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ADJUSTMENT OF MATHEMATICAL MODELS TO DETERMINE QUALITY CHARACTERISTICS OF PINEAPPLE FRUITS VITÓRIA CULTIVAR

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Abstract: The objective of this study was to adjust and validate mathematical models to estimate physical and chemical characteristics of pineapple fruits (*Ananas comosus* L.) through their linear dimensions. For this purpose, 130 fruits of the cultivar BRS Vitória were used, produced at the experimental farm of the Capixaba Institute of Research, Technical Assistance and Rural Extension, located in the municipality of Sooretama, North of the State of Espírito Santo, Brazil. Of all fruits, the length (L), diameter (D), mass (M), titratable acidity (TA) and soluble solids (SS) were determined. For the modeling, the characteristics M, TA and SS were used as a dependent variable in function of L and

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D of the fruits, being adjusted the models of equation of first degree linear, quadratic and power. All equations were valid, thus obtaining the mean absolute error, root mean square error and Willmott d index. The diameter showed a better relationship with the physical and chemical characteristics of the pineapple fruit cultivar BRS Vitória, the equations being $M = 0.0015(D)^{2.7451}$, $TA = 1.076350 - 0.261046(D) + 0.018081(D)^2$ e $SS = 21.91682 - 4.58785(D) + 0.31048(D)^2$ more suitable for estimating the mass, titratable acidity and soluble solids respectively, in a simple, safe and without the need to destroy the fruits.

Keywords: *Ananas comosus* L., non-destructive method, statistical modeling, mathematical equations

1 INTRODUCTION

The pineapple culture (*Ananas comosus* L.) has been increasing its participation in brazilian agribusiness every year (PEREIRA *et al*., 2009). This is due to the knowledge of the physical and chemical characteristics of the fruits, which is extremely relevant for decision-making in relation to the crop, mainly in the harvest and in the post-harvest processes, having a direct influence on the acceptability of the products by the consumer market (BERRILI *et al*., 2014).

For the determination of fruit quality, the physical and chemical parameters commonly analyzed are mass, length, diameter, shape, color, firmness, titratable acidity, pH and soluble solids (PEREIRA *et al*., 2009). In relation to these characteristics, we can mention that the most desirable fruits are those with moderate acidity and high sugar content, in addition, characteristics such as high productivity, tolerance or resistance to pests and diseases can also be highlighted (BRITO *et al*., 2008).

In relation to the BRS Vitória cultivar, its fruits have a weight of approximately 1.5 kg, with white pulp, soluble solids content around 15.8 ºBrix and titratable acidity in approximately 0.8% citric acid, characteristic that favor the consumption of the fruit in the fresh market or in agroindustrialization, in addition, the plants present resistance to fusariosis, a fundamental characteristic since this disease has been generating enormous damages to the plantations of this culture (VENTURA *et al*., 2009; BERRILI *et al.* , 2014).

The determination of the physical and chemical characteristics of the fruits can be laborious, require specific equipment, qualified labor, and it is often necessary to destroy the fruits. As an alternative to these problems, we can mention the use of mathematical equation models, for practical purposes, the application of these models allows the rapid estimation of characteristics difficult to measure relating them to an easily measured characteristic, being able to estimate the desirable characteristic without the need for destruction of the fruits, enabling better management of the crop and favoring both researchers, producer and the final consumer.

Given the notorious importance of culture and the lack of studies involving the estimation of physical and chemical characteristics of pineapple fruits BRS Vitória cultivar, the objective of this study was to adjust and validate mathematical models to estimate the mass, the titratable acidity and soluble solids using the dimensions of the length and diameter of the fruits.

2 METHODS

The study was conducted at the experimental farm of the Capixaba Institute for Research, Technical Assistance and Rural Extension, located in the municipality of Sooretama, North of the State of Espírito Santo, Brazil, located at the following geographical coordinates: 19° 114' south latitude and 40° 079' west longitude. During the period from October 30 to December 2 of the year 2019. The region is characterized by the tropical Aw climate according to the Köppen classification, with dry winter and predominance of rain during the summer (ALVARES *et al*., 2014).

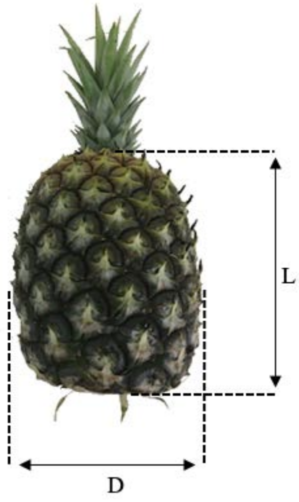
In total, 130 pineapple fruits were collected from plants of the BRS Vitória cultivar with 532 days after planting and which had all their flowers completely closed. The fruits were collected at random at different stages of development (Figure 1), with their peel classified as completely green or painted (up to 25% of the yellow-orangish peel) (BRASIL.MAPA, 2002), packed in a plastic box with capacity 47 liters and transported to the laboratory where physical and chemical analyzes were carried out.

Figure 1. Representation of different stages of development of pineapple fruits (*Ananas comosus* L.) BRS Vitória cultivar.

Source: Authors.

For the physical characteristics, initially all fruits were measured the longest length (L) without considering the crown and the lorgest diameter (D), both measures were obtained with the aid of a graduated ruler, the values being expressed in cm (Figure 2). To obtain the mass (M), the crown of the fruits was removed and weighed using a precision digital scale where the values were expressed in g and later converted to kg.

Figure 2. Representation of the length (L) and diameter (D) measurements of pineapple fruits (*Ananas comosus* L.) BRS Vitória cultivar.



Source: Authors.

To determine the chemical characteristics, the peel of the fruits was removed, which were chopped and crushed to form a pulp juice. Subsequently, the titratable acidity (TA) was measured by titrating with a 0.1 N NaOH solution, previously standardized, with a turning point at pH 8.2, the results were expressed in g of citric acid / 100 g of juice. For the measurement of soluble solids (SS), the juice was evaluated with a Schmidt Haensch ATR-BR® digital refractometer, the values being expressed in ºBrix, both analyzes were in accordance with IAL, (2008).

For the modeling, 100 fruits were used where the observed values (OV) of mass (M), titratable acidity (TA) and soluble solids (SS) were used as a dependent variable (y) in function to the longer length (L) or the larger diameter (D) as an independent variable (x). Six equations were adjusted for each dependent variable, and the models first degree linear represented by: $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$, quadratic represented by: $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x + \hat{\beta}_2 x^2$ and power represented by: $\hat{y} = \hat{\beta}_0 x^{\hat{\beta}_1}$ were tested. Its determination coefficient (R^2) was also determined for each equation. The parameters $\hat{\beta}_0$ (linear coefficient), $\hat{\beta}_1$ (slope coefficient) and $\hat{\beta}_2$ (quadratic coefficient) were defined using the least squares method.

For better analysis, the models adjusted in the modeling were validated. For this, the values of mass, titratable acidity and soluble solids of 30 fruits were replaced in their respective equations, thus obtaining the estimated values (EV) for each equation. The mean absolute error (MAE), root mean square error (RMSE) and Willmott index (d) (WILLMOTT, 1981) were calculated for all models using the expressions:

$$\mathrm{MAE} = \frac{\sum_{i=1}^{n}|\mathrm{EV}-\mathrm{OV}|}{n}$$

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(\mathrm{EV}-\mathrm{OV})^2}{n}}$$

$$d = 1 - \left[\frac{\sum_{i=1}^{n}(\mathrm{EV}-\mathrm{OV})^2}{\sum_{i=1}^{n}(|\mathrm{EV}-\overline{\mathrm{OV}}| + |\mathrm{OV}-\overline{\mathrm{OV}}|)^2}\right]$$

Where, EV are the estimated values of the mass or titratable acidity or soluble solids, OV are the observed values of the titratable mass or acidity or soluble solids, $\overline{\mathrm{OV}}$ is the average of the observed values of the mass or titratable acidity or soluble solids and n is the number of fruits used for validation, n = 30 in the present study.

As a selection criterion of the mathematical models that best represented the mass, titratable acidity and soluble solids in relation to the linear measurements of the pineapple fruits of the BRS Vitória cultivar adopted the values of MAE and RMSE closer to zero and the value of the Willmott d index with greater proximity one (WILLMOTT, 1981), in addition, the R^2 values were used as an auxiliary criterion.

All statistical analyzes and the elaboration of graphs were performed using software R version 3.6.1 (R CORE TEAM, 2020), the ExpDes.pt version 1.2 data package was also used as an aid to statistical inferences (FERREIRA *et al.*, 2018).

3 RESULTS AND DISCUSSION

The nine adjusted equations, their respective determination coefficient (R^2) and the values of the validation criteria adopted to estimate the mass of pineapple fruits BRS Vitória cultivar are represented in Table 1. It is possible to observe that the larger diameter (D) better explained the mass obtained by the fruits with values of R^2 exceeding 0.90, which is indicative of the precision of models that estimate the mass of fruits (ROJAS-LARA *et al.*, 2008). However, in mathematical modeling studies, only the adoption of the R^2 value for the selection of the equations to be indicated is not recommended since its individual use can lead to mistaken estimates on the part of the models, so R^2 should be used only with one criterion assist in making the decision.

When analyzing the validation criteria of the mean absolute error (MAE) and root mean square error (RMSE), it is possible to observe that the power model equation adjusted from the largest diameter stands out from the other equations with values closer to zero, indicating less presence of errors that may arise in the estimated values of this model.

Table1. First degree linear model equations, quadratic and power adjusted using using mass (M) in function of length (L) and diameter (D) and their respective coefficients of determination (R^2) to estimate the mass of pineapple fruits BRS Vitória cultivar, in addition to the mean absolute error (MAE), root mean square error (RMSE) and Willmott index (d).

Model	Equation	R	MAE	RMSE	d
Linear	$M = -1.87098 + 0.18866(L)$	0.7605	0.2073	0.2342	0.9374
Linear	$M = -1.524201 + 0.236922(D)$	0.9147	0.1094	0.1387	0.9738
Quadratic	$M = -0.770592 + 0.038072(L) + 0.005101(L)^2$	0.7626	0.1774	0.2108	0.9452
Quadratic	$M = 0.374806 - 0.138556(D) + 0.018272(D)^2$	0.9272	0.1055	0.1375	0.9700
Power	$M = 0.0003(L)^{3.0223}$	0.7509	0.1479	0.1946	0.9534
Power	$M = 0.0015(D)^{2.7451}$	0.9271	0.1090	0.1345	0.9716

Source: Authors.

For the d index, it is clear that the three equations obtained from the largest diameter had a similar performance (≤ 0.97) with slightly higher values for the quadratic model equation, followed by the power model and the linear model.

Taking into account all validation criteria, it is possible to infer that for estimating the mass of pineapple fruits of BRS Vitória cultivar the power model equation based on the largest diameter of the fruits is the most accurate. The use of this model, allows the adoption of treatments with the culture based on the estimated productivity, being able to identify the production by plant or in predefined areas, knowing where the highest and lowest yields are concentrated, in addition, these models contribute to the management of fertilization , since the recommendation of the dosages has as a criterion the estimated production, however, due to the fact that the values are estimated, there may be errors, generating overestimated or underestimated values, therefore, the use of certified scales is indispensable for the commercialization of the product (ZUCOLOTO *et al*., 2013).

Regarding the titratable acidity (TA), according to the validation criteria adopted for the nine adjusted models, the best performances were obtained from the largest diameter of the fruits, and the quadratic model presented values of MAE and RMSE closer to zero, index d closest to one, in addition to a higher R^2 value (Table 2). The determination of TA is based on the amount of acid predominant in the fruits, in the case of pineapple culture, citric acid stands out, and the amount of this compound tends to decrease with the progress of the maturation process; (CHITARRA; CHITARRA, 2005).

Table 2. First degree linear model equations, quadratic and power adjusted using using titratable acidity (TA), in function of length (L) and diameter (D) and their respective coefficients of determination (R^2) to estimate the titratable acidity, of pineapple fruits BRS

Vitória cultivar, in addition to the mean absolute error (MAE), root mean square error (RMSE) and Willmott index (d).

Model	Equation	R^2	MAE	RMSE	d
Linear	$TA = -0.832133 + 0.079014(L)$	0.4448	0.1285	0.1385	0.8212
Linear	$TA = -0.802832 + 0.110513(D)$	0.6636	0.1029	0.1153	0.8692
Quadratic	$TA = 0.171166 - 0.058283(C) + 0.004651\,(L)^2$	0.4507	0.0983	0.1119	0.8607
Quadratic	$TA = 1.076350 - 0.261046(D) + 0.018081(D)^2$	0.7045	0.0463	0.0627	0.9458
Power	$TA = 0.00003(L)^{3.4791}$	0.4392	0.0905	0.1154	0.8587
Power	$TA = 0.00006(D)^{3.6449}$	0.7032	0.0576	0.0688	0.9381

Source: Authors.

However, it is possible to observe that there was an increase in TA as the diameter of the fruits increased, this fact can be explained since the fruits were not in the full stage of maturity where the fruits closest to this had 25% of the peel yellow-orangish. In addition, in agreement with the results of this study Berrili *et al*. (2014), points out that in comparison with the cultivars Pérola, Gold and EC-93, BRS Vitória presents higher TA values for fruits with a high degree of ripeness (greater than 90% of the yellow peel), indicating that this is a characteristic strongly present in the fruits of this cultivar.

For estimate the soluble solids (SS) values of pineapple fruits of BRS Vitória culivar, the quadratic model equation based on the largest diameter proved to be more accurate, with higher values of R^2, MAE and RMSE with greater proximity to zero, in addition to the d index closest to one. Due to metabolic processes, mainly the degradation of polysaccharides, the SS content tends to increase as the fruits proceed with maturation (CHITARRA; CHITARRA, 2005). This increase is observed in the pulp and peel of pineapple fruits in the final stage of ripening (CUNHA *et al*., 1999).

It is worth mentioning that the soluble solids have a positive correlation with the sugar content found in the fruits, generally associated with a quality standard (TEHRANI *et al*., 2011), this being a relevant characteristic, which may provide greater acceptance of the fruits in natura. In addition, with regard to the industrialization of pineapple fruit, in the form of pulp, this equation can collaborate in decision making, since brazilian laws establish minimum values of 12º Brix of this characteristic for the commercialization of this product (BRASIL.MAPA, 2002).

Table 3. First degree linear model equations, quadratic and power adjusted using using soluble solids (SS), in function of length (L) and diameter (D) and their respective coefficients of determination (R2) to estimate the soluble solids, of pineapple fruits BRS Vitória cultivar,

in addition to the mean absolute error (MAE), root mean square error (RMSE) and Willmott index (d).

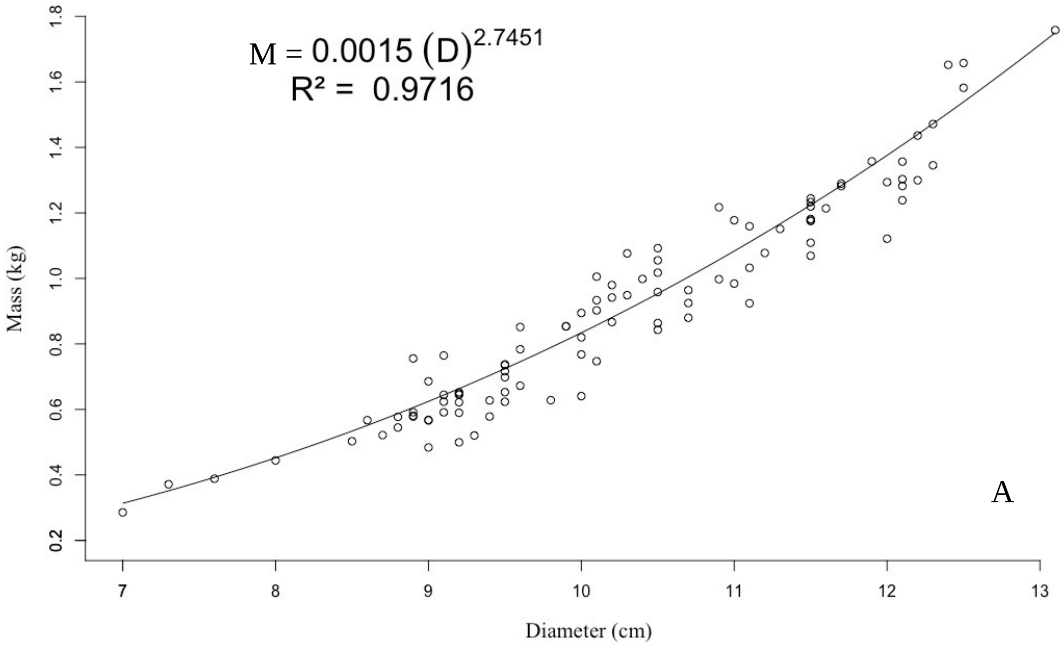
Model	Equation	R^2	MAE	RMSE	d
Linear	$SS = -9.7142 + 1.2060\ (L)$	0.4023	2.4514	2.9102	0.7527
Linear	$SS = -10.3516 + 1.7924(D)$	0.6776	2.4207	2.7566	0.7704
Quadratic	$SS = 0.70951 - 0.22040\ (L) + 0.04832\ (L)^2$	0.4047	2.0539	2.5483	0.7875
Quadratic	$SS = 21.91682 - 4.58785(D) + 0.31048(D)^2$	0.7244	1.2865	1.6698	0.8894
Power	$SS = 0.0203(L)^{2.2197}$	0.4031	2.0372	2.5348	0.7889
Power	$SS = 0.0271(D)^{2.4329}$	0.7160	2.0298	2.3257	0.8241

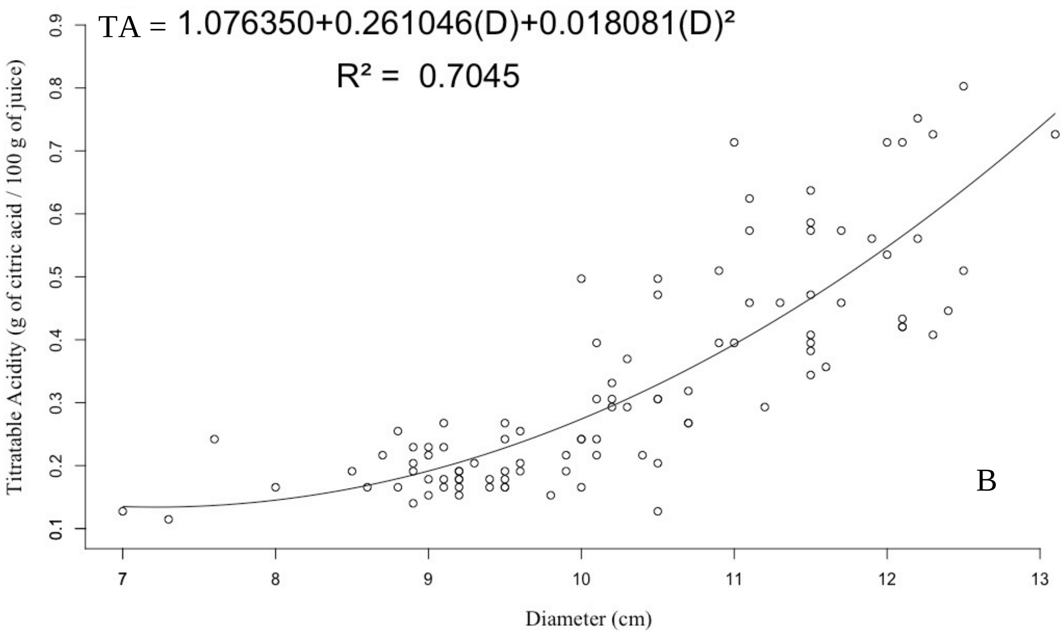
Source: Authors.

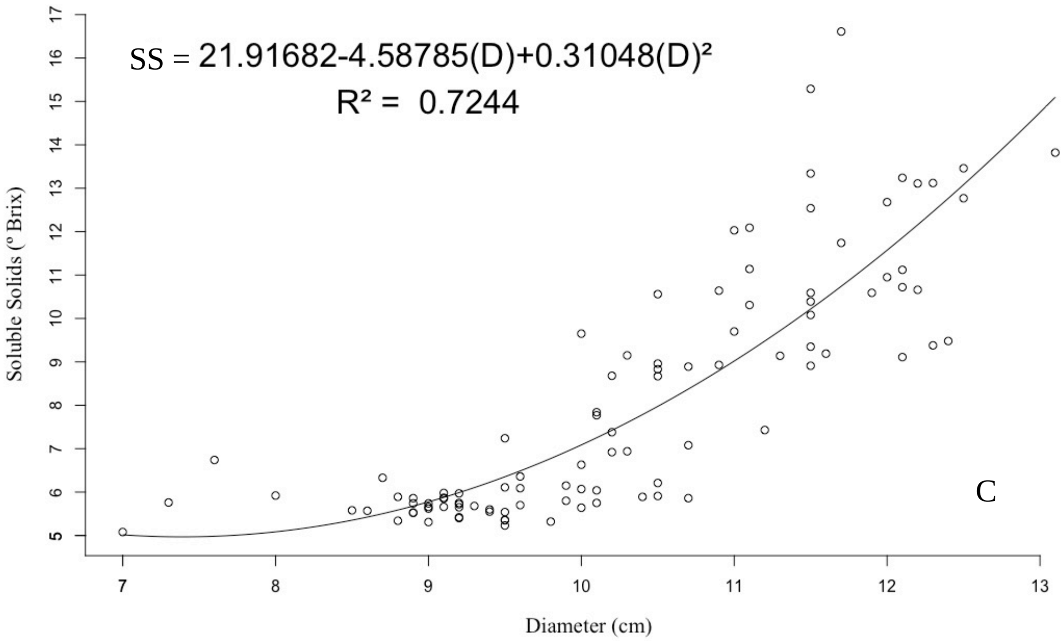
Based on the analyzed data, we can say that the mass, titratable acidity and soluble solids of pineapple fruits of BRS Vitória cultivar can be estimated from its largest diameter (D) by the equations equações $M = 0.0015(D)^{2.7451}$, $TA = 10.76350 - 2.61046(D) + 0.18081(D)^2$ e $SS = 21.91682 - 4.58785(D) + 0.31048(D)^2$ respectively, whose behavior can be seen in Figure 3. It should be noted that these equations were the ones that best met the selection criteria established in this study and can be used accurately to determine these characteristics faithfully.

In addition, despite the removal of fruit from the plant for the preparation of the equations in this study, after adjustment these equations can be used without the need for further removal, and can be used in the field, in future research or by producers, assisting in the treatment of culture, especially in the harvest, because it is essential to determine the ideal harvest point since the physical and chemical characteristics of the fruits directly influence this practice, since they are closely related to the acceptability of the fruits by the final consumer (PEREIRA *et al*., 2009). However, only one of these characteristics individually cannot define the appropriate point of maturation of the fruits, being necessary the evaluation together. We must highlight, that these equations should only be used when the target of the analyzes are fruits of the BRS Vitória cultivar, since the countless varieties of pineapple can suffer variations in their physical and chemical characteristics as reported by Berilli *et al*. (2014), another fact that must be evidenced is that these equations refer to fruits collected when the plants present the total closure of the flowers, so this stage must be respected.

Figure 3. Adjusted equations and determination coefficient (R^2) to estimate the mass (M) (A), titratable acidity (TA) (B) and soluble solids (SS) (C) in function of the diameter of pineapple fruits (*Ananas comosus* L.) BRS Vitória cultivar.


M = 0.0015 (D)^2.7451
R² = 0.9716
Mass (kg)
Diameter (cm)
A


TA = 1.076350+0.261046(D)+0.018081(D)²
R² = 0.7045
Titratable Acidity (g of citric acid / 100 g of juice)
Diameter (cm)
B



Source: Authors.

4 CONCLUSIONS

The diameter (D) showed a better relationship with the physical and chemical characteristics of the pineapple fruits cultivar BRS Vitória. Fruit mass can be determined by the power model equation $M = 0.0015(D)^{2.7451}$, titratable acidity can be defined by the quadratic model equation $TA = 1.076350 - 0.261046(D) + 0.018081(D)^2$, and soluble solids can be estimated by the quadratic model equation $SS = 21.91682 - 4.58785(D) + 0.31048(D)^2$. All these equations were better suited to the established statistical criteria, and as long as the similar conditions presented in this study are respected, they can be used to estimate the characteristics in a simple, safe way and without the need to destroy the fruits.

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