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UNIVERSITÀ DEGLI STUDI DI TORINO

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1 **Investigating the use of gradient boosting**
2 **machine, random forest and their ensemble to**
3 **predict skin flavonoid content from berry**
4 **physical-mechanical characteristics in wine**
5 **grapes**

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6 **Abstract**

7 Flavonoids are a class of bioactive compounds largely represented in grapevine and
8 wine. They also affect the sensory quality of fruits and vegetables, and derived products.
9 Methods available for flavonoid measurement are time-consuming, thus a rapid and
10 cost-effective determination of these compounds is an important research objective.
11 This work tests if applying machine learning techniques to texture analysis data allows
12 to reach good performances for flavonoid estimation in grape berries.

13 Whole berry and skin texture analysis was applied to berries from 22 red wine grape
14 cultivars and linked to the total flavonoid content. Three machine-learning techniques
15 (regression tree, random forest and gradient boosting machine) were then applied.
16 Models reached a high accuracy both in the external and internal validation. The R^2
17 ranged from 0.75 to 0.85 for the external validation and from 0.65 to 0.75 for the
18 internal validation, while RMSE ([Root Mean Square Error](#)) went from 0.95 mg g⁻¹ to
19 0.7 mg g⁻¹ in the external validation and from 1.3 mg g⁻¹ to 1.1 mg g⁻¹ in the internal
20 validation.

21

22 **Key-words:** random forest; gradient boosting machine (GBM); wine-grape; flavonoids;
23 texture analysis

24

25 **1. Introduction**

26 Flavonoids are a group of secondary metabolites widely distributed in plants, which
27 greatly affect the sensory and nutritional quality of fruits and vegetables (Harnly et al.,
28 2006). They represent a huge portion of soluble phenols present in grapevine (Braidot et
29 al., 2008). Flavonoids are among the most important compounds for the quality of red

30 wine grapes because of their effect on wine sensory attributes (Ristic et al., 2010 is an
31 example) and aging. The concentration of these compounds in wine depends, among
32 other factors, on the quantity originally present in grapes (González-Neves et al., 2004).
33 In the last ten years, flavonoids have received a very great attention from both
34 researchers and the general audience because of their beneficial effect on human health
35 (Yao et al., 2004). They have shown antioxidant (Lourenço et al., 2008),
36 hypocholesterolemic (Gonzalez et al., 2014) and anti-inflammatory effects (Noll et al.,
37 2009). Their nutraceutical properties are exploited in fresh table grapes, in
38 pharmaceutical and cosmetic products derived from grape, and are a very appealing
39 argument for wine marketing purposes.

40 Red grapes are richer in flavonoids than white ones, but their biosynthesis and
41 concentration greatly depend on cultivar, vineyard practices, soil and climate
42 (Kondouras et al., 2006). Grape maturity, and therefore the harvest date, is also another
43 very important parameter because quantitative and qualitative modifications of tannins
44 and anthocyanins (the two most represented flavonoid families in grape) happen during
45 ripening (Kuhn et al., 2013).

46 Different methods based on spectrophotometry, chromatography, and mass spectrometry
47 are usually used for the determination of flavonoids in fruits and vegetables (see Ignat et
48 al., 2011 for a generic review and Lorrain et al., 2013 for the case of grapes and wine).
49 Regarding grape analysis, these methods are all very accurate but they often require
50 sample preparation and long analysis times. The problem is especially the time required
51 for the extract preparation and purification, which has to be made by hand and can
52 require berry peeling, solvent extractions, and other manipulations that strongly increase
53 costs and limit the number of acquirable data. Industry and research will greatly benefit
54 from a rapid and cost effective method to obtain a faster screening of flavonoids in

55 grapes. Such a method is at today lacking, although recently great advances have been
56 made in this field by the use of Near InfraRed (NIR) spectroscopy coupled to
57 chemometrics, in particular using partial least squares (PLS) regression models (Ferrer-
58 Gallego et al., 2011, Rolle et al., 2012a, Cozzolino 2015).

59 During grape ripening, berries change not only their chemical composition, but also
60 their mechanical properties: they soften, become less resilient, and the skin generally
61 harden (Rolle et al., 2012b). In industry, these textural modifications are currently
62 evaluated by sensory panels to help in the choice of the harvest date. Texture Analysis
63 (TA) has shown to be an effective instrumental technique for an accurate evaluation of
64 physical-mechanical characteristics of grapes (Letaief et al., 2008, Giordano et al.,
65 2013, Battista et al., 2015). It is cost-effective as it [does not](#) require long times and
66 reagents for sample preparation and analysis.

67 Although flavonoids and texture parameters belong to different grape properties, their
68 values are both influenced by the berry ripening process. The phenolic ripeness of grape
69 skin was found to be well assessed when the TA values were used (Río Segade et al.,
70 2008), but the possibility of a predictive model has been never investigated, and neither
71 an evaluation of possible chemometrics approaches to these parameters exists. A model
72 linking the differences in berry mechanical properties and chemical composition
73 induced by the grape ripeness could be an alternative to NIR methods for rapidly
74 assessing the flavonoid contents at the berry level.

75 TA data are different from those obtained with NIR. In the first method, the number of
76 measured parameters available as predictors is limited, and it is generally lower than the
77 number of observations, i. e. the dataset is in a long format. Conversely, NIR datasets
78 are wider, the number of wavelengths available as predictors is large and therefore PLS,
79 a regression algorithm well suited to these situations, has been extensively applied

80 (Cozzolino 2015). With the reduced number of predictors present in TA, other learning
81 algorithms could be effectively applied as an effort to better exploit the available
82 information.

83 In this work, we will evaluate the use of regression trees and of two ways of combining
84 them in order to achieve greater performances in predictions: Random Forest, RF
85 (Breiman 2001), and gradient boosting machine, GBM (Friedman 2001). RF has shown
86 to be a state-of-the art method, allowing the highest accuracy, but it is still not
87 widespread to date. According to a [recent review by Scott et al., 2013](#) for chemometric
88 classification problems (286 reviewed papers), RF is used in only 4.5% of the articles
89 where machine-learning algorithms are applied. The same source evidences that
90 boosting algorithm is even less used (1%).

91 The aim of the work was to evaluate different chemometric approaches in the evaluation
92 of data obtained from parameters influenced by the grape ripening process, such as
93 berry mechanical properties data and flavonoid content in berry skins. For this, the
94 performances of RF and GBM algorithms were compared on a large dataset composed
95 of approx. 800 berries belonging to 22 grapevine cultivars, their suitability for flavonoid
96 content prediction in grape berries was evaluated on the basis of mechanical properties,
97 and an informal explanation of the underlying algorithms was suggested. Furthermore, a
98 predictive model was also developed. This approach could be used as an example for
99 other compounds and fruits.

100

101 **2. Materials and Methods**

102 **2.1 Grape sampling**

103 Grapes from 22 red grapevine cultivars (*Vitis vinifera* L.) were sampled in the CRA-VIT

104 experimental collection (1.2 ha) located in Susegana (TV), Veneto Region (North-East
105 Italy), in 2010 and 2011. Vines were 15 years old, grafted on SO4 rootstock
106 (interspecific cross between *Vitis riparia* Michx. and *Vitis berlandieri* Planch.), and
107 planted at 3.0 m between rows and 1.5 m between vines. They were Sylvoz pruned and
108 trained with a vertical shoot position system. For each cultivar, samples were composed
109 of approx. 3 kg of grape berries, which were picked up randomly from ten vines. In
110 order to successfully compare berries at ripeness with adequate sugar content, the
111 berries were calibrated using a densimetric method by berry flotation in different saline
112 solutions (Rolle et al., 2011). This study was carried out only on the berries with sugar
113 contents comprised between 183 ± 8 g L⁻¹ and 217 ± 8 g L⁻¹ corresponding to $11.0\pm 0.5\%$
114 (v/v) and $13.0\pm 0.5\%$ (v/v) potential alcohol, respectively.

115 The sorted berries were visually inspected before analysis; those with damaged skins
116 were discarded. For each variety studied, a sub-sample of 36 sorted berries (therefore a
117 total of 792 berries for all cultivars together) was randomly selected for the
118 determination of the physical-mechanical properties and then for the flavonoid content.
119 As described in the successive section, single berries measurements were then averaged
120 by three to compose a single sample for predictive modeling.

121

122 **2.2 Physical and mechanical properties**

123 Grape berries were singularly weighed, with an analytical laboratory balance Radwag
124 AS 220/X (Radwag, Radom, Poland), and then a Texture Profile Analysis (TPA) non
125 destructive mechanical test was performed for each of them as described by Letaief et
126 al., 2008. It allowed the measurement of berry hardness (N, as H), cohesiveness
127 (adimensional, as Co), gumminess (N, as G), springiness (mm, as S), chewiness (mJ, as
128 Ch) and resilience (adimensional, as R). A puncture test (Letaief et al., 2008) was then

129 carried out on the same berries taken singularly to measure skin break force (N, as F_{sk}),
130 skin break energy (mJ, as W_{sk}) and skin resistance to axial deformation ($N\ mm^{-1}$, as
131 E_{sk}). All these measurements were performed on the equatorial position of whole berry,
132 while skin thickness (μm , as Sp_{sk}) was measured in the skin after manual removal from
133 the pulp with a razor blade (Letaief et al. 2008, Río Segade et al. 2011a). Analyses were
134 made with a Universal Testing Machine (UTM) TAxT2i texture analyzer (SMS-Stable
135 Micro Systems, Godalming, Surrey, UK) equipped with a 5 kg load cell and a HDP/90
136 platform. A SMS P/35 flat probe under 25% deformation, with a waiting period of 2s
137 between the two compressions and a speed of $1\ mm\ s^{-1}$, was used for the TPA test. A
138 SMS P/2N needle probe, with a test speed of $1\ mm\ s^{-1}$ and a penetration depth of 3 mm,
139 was used for the puncture test. A SMS P/2 flat probe, with a test speed of $0.2\ mm\ s^{-1}$
140 was used to measure Sp_{sk} . All data were acquired at 400 Hz and evaluated using the
141 Texture Expert Exceed software, version 2.54.

142

143 **2.3 Skin flavonoid content**

144 After the skin thickness test, each berry skin was individually immersed for 4 hours in
145 5 mL of a buffer solution containing 12% v/v ethanol, $2\ g\ L^{-1}$ of $Na_2S_2O_5$, $5\ g\ L^{-1}$ of
146 tartaric acid and adjusted to pH 3.20 with NaOH (Di Stefano et al., 1991). Each skin
147 was then homogenized at 8000 rpm for 1 min with an Ultraturrax T18 (IKA
148 Labortechnik, Staufen, Germany), and the extract was centrifuged for 10 min at $3500 \times$
149 g and $20\ ^\circ C$. The supernatant was then used for analysis after dilution with an ethanolic
150 solution of HCl (70:30:1, ethanol:water:HCl, v/v) (Di Stefano et al., 1991). Total
151 flavonoid index (TF) was determined by a spectrophotometric method, [reading the](#)
152 [absorbance at 280 nm](#), using an Uvmini-1240 PC spectrophotometer (Shimadzu
153 Scientific Instruments, Columbia, MD, USA) and expressed as $mg\ g^{-1}$ berry of (+)-

154 catechin (Rolle et al., 2011, Di Stefano et al., 1991).

155 **2.4 Predictive modelling**

156 **2.4.1 Description of the used machine-learning techniques**

157 The relationship between predictors and the outcome was modeled using Regression
158 Trees, RT (Breiman et al., 1984) and two derived techniques: RF (Breiman, 2001) and
159 stochastic gradient boosting with trees as base learners; the latter will be here called
160 Gradient Boosting Machine (GBM) in reference to the work where this technique first
161 appeared (Friedman, 2001). A comprehensive description of these techniques cannot be
162 given in few words, nevertheless the following paragraphs will try to briefly and lightly
163 introduce the subject. Readers interested in more technical details can find worthwhile
164 information in (Hastie, 2009) and in the help and vignettes of the cited R packages.

165 Regression trees are rule based models that split the whole dataset in groups where data
166 tend to be homogeneous with respect to the response. In the technique used in this work,
167 which is known as Classification And Regression Tree, CART (Breiman et al., 1984),
168 data in the terminal nodes (the final groups that are no further partitioned) are simply
169 averaged to predict the outcome. At the beginning, the entire dataset is split in two
170 groups to minimize the overall sum of squares, by searching every value of every
171 predictor. The technique is then recursive, these two groups are split again in two parts
172 each to further reduce the prediction error, according to the available predictor values.
173 This technique is also known as recursive partitioning because of its iterative nature.
174 The number of groups duplicates at each split until the terminal nodes are so small that
175 they cannot be further partitioned. However, these “full grown” trees generally overfit,
176 in the sense that they tend to fit the noise other than the structure in the training data.
177 Therefore, they achieve poor performances on the validation data despite having great
178 performances on the training data. Their growth must therefore be controlled, and this

179 can be obtained by cross-validation procedures. Cross-validation is a form of internal
180 validation, which is based on the use of a fraction only of the whole training data to
181 develop the model, while using the remaining part for the validation. In k-fold cross
182 validation, the training dataset is divided in k parts; k-1 parts are used to fit the model
183 and the kth part is used to evaluate the structure of the model on simulated new data. The
184 procedure is then iterative, and all k parts serve as validation once at a time. This allows
185 determining the size of the trees enabling the best results on future unseen data.

186 A characteristic of regression trees is their instability, their structure can greatly vary
187 with the data available for modeling. This property can appear at a first sight a
188 deficiency of the method, instead it has become to be really useful and extremely well
189 exploited by two state-of-the-art techniques in statistical learning such as bagging and
190 boosting. These techniques are based on the “perturb and combine” strategies (Breiman,
191 1996a) and on the idea that combined learners can outperform single ones. For this
192 combination to be effective, single learners must be able to capture a part of the
193 structure in the data that is not modeled by other learners. The plasticity of trees can be
194 exploited for this purpose: by artificially varying the available data through re-sampling
195 techniques, they can be induced to learn different aspects of the dataset. Partial
196 predictions from ensemble of trees are then combined to obtain the final predictions.
197 Bagging (Breiman, 1996b) and boosting (Freund & Schapire 1997) are two ways of
198 combining learners. In bagging, trees are grown in parallel on a part of the available
199 data, and predictions are then averaged across all trees. However, in boosting, trees are
200 grown sequentially, and each successive tree models the residuals of the previous tree
201 predictions. Bagging and boosting are the two techniques that, further optimized by
202 increasing randomization, are respectively used in RF and GBM. In RF, trees are grown
203 on re-sampled subsets of the training data by using only some of the available

204 predictors, randomly chosen at each split. Final predictions for each tree are then
205 averaged. This parameter is called *mtry* and has to be set by the user, as well as the
206 number and depth of trees in the forest. In GBM, trees are sequentially built to reduce
207 the errors of the previous trees, but residuals are resampled and just a fraction is
208 available for modeling at each iteration. Furthermore, learning is regularized through
209 shrinkage, i.e. learning rate is slowed by allowing the use of just a fraction of the whole
210 value for each residual. As occurred in RF, even in GBM, the number and depth of trees
211 have to be selected by the user. Parameter selection, also called parameter tuning, is
212 generally made using cross-validation or bootstrap techniques in order to minimize the
213 performances of the algorithm on simulated new data, being not the error on the training
214 set a robust choice because of overfitting.

215

216 **2.4.2 Details about the used procedure**

217 A predictive model was built to predict the flavonoid content in berry skin using
218 physical and mechanical properties of the whole berry and skin as inputs. The 792
219 berries data (36 berries x 22 cultivars) were averaged by three, randomly selected inside
220 the same cultivar, to obtain 264 averaged samples (12 samples composed by 3 berries
221 for 22 cultivars). Prior to model fitting, data were partitioned and a random approx. 20%
222 of data (53 samples) were left out from the training set for later use as test set. Data
223 were then centered and scaled. In this work, models were tuned using 10 repetitions of 5
224 folds cross-validation in order to optimize the Root Mean Square Error (RMSE) on the
225 resampled data (more than 10 000 possible combinations were evaluated). Performances
226 of the models were then compared on the same set of 100 bootstrap re-samples always
227 using RMSE as a metric.

228 Data were analyzed with the R statistical software 3.1.2 (R Core Team, 2014) using the

229 packages rpart (Therneau et al., 2015), randomForest (Liaw & Wiener, 2002), gbm
230 (Ridgeway, 2013), caret (Kuhn, et al., 2014).

231 **3. Results and Discussion**

232 **3.1 Descriptive analysis**

233 Fig. 1 shows the TF content for the 22 cultivars used in the experiment. Raboso,
234 Ancellotta and Teroldego had the highest amount of TF in the skin of fresh berries (with
235 a median of 8.72, 6.52 and 5.35 mg g⁻¹ berry, respectively) but also had the highest
236 variance (1.52, 4.20 and 0.71 mg g⁻¹ berry, respectively). Gamay, Schiava gentile and
237 Aleatico had the lowest concentration in these compounds (with a median of 0.97, 0.91
238 and 0.98 mg g⁻¹ berry, respectively) and the lowest variance (0.01, 0.01 and 0.01,
239 respectively). In the global dataset (Table 1), TF had a mean of 2.60 mg g⁻¹ berry, a
240 median of 2.07 mg g⁻¹ berry and a variance of 4.16 mg g⁻¹ berry. The registered
241 minimum was 0.69 mg g⁻¹ berry (Aleatico), while the maximum was 12.87 mg g⁻¹ berry
242 (Ancellotta). Descriptive statistics for the physical-mechanical characteristics in the
243 global dataset is shown in Table 1. Data were in agreement with those reported in
244 scientific literature in several works (Zouid et al., 2013, Letaief et al., 2008, Río Segade
245 et al., 2011a).

246 Table 2 shows Pearson correlations in the global dataset. Being TF the outcome of the
247 developing model, good correlations with the available predictors would be welcomed,
248 but *r* values for this variable were moderate. BW and S showed the highest correlations
249 with TF (*r* values of -0.59 and -0.53, respectively, *p*-value < 0.001), followed by E_{sk} and
250 Sp_{sk} (*r* values of 0.34 and 0.34, respectively, *p*-value < 0.001). The less related
251 predictors were W_{sk}, H and G, which did not show significant correlations. It should be
252 noticed that the last two variables were well related to the anthocyanin extractability in
253 the study published by (Zouid et al., 2013). In the present work, the number of cultivars

254 taken in account is greatly higher compared to the cited work, where only Cabernet-
255 Franc was measured. Given the lack of significance, it could be hypothesized that the
256 relation is not uniform but depends on the cultivar. The Spearman's method, used to
257 highlight possible monotonic, but non-linear relations with TF, did not give association
258 values higher than those already observed (data not shown).

259 The strongest correlations observed in the dataset (r values higher than 0.75, p -value <
260 0.001) were those among the physical-mechanical predictors (H with G and Ch; F_{sk} with
261 W_{sk} and E_{sk} ; BW with S and SW), which is a consequence of the way they were
262 measured or calculated (Letaief et al., 2008). H, G and Ch were strongly positive-related
263 because G and Ch were calculated from H. Therefore, harder berries were also more
264 gummy and chewy. Considering skin related mechanical properties, F_{sk} corresponds to
265 the skin resistance to the needle probe penetration, while W_{sk} is represented by the area
266 under the force/time curve. E_{sk} is defined as the slope of the stress–strain curve in the
267 linear section. W_{sk} and E_{sk} were strongly positive-related to F_{sk} , so stiffer skins were
268 also more resistant to the penetration and therefore harder. Furthermore, heavier berries,
269 which are also bigger ones, had higher value of S and had, obviously, higher amount of
270 skin. BW was retained instead of S because the relationship of BW with TF is well
271 known in the literature.

272 It is important to highlight that the sugar content of berry showed some significant
273 relations (alpha risk < 0.1) with other variables in the dataset, table 2, but the correlation
274 was strong with none of them. The effect of stage of ripening on mechanical properties
275 values was in general less determining in comparison to variety effect (Rio Segade et
276 al., 2008). Cultivar variability of these properties across the 22 cultivars studied clearly
277 dominated. Before continuing, it should be cleared that even if the correlations in Table
278 2 let to make an idea of the main relationships in the dataset, possible multidimensional

279 relations were not taken into account. As an example, it seems logical that total skin
280 weight could be the result of a linear combination between the berry size and the skin
281 thickness for each berry. SW was highly related to a combination of BW and Sp_{sk} with a
282 r value of 0.87. This value was clearly higher than those of the single relations, being
283 probably redundant the information of SW if used in a model also containing BW and
284 Sp_{sk} .

285

286 **3.2 Predictor filtering**

287 Sensibility to correlated predictors depends on the used statistical learning technique,
288 but it is generally not welcomed because redundant and non informative inputs reduce
289 model performances. When inference is the objective, the negative effect of correlated
290 variables is even worse than for predictions alone. Furthermore, the measurement of a
291 greater number of variables in order to apply a model would increase costs and time,
292 and therefore a justification is required. Any of the three used learning techniques (RT,
293 RF, GBM) completely fail when correlated predictors are present, the less sensitive
294 technique probably being GBM because it shrinks effect estimates (Maloney et al.,
295 2012), and the most sensitive one being RF (Strobl et al., 2007). In general, tree based
296 techniques implicitly run feature selection because, if a predictor does not permit to
297 reduce the residual sum of squares at any tree split, its contribution to the model is zero.
298 However, if highly correlated predictors are present, the choice between them is
299 somewhat random because they similarly reduce the sum of squares, and have a similar
300 probability to be chosen for a given split. In RF, where an $mtry$ number of predictors is
301 sampled at each split (see section 2.4), the presence of correlated predictors increases
302 the chance to sample similar information. It reduces randomization and therefore
303 independence across trees; important assumption to optimize performances. In addition,

304 it dilutes the importance of key predictors and increases the importance of weak
305 variables correlated to important ones (Strobl et al., 2007).

306 To account for these problems and to optimize model performances, predictors were
307 first filtered to avoid correlation levels higher than 0.7 (according to Pearson correlation
308 coefficients, Table 2) and therefore to reduce redundancy. The relationships of the
309 predictors with the outcome were not considered for selecting predictors in this first
310 phase. Feature selection was indeed performed successively using Recursive Feature
311 Elimination (RFE). Four predictors were eliminated by this filtering step, which were
312 F_{sk} , W_{sk} , H, and G. F_{sk} and W_{sk} were highly related ($r = 0.92$, $p < 0.001$). W_{sk} was not
313 related to TF, contrarily to F_{sk} , but this last was also strongly related to E_{sk} ($r = 0.81$, $p <$
314 0.001). A previous study has reported that E_{sk} is related to cellular maturity index
315 (EA%) as predictors of anthocyanin extractability (Río Segade, et al., 2011b). Among
316 H, G and Ch ($r = 0.91-0.97$, $p < 0.001$), this last was retained because it was also well
317 related to anthocyanin extractability (Zouid et al., 2013). The information provided by
318 SW in a model can be well approximated by a combined use of BW and Sp_{sk} , as
319 previously explained. Furthermore, Sp_{sk} is considered as main texture parameter to
320 predict anthocyanin extractability in winegrapes (Río Segade et al., 2011c). The final set
321 of filtered predictors included BW, E_{sk} , Co, Sp_{sk} , Ch, W_{sk} , and R.

322 **3.3 Recursive feature elimination and model tuning**

323 Recursive feature elimination (RFE) (Guyon et al., 2002), a backward selection
324 algorithm, was used in the way optimized by Ambroise & McLachlan 2002, and
325 therefore including feature selection in the model building process. Predictors
326 elimination was evaluated on the basis of the performances achieved on re-sampled sets
327 obtained by k-fold cross validation ($k = 5$). The process was run for RT, RF, and GBM,
328 and models were also tuned to optimize performances during the process (see section

329 2.4). RT, RF, and GBM were all tuned using the same set of re-samples therefore
330 ensuring consistency in the evaluation and allowing comparison across model
331 performances.

332 In all three cases (RT, RF, and GBM), RFE suggested the use of all seven available
333 predictors (BW, E_{sk} , Co, Sp_{sk} , Ch, W_{sk} , and R), and therefore all of them had some
334 influence on the techniques evaluated. The relative predictor importance in all models is
335 shown in Table 3. In this table, the influence was scaled between 0 and 100 to allow an
336 easier comparison between models, but as already stated some of the selected predictors
337 had zero influence. The 0 and 100 are relative values obtained by subtracting the
338 minimum registered influence (across all predictors) from the individual influence for
339 each predictor, and then by dividing for the difference between the maximum and the
340 minimum registered influence. The influence of each predictor in the model varied
341 according to the model. Considering a single tree (RT), the overall relative influence of
342 each predictor was higher, because all predictors were used once or few times, and this
343 avoided the predominance of very strong predictors such as BW. In RT, Sp_{sk} was the
344 predictor that allowed the greatest error reduction. In ensembles, and with the
345 perturbation of data imposed in RF and GBM methods, the influence of some strong
346 predictors popped up and seems to take advantage over the others. This was more
347 evident in GBM than in RF, which had an intermediate behavior. These comments are
348 valid only for this study.

349 Model tuning suggested the use of 7 splits for RT, 1000 trees and $mtry = 4$ for RF, 5000
350 trees having 4 splits each and a shrinkage of 0.005 for GBM. Fig. 2 shows the tuned RT
351 with the aim of illustrating the basic element also composing RF and GBM ensembles.
352 Single trees are very easy to interpret and to allow making an idea of the relationships in
353 the dataset. It is important to remember that they are fairly unstable, and small

354 perturbations in the dataset can completely change their structure. Therefore, trees just
355 describe relationships relative to the data observed, and interpretations are difficultly
356 generalizable. This is especially true for the lower splits. However, it is worthwhile to
357 note that Sp_{sk} , which was the variable with the largest influence for RT (Table 3), acts in
358 a controversial fashion. For the smallest berries, which were also the richest in
359 flavonoids, a higher Sp_{sk} indicated a lower content of TF, while for the biggest berries,
360 the inverse was true. It is also important to note the role of BW, which was negatively
361 related to the amount in phenolic compounds as widely discussed in the literature
362 ([Barbagallo et al., 2011](#)). Also E_{sk} seems to be an important parameter because elastic
363 skins were associated to higher content in TF. BW, E_{sk} , and Sp_{sk} were the predictors
364 with the highest influence in all models (Table 3).

365

366 **3.4 Model comparison**

367 Results of the tuned models are shown in Table 4 for both training and test data and for
368 the cross-validated re-samples. It appears that all algorithms, starting from RT, tended to
369 overfit the training set, which is probably a consequence of a training set too small
370 when compared to the complexity of the relationships among predictors and between
371 these and the outcome, as suggested by the weak correlations observed in Table 2.
372 Despite this, the model accurately predicted the test set used as external validation.
373 Predictions for the test set exceeded those obtained with 5-fold cross-validation, which
374 can be considered an internal validation. Test sets are considered the ultimate proof of
375 model performances, often neglecting cross-validation and bootstrap assessment
376 methods. However, observations like the present one make us think about the method to
377 prefer in model assessment. The performances observed over a test set could also be
378 attributed to random select observations easier to predict than those contained in the

379 training set used in cross-validation. Resampling methods are more robust from this
380 point of view, but they can be upward (i. e. pessimistic) biased, especially the bootstrap,
381 even if an alternative to avoid such bias is available, but only for classification problems
382 (Efron & Tibshirani 1997).

383 Fig. 3 shows the predictions on the [train and test sets](#) for all methods. Figs. 3a and 3b
384 shows the blocky structure used in prediction by RT, where similar data were just
385 predicted by the mean of the group they belong according to the rules in Fig. 2, and are
386 therefore grouped also in predictions. In GBM and RF ensembles, the predictions are
387 averaged from many trees and allow the methods to be more adaptable to the form of
388 data and to also model non-linearity (and interactions). In Figs. 3c/d and 3e/f,
389 predictions were no longer grouped for the same values of predictions. Comparing
390 Figs 3c/d with 3e/f, it appears that both RF and GBM methods well predict the test set,
391 but predictions, as shown by the location of points in the scatterplots, although similar
392 were not exactly identical. Predictions obtained on the same re-sampled data by GBM
393 and RF were highly correlated (0.82), however looking at Table 3 it appears that they
394 did not make use of the same predictors in the same way. It will be possible that
395 combining both methods in a single ensemble will boost the overall accuracy a little bit.
396 These algorithms were combined by weighted average of their predictions, using a
397 greedy optimization method as described in (Caruana et al., 2006). Combining methods
398 in a single ensemble of models has the highest efficacy when algorithms are different,
399 and therefore predictions uncorrelated. It is not the case here, where these assumptions
400 are not really respected. However, the combination of RF and GBM brings to a nice
401 improvement in model predictions. GBM and RF predictions were weighted 0.51 and
402 0.49, respectively, for averaging, and the resulting RMSE of their ensemble was 1.05
403 mg g^{-1} , which was slightly lower than that obtained by single methods (Table 4). The

404 result on the test set for the RMSE was 0.701 mg g^{-1} and for R^2 was 0.85. The
405 corresponding predictions on the train set are in Fig. 3g and in the test set are shown in
406 Fig. 3h.

407 To compare the results of this work with others found in the literature is somewhat
408 difficult, because the use of texture analysis to predict flavonoid content in grape berries
409 is novelty, and also a so varied dataset, containing 22 cultivars, is rare to be found.
410 Texture analysis was already used to develop rapid method for the evaluation of total
411 phenolic content and phenol extractability in grape seeds with a good accuracy (Rolle et
412 al., 2013), and in skins but limited to the anthocyanin content (Rolle et al., 2012b, Rio
413 Segade 2011c). In grape berries, however, a rapid evaluation of the phenolic content has
414 generally been made using NIR spectroscopy, and several works have reached very
415 good performances (Ferrer-Gallego et al., 2011). This work was performed on a single
416 cultivar (Graciano), and data were expressed in mg g^{-1} of berry skins. In the present
417 work, data were expressed in mg g^{-1} of whole berry, which from an industrial point of
418 view could be more practical. The results of the last two studies are therefore not
419 directly comparable.

420 The results obtained showed that RF and GBM, and even their average can reach a very
421 high accuracy for TF prediction from physical-mechanical data obtained for many
422 different cultivars. RF is simpler to perform and accurately tune than GBM.
423 Furthermore, its use of features in the dataset less overfitted BW influence.

424 However, even if the performances of those algorithms were very high, it is also true
425 that for real world application, model performances were still too low to be practically
426 used in a generalized way. Results obtained with prediction could be useful for the
427 comparison of the phenolic maturity of different vineyards, but at this time they were
428 hardly suitable for the monitoring of TF during ripening for cultivars with low amounts

429 of flavonoids. Conversely, they could be used for those cultivars with very high
430 amounts of flavonoids (such as Raboso, Ancellotta and Teroldego), because a reduced
431 relative error in prediction.

432 It is possible that, being the physical-mechanical characteristics linked to total
433 flavonoids in a way that depends on the cultivar and is not universal, cultivar-specific
434 calibration will be necessary to improve model performances. This will probably allow
435 the use of TA to monitor grape ripening even for cultivars with low amount in
436 flavonoids. Cultivar- specific calibration or the inclusion of the cultivar as a categorical
437 term in the developed models was not possible in this work because the number of
438 observations by cultivar was too low.

439 To further increase model accuracy, it will also be interesting to test the average of more
440 than three berries for a single sample in order to improve the accuracy in the TA
441 predictors. It could also be interesting to normalize the results using other properties or
442 evaluated parameters. Finally, it will be important to acquire more data and to develop
443 cultivar-specific calibrations. Indeed, except BW, which had a homogeneous behavior
444 for all 22 cultivars in the dataset, other physical-mechanical parameters greatly varied
445 by the cultivar, and general patterns were weak.

446

447 **4. Conclusions**

448 This work collected and assessed a large and varied dataset of texture analysis data and
449 flavonoid content from the analysis of every single berry. It tried to evaluate different
450 machine-learning algorithms to assess their suitability to model the relationships
451 between physical-mechanical characteristics of grape and the concentration of skin
452 flavonoids. The reason for modeling such a relation is that grape berries show changes
453 in their physical-mechanical properties during ripening, which are variety dependent.

454 The approaches evaluated here (RF and GBM) are state-of-the art techniques, but have
455 still rarely been used in chemometrics. This work brings an interesting case-study while
456 also trying to simply and informally explain the way these methods work, starting from
457 their basic element, RT. It will serve as an introduction and will offer some valuable
458 insights for food scientists interested in learning more about these techniques or
459 searching for domain-specific examples of application.

460 Presented models are able to capture a huge portion of the variability in the dataset, as
461 shown by the reached R^2 and accuracy (given by the RMSE), and they can be useful for
462 a fast screening of many cultivars, because it does not ask for sample preparation and
463 extraction, but not yet for fine measurements. It should also be considered that, even if
464 the number of cultivars in this study was high, universal considerations cannot be
465 inferred because, as already reported in the discussion, the evolution of physical-
466 mechanical parameters with ripening could be different across cultivars. Therefore it is
467 probable that conclusions obtained from this study could be different when developing
468 models for a single cultivar, especially in the role and importance of the used physical
469 predictors. It is also highly probable that machine-learning techniques, once applied on
470 single cultivars or on groups of cultivars presenting a similar evolution of physical-
471 mechanical properties with the ripening, will reach outstanding performances and could
472 allow a rapid and accurate estimation of ripening-influenced parameters like TF in grape
473 berries.

474 **Abbreviations**

475 **BW** Berry Weight

476 **CART** Classification And Regression Tree

477 **Co** Cohesiveness

478 **Ch** Chewiness

479 **E_{sk}** Skin Young's modulus

480 **F_{sk}** Skin break force
481 **G** Gumminess
482 **GBM** Gradient Boosting Machine
483 **H** Hardness
484 **R** Resilience
485 **RF** Random Forest
486 **RFE** Recursive Feature Elimination
487 **RT** Regression Tree
488 **S** Springiness
489 **Sp_{sk}** Skin thickness
490 **SW** Skin Weight
491 **W_{sk}** Skin break energy
492 **TA** Texture Analysis
493 **TF** Total Flavonoids Index

494

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Table 1. Descriptive statistics for the global dataset of physical-mechanical properties and total flavonoid content composed of 792 berries from 22 red wine grape cultivars.

	Min.	Max.	Mean	Median	Var.
BW (g)	1.31	4.13	2.57	2.54	0.331
F_{sk} (N)	0.18	1.01	0.65	0.66	0.024
W_{sk} (mJ)	0.11	1.47	0.64	0.64	0.040
E_{sk} (N mm⁻¹)	0.15	0.47	0.29	0.29	0.004
Sp_{sk} (μm)	122.33	315.00	209.69	201.00	1599.699
SW (g)	0.12	0.45	0.26	0.25	0.005
H (N)	1.36	5.68	3.19	3.05	0.655
Co (adimens.)	0.60	0.89	0.79	0.80	0.003
G (N)	1.13	4.45	2.51	2.43	0.377
S (mm)	1.62	3.00	2.43	2.48	0.069
Ch (mJ)	1.86	11.89	6.21	6.01	3.193
R (adimens.)	0.31	0.51	0.45	0.41	0.001
TF (mg g⁻¹)	0.69	12.87	2.60	2.07	4.164

Table 2. Pearson correlations for the global dataset of physical-mechanical properties, total flavonoid and total soluble solids content obtained from 792 berries from 22 red wine grape cultivars

	BW	F _{sk}	W _{sk}	E _{sk}	Sp _{sk}	SW	H	Co	G	S	Ch	R	TSS
BW													
F_{sk}	-0.13 *												
W_{sk}	0.04 ***	0.92 ***											
E_{sk}	-0.29 ***	0.81 ***	0.54 ***										
Sp_{sk}	0.06	-0.07	-0.12	0.03									
SW	0.76 ***	-0.21 ***	-0.11	-0.25 ***	0.46 ***								
H	0.17 **	0.54 ***	0.30 ***	0.75 ***	0.06	0.14 *							
Co	0.03	-0.11	-0.06	-0.17 **	-0.01	0.08	-0.22 ***						
G	0.19 **	0.53 ***	0.31 ***	0.73 ***	0.05	0.16 **	0.97 ***	0.01					
S	0.88 ***	-0.06	0.02	-0.10	-0.06	0.62 ***	0.31 ***	0.15 *	0.36 ***				
Ch	0.44 ***	0.42 ***	0.26 ***	0.57 ***	0.04	0.35 ***	0.91 ***	0.05	0.95 ***	0.61 ***			
R	0.06	-0.23 ***	-0.15 *	-0.29 ***	-0.20 **	0.01	-0.38 ***	0.58 ***	-0.24 ***	0.25 ***	-0.14 *		
TSS	-0.11	-0.01	-0.02	0.01	-0.02	0.00	-0.05	0.04	-0.05	-0.11	-0.07	0.04	
TF	-0.59 ***	0.13 *	-0.03	0.34 ***	0.34 ***	-0.18 **	0.00	-0.13 *	-0.03	-0.53 ***	-0.20 **	-0.19 **	0.03

*** = p -value < 0.001, ** = p -value < 0.01, * = p -value < 0.05, . = p -value < 0.1

Table 3. Relative influence of each predictor in all tested algorithms. Influence was scaled between 0 and 100 to allow an easier comparison.

	RT	GBM	RF
C	0.00	6.20	4.23
R	17.00	0.00	0.00
W_{sk}	51.25	1.31	0.98
Ch	35.41	2.79	15.80
Sp_{sk}	56.41	3.49	3.03
E_{sk}	100.00	4.77	26.77
BW	42.07	100.00	100.00

Table 4. Results (R^2 and Root Mean Squared Error, RMSE) of the tested algorithm on the training set, the external validation (test set) and the internal validation (10 repetitions of 5-fold Cross-Validation, CV). For cross-validation estimations of the standard deviation for both metrics are also shown. RMSE results are expressed in mg g^{-1} berry, lower the error better the performances of the model.

	Train RMSE	Train R2	Test RMSE	Test R2	CV RMSE	CV R2	CV RMSE SD	CV R2 SD
RT	0.817	0.849	0.951	0.752	1.286	0.650	0.198	0.101
RF	0.419	0.965	0.729	0.836	1.071	0.754	0.148	0.063
GBM	0.364	0.971	0.745	0.836	1.074	0.753	0.147	0.058

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E_{sk}	100.00	4.77	26.77
BW	42.07	100.00	100.00

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GBM	0.364	0.971	0.745	0.836	1.074	0.753	0.147	0.058

Figure Captions:

Fig. 1. Flavonoid content for all cultivars in the experiment. Flavonoid content ($\text{mg g}^{-1}_{\text{berry}}$) for the 22 red wine grape cultivars used in the experiment.

Fig. 2. Best regression tree model to predict total flavonoids from texture analysis data Figure representing the tuned RT on the training dataset. The whole training dataset is recursively splitted in two parts, according to the predictor that allows the greatest reduction in the residual sum of squares. The selected predictor at each split is shown inside the ellipse, while just under there is the rule used for splitting which is a corresponding predictor value. Here numbers are expressed in the original measure unit of each predictor, readers are kindly referred to table 1 for the complete list. The optimal number of splits according to the results of the cross-validation procedure was equal to 7.

Fig. 3. Results of the machine-learning techniques on train and test data-sets. Relationships between observed and predicted TF data (mg g^{-1}) over the train test and the test set used as external validation for all algorithms. Solid black line is the identity line, while the dashed gray line is a linear regression (OLS) applied to the data and the filled gray region is its 95% confidence interval.

Figure 1

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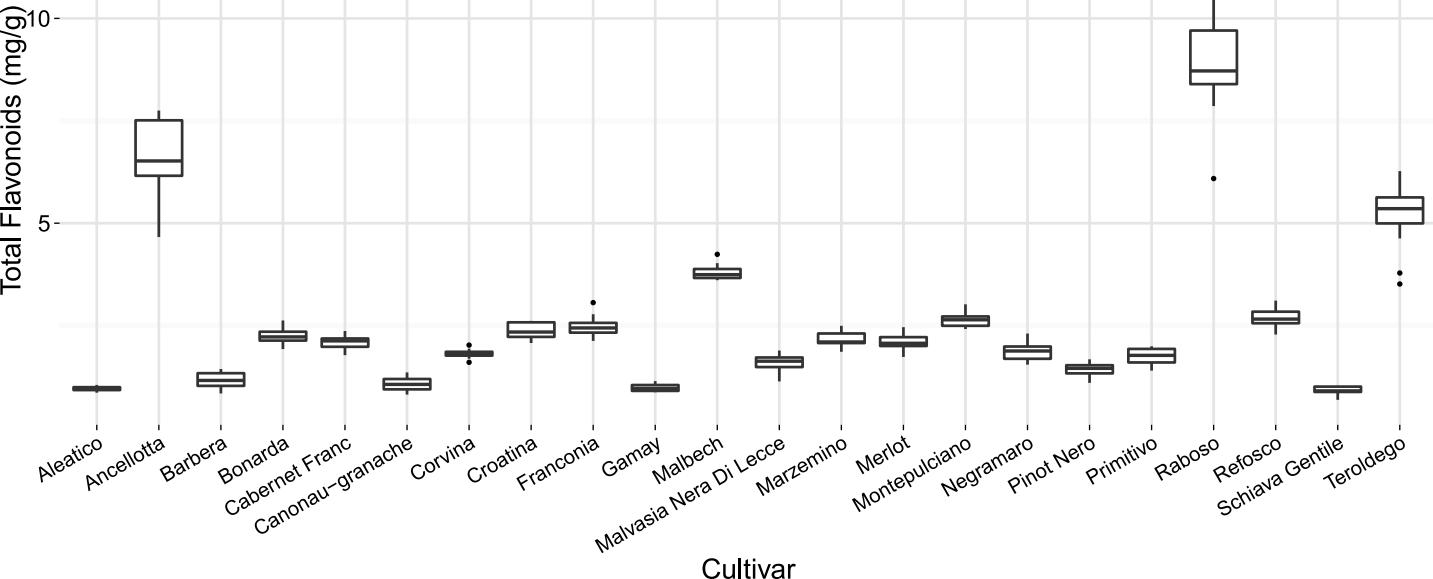


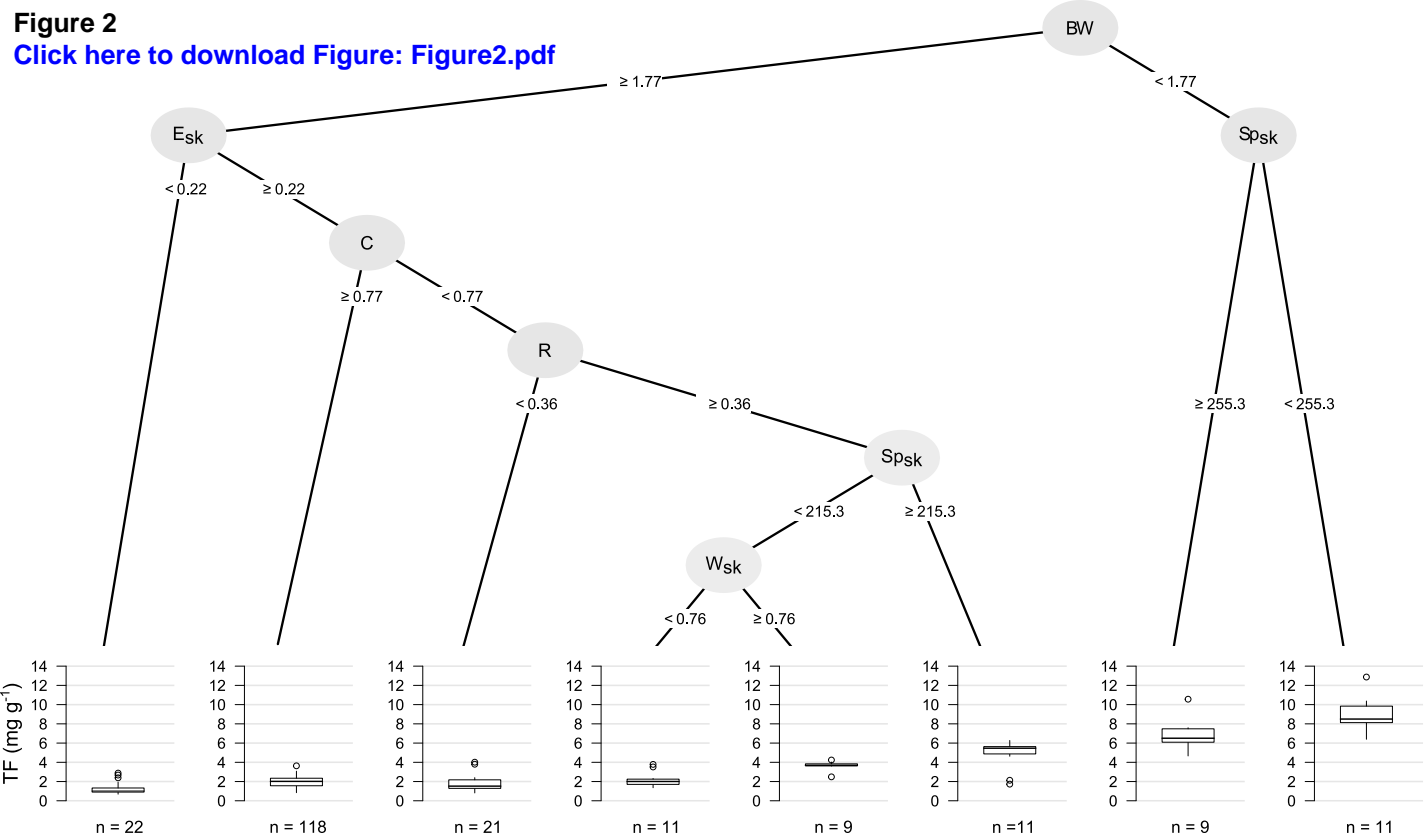
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