

Size estimation of tomato fruits based on spectroscopic analysis

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Abstract. This study used visible and near-infrared (VIS-NIR) spectroscopy for size estimation of tomato fruits of three cultivars. A mobile, fibre-type, VIS-NIR spectrophotometer (AgroSpec, Tec 5, Germany) with spectral range of 350-2200 nm, was used to measure reflectance spectra of on-vine tomatoes growing from July to September 2010. Spectra were divided into a calibration set (75%) and an independent validation set (25%). A partial least squares regression (PLSR) with leave-one-out cross validation was adopted to establish calibration models between fruit diameter and spectra. Furthermore, the latent variables (LVs) obtained from PLS regression was used as input to back-propagation artificial neural network (BPANN) analysis. Result shows that the prediction of PLSR model can produce good performance with coefficient of determination (R^2) of 0.82, root-mean-square error of prediction (RMSEP) of 4.87 mm and residual prediction deviation (RPD) of 2.35. Compared to the PLSR model, the PLS-BPANN model provides considerably higher prediction performance with R^2 of 0.88, RMSEP of 3.98 mm and RPD of 2.89. It is concluded that VIS-NIR spectroscopy coupled with PLS-BPANN can be adopted successfully for size estimation of tomato fruits.

Introduction

Fruit size has been one of important focuses for tomato growers, fruit retailers and cultivar genetic researchers. Firstly, as a market grading standard, fruit size is considered as a direct indicator of tomato quality [1]. Although fruit grading for market is mostly based on the conditions and the quality of the fruits, retailers have differential prices for size-graded fruits as against size-ungraded ones. For export, tomatoes are usually packed in cardboard boxes with a certain standard volume. Size-graded fruits are pattern-packed in layers to make best use of the box. Secondly, fruit size, expressed as fresh fruit mass or weight [2,3], is an important parameter for yield prediction and growth mode characterization of greenhouse tomatoes [4]. Yield is of interest to greenhouse growers for developing short-term crop management strategies and long-term marketing and labor management. Finally, fruit size of tomatoes has been one of important targets for genetic research on tomato cultivars. Domesticated tomatoes can be up to 1000 times larger than their wild relatives due to historical selection of large-size cultivars and modern transgenic variety improvement [5]. Although it has been known that tomato size is manipulated by gene and can be inherited by reproduction [6,7], it has been difficult to clone these genes in tomatoes even with modern advanced genomics tools. The challenges is owing to the fact that fruit size of tomatoes is not influenced by one gene, but many genes acting

together, which are called quantitative trait loci (QTLs). Size measurement of fruit can help plant breeders to identify phenotypic expression of target genes possibly linked with fruit size.

Size measurement of tomato fruits has been conducted in history for a long time by mechanic way [8]. Human operation is often a labor intensive, tedious and subjective task. Based on the close relationship between size and fresh fruit weight [2], electronic weigh buckets for processing tomatoes based on impact principles have been tested in laboratory and in-field for fruit grading of tomatoes [9]. However, the majority of these fruit-grading systems for tomatoes is often cumbersome, only available for off-vine fruit measurement, and cannot be used for *in situ* measurement of on-vine tomato fruits. With the development of image sensing and processing techniques, the measurement of fruit size could be conducted based on machine-vision technique [1, 10-12]. One method for size measurement of fruits was to use the area occupying fruit and an equivalent circle diameter after binarization based on the color information [13]. Alternatively, digital reflective near-infrared imaging was examined for automatic fruit grading [14]. Although these optical methods for size measurement of fruits are much convenient for in-field conditions compared to the mechanical predecessors, they often suffered from the ambiguity of computer vision due to the quality of captured images. Often due to the unstructured nature of typical agricultural settings and biological variation of plants within them, object identification based on machine vision is considerably more difficult [12].

Recently, due to relative low cost, fast acquisition rate of data and excellent repeatability, visible and near infrared (VIS-NIR) spectroscopy [15-17] has become a successful technique for the measurement of physicochemical qualities of tomato fruits. Of them, some of growth-related parameters, including ripeness, firmness and concentration of some chemicals, like sugar and acidity have been tested under laboratory conditions [18-20]. Tomato color has been correlated with firmness maturity [18-19] or with lycopene [23-25]. Although these studies on internal qualities of tomato fruits using VIS-NIR spectroscopy may lead to fast determination of what degree of ripeness a tomato fruit is, there is still lack of information about how large a tomato fruit is. To our knowledge, no published studies have addressed the use of VIS-NIR spectroscopy for *in situ* measurement of tomato fruit size.

The aim of the paper is to implement the VIS-NIR spectroscopy for *in situ* size estimation of tomato fruits with different cultivars. Performance of different calibration models is to be compared

Materials and Methods

Tomato Samples. Three tomato cultivars were planted at the Silsoe Horticultural Centre, Bedfordshire, the United Kingdom, in the summer growing season from July to September 2010. Spectral measurement started on the 24th July and was repeated every 2-3 days until the target tomatoes were fully ripen and picked. Fruit diameter was measured using a digital calliper (0-150±0.01mm, Neiko, UK). The sample statistics are listed in Table 1.

Table 1. Sample statistics of tomato fruits

Data set	Sample number	Fruit diameter			
		Range (mm)	Mean (mm)	Standard deviation	Coefficient of variation
Calibration	618	12.67-62.20	35.41	11.65	0.329
Independent validation	202	13.26-58.52	35.52	11.50	0.324

Optical measurement. The reflectance spectra of tomato fruits were measured by a mobile, fibre-type, VIS-NIR spectrophotometer (AgroSpec, Tec5 Co., Germany) with spectral range of 350-2200 nm. A 100% white reference was used before scanning. Spectral measurement was made in three separate positions on the equator of a fruit. A total of ten scans were measured at each position and the spectra from the three positions were averaged in one spectrum.

Spectral Pretreatment and Data Analysis. Due to the low signal-to-noise ratio of both ends of each spectrum, only the region of 400-2100 nm was used. Several spectral pretreatment algorithms,

including Savitzky-Golay smoothing, multiplicative scatter correction (MSC), standard normal variation (SNV), 1st and 2nd order de-trending, baseline offset correction and 1st and 2nd derivatives were investigated. Spectra were divided into a calibration set (75%) and an independent validation set (25%). The calibration spectra were subjected to a partial least squares regression (PLSR) with leave-one-out cross validation. The optimal number of latent variables (LVs) was determined by minimizing the predicted residual error sum of squares (PRESS). The PLSR calibration models were evaluated using coefficient of determination (R^2) in calibration and cross-validation, root-mean-square error of calibration (RMSEC) and cross validation (RMSECV). The coefficient of determination (R^2) and root-mean-square error of prediction (RMSEP) were used for the evaluation of prediction performance of the established PLS models based on the independent validation set. Also, the prediction accuracy of each PLS model was evaluated using the residual predictive deviation (RPD), which is the ratio of standard deviation of reference size to RMSEP of the independent validation set. We propose that RPD between 1.8 and 2.0 indicates good, quantitative model/prediction; RPD between 2.0 and 2.5 indicates very good, quantitative model/predictions; and RPD>2.5 indicates excellent model/predictions. Generally, a good model would have high values of R^2 and RPD, and low values of RMSEC, RMSECV and RMSEP. Spectra pretreatment and PLSR were conducted using the Unscrambler software (CAMO Software AS, Oslo, Norway).

After PLSR analysis, the optimal number of latent variables (LVs) enabling the minimization of PRESS was used as input to a standard three-layer back-propagation artificial neural network (BPANN) to build PLS-BPANN models aiming at improving the results obtained with the PLS. The tan-sigmoid function and a linear function were adopted in the hidden and output layers, respectively. The momentum was set as 0.9, the learning rate as 0.05, the threshold residual error as 0.001 and the training epochs as 8,000. After training, the number of neural nodes in the hidden layer was adjusted to achieve the best results. To avoid over-fitting, the cross-validation option was adopted. PLS-BPANN was conducted using Matlab software (The Math Works, Natick, MA, USA).

Results and Discussion

PLSR Models. Table 2 reports the results of the PLSR models. In general, the performance of most of these models for size measurement is good with RPD>1.8. The best prediction accuracy for individual cultivar 1, 2 and 3 is obtained by de-trending with 1st or 2nd order polynomial approximation with R^2 of 0.68-0.74 and RPD of 1.84-1.99. Compared to the models developed for individual cultivars, models developed for mixed spectra are considerably more accurate, although they are calibrated with larger numbers of latent variables (15-20). The general models with mixed spectra provide very good prediction performance achieved after baseline offset correction with R^2 of 0.82 and RPD of 2.35 for the independent validation set (Table 2).

Table 2. Performance of best PLS models built individually for cultivars 1, 2, 3 and for mixed spectra collected from across the whole growing stages

Method	LVs	Calibration		Validation		Independent validation				Model evaluation
		R^2_{cal}	RMSEC	R^2_{val}	RMSECV	R^2_{pre}	RMSEP	Bias	RPD	
None	15	0.78	5.42	0.74	5.98	0.74	5.81	0.23	1.98	Good
SNV	13	0.78	5.52	0.73	6.05	0.72	6.04	0.13	1.90	Good
MSC	12	0.80	5.16	0.77	5.54	0.80	5.03	-0.04	2.28	Very good
1 st Det	15	0.80	5.24	0.75	5.78	0.79	5.27	0.10	2.18	Very good
2 nd Det	18	0.85	4.46	0.81	5.13	0.81	5.02	0.18	2.29	Very good
BOC	20	0.86	4.43	0.81	5.18	0.82	4.87	0.07	2.35	Very good
1 st Der	10	0.77	5.55	0.71	6.18	0.73	5.89	0.12	1.95	Good
2 nd Der	15	0.80	5.24	0.68	6.60	0.69	6.46	0.30	1.80	Good

PLS-BPANN Models. Although it is successful to establish models for tomato size prediction using PLSR models, the prediction accuracy is still low. Table 2 also shows large number of LVs (10-20) needed to establish PLSR models. These high dimensional data structures may not be dealt well with linear calibration methods like PLSR. Alternatively, non-linear methods might be more suitable.

BPANN is one of best candidates due to its flexible data structure and adaptive training process. Compared to the best PLSR model, the PLS-BPANN model produces better prediction performance with R^2 of 0.88, RMSEP of 3.98 mm and RPD of 2.89, which is regarded as excellent.

Conclusions

The visible and near-infrared (VIS-NIR) spectroscopy was used for size estimation of tomato fruits of three cultivars. Combined with relevant pre-treatment algorithms, the partial least squares regression (PLSR) enabled establishing correlation between fruit diameter and VIS-NIR spectra. Prediction of the PLSR model for independent validation set achieves good or very good performance for the measurement of tomato size. Further improvement in the prediction accuracy of fruit size is obtained using PLS-BPANN analysis. The result shows that the PLS-BPANN model achieves best prediction performance with R^2 of 0.88, RMSEP of 3.98 mm and RPD of 2.89, which suggests that the methodology proposed in this study is worthy of further investigation in other tomato cultivars.

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