data point. The excluded observation is then classified using these new group centroids. The data point is then replaced and the next observation removed from the data set. This process is repeated until all observations have been left out in turn. Thus, the percentage of observations correctly classified can be ascertained by comparing the true class membership with that estimated by LDA. This provides a good indication of the reliability of the classification method. (Zhang and Wang 2007).

Classification performance depends on the selected categorical target variable. Fig.1 shows the case when categorical variable protein content (*Prot*) was used as the target variable. As shown, 90.9% of the originally grouped objects were correctly classified when the discrimination model was calculated and 75% of the objects were correctly classified using leave-one-out cross-validation method.

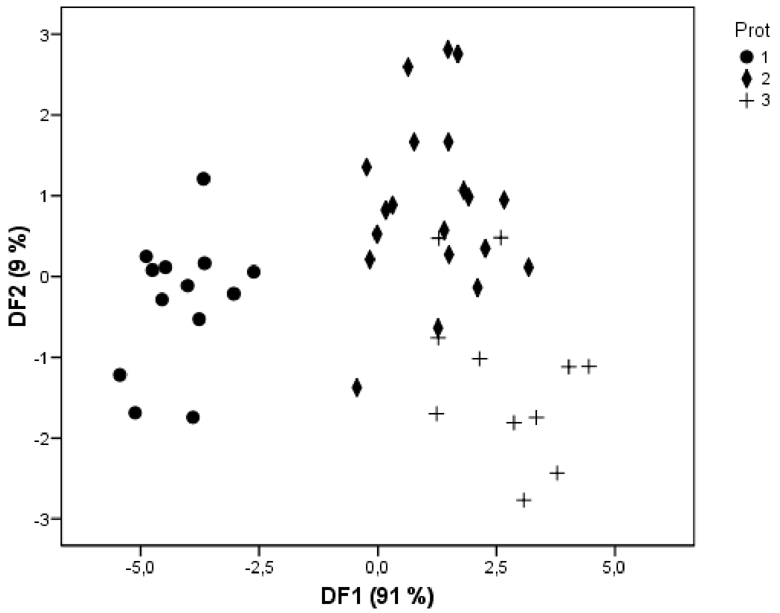

Fig. 1: Plot of discriminant functions (DF's) showing 44 wheat samples clustered by protein content (*Prot*). A 90.9% performance was achieved for the wheat samples classification in discrimination model; 75% performance was achieved for the wheat samples classification using leave-one-out validation. Software SPSS 15. Wheat cultivars were distributed by protein content to three classes in accordance with standard STN 46 1100-2 (classes 1-3 on figure represents STN classes E, A and B respectively). 1= elite class (E), marked with dots; 2= good quality class (A), marked with diamonds; 3= standard class (B), marked with plus signs.

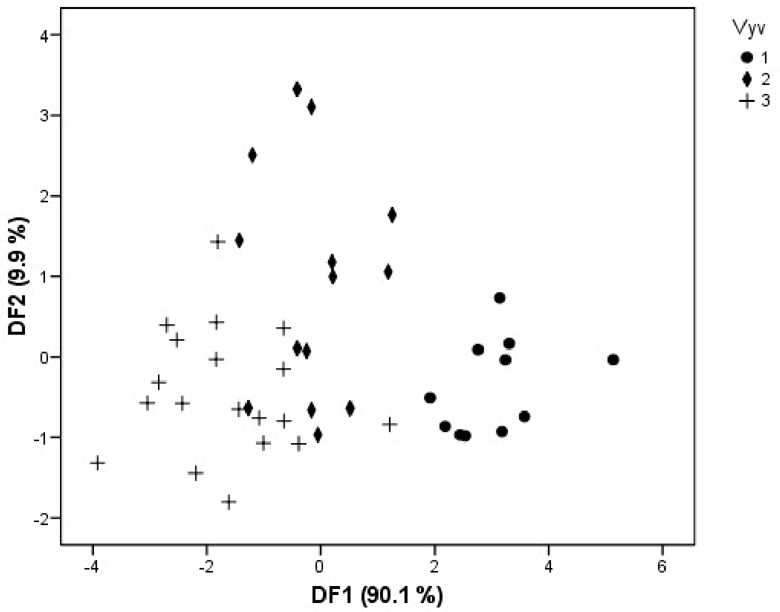

Fig. 2: Plot of discriminant functions (DF's) showing 44 wheat samples clustered by dough development (*Vyv*). A 86.4% performance was achieved for the wheat samples classification in discrimination model; 45.5% performance was achieved for the

wheat samples classification using leave-one-out validation. Software SPSS 15. Wheat cultivars were distributed by dough development values to three classes according to Szemes and Dodok (1998): 1= cultivars with strong flour, marked with dots; 2= cultivars with medium flour, marked with diamonds; 3= cultivars with weak flour, marked with plus signs.

It means that 11 objects out of 44 ones were categorized into a different category then supposed. Classification of wheat samples according to dough development (*Vyv)* was also successful (Fig.2). In this case we observed 86.4% performance for the wheat samples classification in discrimination model and 45.5% performance was achieved for the wheat samples classification using leave-one-out validation. In both cases (*Prot* and *Vyv*) only the class 1 was significantly separated from classes 2 and 3. Successful results obtained by LDA in classification of new wheat genotypes were reported by Kraic et al. (2009).

Conclusion

LSD and Bonferroni tests showed that variable *gluc* (*β*-glucan content) is significant (p=0.05) for the class 7 (American cultivars) and separates this class from the others (categorical variable is country of origin). In the case of categorical variable *Prot*, variable *lepDM* (wet gluten content) was observed to be significant in differentiation of all the three classes from each other (classes 1-3 represent classes E, A and B, respectively, according to standard STN 46 1100-2). For categorical variable *Lep*, the variables *StDM* (starch content), *Tvr* (grain hardness) and *Prot* (protein content) are significant, while only the variable *Prot* can separate the first class (best quality cultivars) from the other classes.

Wheat classification may be conveniently illustrated by linear discriminate analysis, which was proved as an appropriate multidimensional classification technique. Best results were achieved, when categorical variables *Prot* (protein content) and *Vyv* (dough development), respectively, were used as the target variables.

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