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Radial basis network analysis of color parameters to estimate lycopene content on tomato fruits

Virginia Fernández-Ruiz[a], José S. Torrecilla[b], Montaña Cámara[a,*], Mª Cortes Sánchez Mata[a], Charles Shoemaker[c]

[a] Departamento de Nutrición y Bromatología II, Facultad de Farmacia, Universidad Complutense de Madrid, 28040 Madrid, Spain
[b] Departamento de Ingeniería Química, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain
[c] Food Science and Technology Department, University of California, 95616 Davis, CA, USA

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ABSTRACT

With the purpose of estimating the lycopene concentration in tomato food samples, in an non-destructive way, several types of linear models of color parameters have been tested using individual values of L^*, a^* and b^* values, (a^*/b^*), (a^{*2}/b^{*2}) and chroma parameters from tomato juice and fresh tomato fruits obtained with two different apparatus (Minolta CR-200b triestimulus colorimeter and HunterLab LabScan XE). Lycopene concentrations of fresh tomato and tomato juice (used as an input) were analyzed by UV–Vis spectroscopy. For all linear methods applied, the best one to estimate the lycopene concentration in tomato was the L^*, a^* and b^* values of tomato juice measured with Hunter colorimeters (adjusted correlation coefficient, $R_a^2 > 0.86$ and mean prediction error, MPE < 6.59%). Four different RBEF models were designed firstly using three color parameters (L^*, a^* and b^*) designated as "Lab case", and secondly individually by the (a^*/b^*), (a^{*2}/b^{*2}) and chroma parameters. The lycopene concentration estimations were carried out with the lowest MPE and highest R_a^2 values possible. In order to test the reliability of the non-linear models, external validation process was also performed. From the testing of the all non-linear models applied, the RBEF Lab case model was the best to estimate lycopene content from color parameters (L^*, a^* and b^*) using Minolta or Hunter equipments (MPE lower than 0.009 and R_a^2 higher than 0.997). This was a simple non-destructive method for predicting lycopene concentration in tomato fruits and tomato juice, which was reproducible and accurate enough to substitute chemical extraction determinations, and may be a useful tool for tomato industry.

1. Introduction

Tomato fruit color measurement is frequently used in the tomato industry to predict the color of finished tomato products, which is an important quality index and determines the maturity and tomato post harvest life [1]. Color or pigment changes during tomato ripening are characterized by a decrease in chlorophyll and a rapid accumulation of carotenoids, particularly lycopene which is the predominant pigment in tomato and imparts the attractive redness [2].

Instrumental color measurements provide an objective, non-destructive and rapid technique that enables the analyst to obtain a series of parameters in a few seconds, and it is an useful tool for food quality control [3,4]. Fruit chromaticity can be evaluated by the color space coordinates L^* (degree of lightness, value), a^* (a measure of the degree of redness or greenness) and b^* (a measure of the degree of yellowness or blueness). From these parameters, (a^*/b^*), (a^{*2}/b^{*2}) and chroma $((a^*)^2 + (b^*)^2)^{0.5}$ values can be calculated to characterize the three dimensionally of colors.

The processing tomato industry is also interested in the measurement of lycopene as it is considered as an important bio-active compound or an nutraceutical ingredient [5,6]. It has a high antioxidant activity with likely involvement in the prevention of certain types of cancer and a broad range of degenerative diseases [7–11]. With an increased consumer demand on food products with health benefits [12], scientists and the industry are focused on developing food and nutritional supplements enriched in lycopene from natural resources. A rapid method for lycopene quantification in fruits and vegetables and their products is required [13].

The main problem in measuring lycopene concentrations is its insolubility in aqueous solution. Lycopene concentration in tomato can be determined accurately by spectrophotometry and HPLC analysis after extraction in organic solvents [14–16]. However, this procedure is time-consuming and destructive.

Considering all the inconveniences of analytical determination of lycopene some studies have been focused on developing non-

* Corresponding author. Tel.: +34 913941808; fax: +34 913941799.
E-mail address: mcamara@farm.ucm.es (M. Cámara).

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destructive methods for lycopene quantification using the linear correlation of color measurements to predict lycopene content of tomato obtaining correlation coefficients (R^2) equal to 0.83 and 0.96 in tomato fruits [2,17]. Other authors use color absorbance method for lycopene assay of tomato puree obtaining a $R^2 = 0.96$ [18,19]. However, these lab methods are not portable for field applications. Chourdhary et al. [20] proposed chemometric models for rapid quantification of lycopene content in tomato puree ($R^2 = 0.62$) and watermelon ($R^2 = 0.90$) by a fiber optic reflectance spectroscopy.

Considering the interest on lycopene research and the inconveniences of chemical and destructive assays, the objective of this study was to perform a radial basis network analysis of color instrumental parameters in order to estimate lycopene content in tomato food samples, in a non-destructive way, economical, fast and accurate enough to be used for tomato industry for quality control.

2. Materials and methods

2.1. Samples

Six batches of fresh tomato fruit from *Lycopersicon esculentum* were purchased from local markets in Davis, CA. Sample treatments to obtain tomato juice from fresh tomato was as follows: whole tomatoes were cut in halves face down (1.300 g) and microwaved. Afterwards, water was added to regain the original sample weight. Tomato juice was obtained from an industrial blender and the juice degassed to remove air. Samples of each batch were immediately analyzed for color and lycopene content.

2.2. Color measurement

Two different equipments were used for the evaluation of color in samples considered for study, Minolta CR-200b portable tri-estimulus colorimeter consisting on a head with an 8″ diameter measuring area and a diffuse illumination/0° viewing and Hunter-Lab LabScan XE (Hunter Associates, USA) with a view area of 0.25″ and a size port of 0.40″ and 2° Standard Observer was used for measurements. The illuminant used for the color study was CIE illuminant C [21]. Both colorimeters were calibrated with a white, black and red standard tiles. L^*, a^* and b^* values, (a^*/b^*), (a^{*2}/b^{*2}) and chroma value ($((a^*)^2 + (b^*)^2)^{0.5}$ were calculated to characterize the viewing colors three dimensionally.

For the fresh tomato samples, two color measurements were taken in opposite positions on the surface of each fruit, taking care to avoid areas with stripes. In each case, the final color score of each sample was obtained by mean of three replicates.

2.3. Chemical analysis in tomato

Determination of soluble solids at 20 °C was performed by a direct measurement of refraction index, expressed as the percentage of sucrose at 20 °C [22]. Samples showed Brix values ranging between 4.2 and 5.3, which means similar maturity index in all fruits from each batch to avoid differences in color due to the ripening stage.

Lycopene extractions were carried out immediately after processing the tomatoes into juice, using organic solvents in darkness to prevent light-induced oxidation. Samples were extracted in a mixture of hexane/acetone/ethanol (50/25/25). After 30 min in magnetic stirring, 10 mL of water was added and the upper hexane layer was separated for spectrophotometric analysis at 446 and 502 nm, according to Olives Barba et al. [15]. Every sample was prepared in triplicate, and then, each one was monitored also three times.

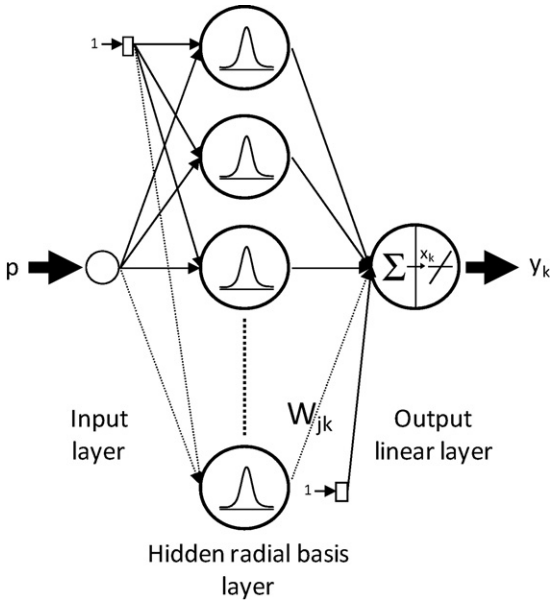

Fig. 1. Scheme of calculation of radial basis network (■,bias node).

2.4. Linear models

Linear and multiple linear regressions are the most widely used and known modelling method. It has been adapted to a broad range of situations. In a multivariate case, when there is more than one independent variable, the regression line cannot be visualized in a two dimensions space. In this case, a linear equation similar to those used here, containing all required independent variables

$$y = \alpha_0 + \sum_{i=1}^{n} \alpha_i x_i + \varepsilon \quad (1)$$

where y represents the response variable or dependent variable (lycopene concentration), n the number of observations, α_i (α_0, α_1,. . ., α_n) of the model, x_i ($i = 1, 2,. . ., n$) the independent variables (L^*, a^* and b^*), (a^*/b^*), (a^{*2}/b^{*2}) and chroma value, and ε random error [23,24].

2.5. Radial basis network model

The radial basis model (RBN) consists of three layers: the input, hidden radial basis, and output linear, Fig. 1. The input layer has no calculation power and serves as an input distributor to the hidden radial basis layer. The input to the hidden radial basis neuron is the vector distance between its weight vector (self-adjustable parameter of the net, w), and the input vector, p, multiplied by the bias. The transfer function of radial basis neurons is a Gaussian function, Eq. (2). The radial basis function has a maximum of 1 when its input is 0. As the distance between w and p decreases, the output increases. The bias allows the sensitivity of the radial basis neuron to be adjusted. The operation of the output layer is a linear combination of the radial basis units according to Eq. (3) [25]

$$G_j(x) = \frac{1}{e^{x^2}} \quad (2)$$

$$y_k(x) = \sum_{j}^{n_h} w_{jk} \cdot G_j(x) + w_k \quad (3)$$

In Eqs. (2) and (3), y_k is the kth output unit for the input vector x, n_h is the number of hidden radial basis units, w_{jk} is the weight

between the jth hidden and the kth output neurons, G_j is the notation for the output of the jth radial basis unit, and w_k is the weight of bias.

The network used here was a radial basis networks exact fit (RBEF). The algorithm very quickly designs a radial basis network with zero error on the design vectors, i.e. in this model the performance error is equal to zero. It depends on a matrix of input vectors, a matrix of target class vectors and a spread of radial basis functions (spread constant). The RBEF algorithm returns a new exact radial basis network.

As the spread constant (SC) is the only parameter of the RBEF which can be optimized, it was optimized by testing different spread constant values between 0.001 and 15 [25]. The response variables were the mean prediction error (MPE, %), Eq. (4), and adjusted correlation coefficient (predicted vs. experimental values, R_a^2).

$$\mathrm{MPE} = \frac{1}{N}\sum_{n}\frac{\left|y_n - y_n^{est}\right|}{y_n} \times 100 \quad (4)$$

where N, y_n, and y_n^{est}, are the number of observations, lycopene concentration value and RBEF model estimation, respectively. The RBN model designed was developed taking into account that lycopene concentration estimations should be carried out with the lowest MPE and highest R_a^2 values possible.

Every RBEF model used in this work was designed using Matlab version 7.01.24704 (R14). The statistical analyses were carried out by Statgraphics Plus version 5.1.

2.5.1. Learning, verification and validation samples

The color characteristics of juice (J) and fresh fruit (F) of tomatoes measured by Minolta (M) and Hunter (H) instruments have been distributed in four databases, (JM, FM, JH and FH) consisting in seven columns (L^*, a^*, b^*, (a^*/b^*), (a^{*2}/b^{*2}) and chroma and their respective lycopene concentration, *vide supra*). These databases have been used to design linear models.

To optimize and verify the non-linear models, these databases (JM, FM, JH and FH) have been divided in two groups *viz.* learning and verification. The first one contained 80% used in the learning process and the remaining 20% of the whole data to verify the performance of the RBEF models.

An external validation of two non-linear models (FM and FH databases), was performed using a set of data from tomato fruits taken from literature, including L^*, a^* and b^*, color parameters (Minolta) as an input, and lycopene content by HPLC as an output [17].

3. Results and discussion

3.1. Multiple linear regression models

To estimate the lycopene concentration, four types of linear models have been tested, using individual values of L^*, a^* and b^* values from tomato juice and fresh tomato fruits measured with two different apparatus (Minolta CR-200b triestimulus colorimeter and HunterLab LabScan XE, *vide supra*). Lycopene concentrations of fresh tomato and tomato juice were evaluated by UV–Vis spectroscopy. In the light of MPE (Eq. (4)) and adjusted correlation coefficient values (real vs. estimated concentration), the best model was achieved measuring L^*, a^* and b^* values in tomato juice samples by Hunter equipment ($R_a^2 > 0.86$ and MPE < 6.59%), Table 1. The UV–Vis lycopene concentrations and their linear estimations are shown in Fig. 2.

For a better estimation of lycopene content, twelve linear regression models have also been proposed. These models were designed using individually (a^*/b^*), (a^{*2}/b^{*2}) and chroma parameters (Minolta and Hunter), Table 2. The UV–Vis concentration and their linear estimations are shown in Fig. 2. In the light of MPE (Eq. (4)) and adjusted correlation coefficient values (real vs. estimated concentration), the best results are achieved in tomato juice samples evaluated by Minolta or Hunter apparatus ($R_a^2 > 0.66$ and MPE < 10.38% and $R_a^2 > 0.66$ and MPE < 10.94%, respectively), Table 2.

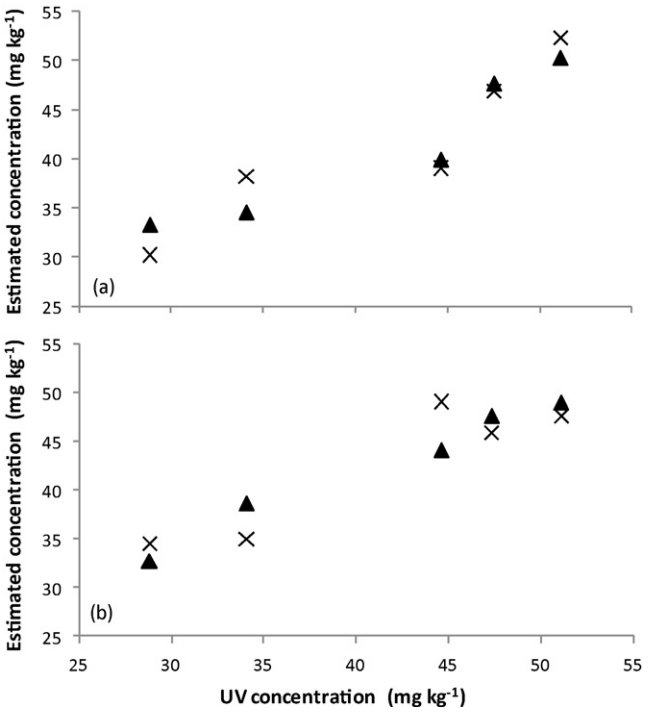

Fig. 2. UV–Vis measured concentration of lycopene vs. its linear estimations. (a) Juice; (b) fresh fruit. (×, Hunter and ▲, Minolta).

For all linear methods applied, the best one to estimate the lycopene concentration in tomato juice consists on using L^*, a^* and b^* values measured with the Hunter ($R_a^2 > 0.86$ and MPE < 6.59%). Nevertheless, there was not an outstanding linear mathematical correlation between lycopene content and the color values. Therefore, to find more reliable estimations of lycopene concentration, the models could be improved using non-linear algorithms as RBEF models.

3.2. Non-linear models

Following the same procedure as in the linear model designs, four different RBEF models were designed to estimate the lycopene concentration, firstly using three color values (L^*, a^* and b^*) designated as "Lab case", and secondly individually by the (a^*/b^*), (a^{*2}/b^{*2}) and chroma parameters. As the number of input nodes and output neurons are fixed by the requirements of the system to be modelled, in all cases there was an output neuron (lycopene content) and the number of input neurons varied depending on the required information, that is, three nodes in the first (Lab case), and one node in the other three RBEF models designed. The hidden neurons number was optimized by the radial basis network itself (*vide supra*) [25].

In the RBEF models optimization, every spread constant value was optimized following the aforementioned method. The design was analyzed taking into account that the estimations should be carried out with the lowest MPE and highest R_a^2 values possible. In every RBEF models, the optimized spread constant was equal to unity.

Table 1
Parameters of linear models and their statistical results of UV-Vis lycopene concentration (mg kg^{-1}) *versus* those estimated by multiple linear regression models[#].

Sample	Equipment	α_0[§]	α_L[§]	α_a[§]	α_b[§]	R_a^2[¥]	MPE (%)[*]
Tomato fruit	Minolta	368.769	−8.934	3.756	−1.233	0.839	9.731
	Hunter	26.664	1.862	1.619	−5.550	0.707	9.711
Tomato juice	Minolta	64.537	−5.296	14.068	0.602	0.804	7.989
	Hunter	30.737	−2.212	4.208	1.412	0.863	6.585

[#] [Lycopene] = $\alpha_0 + \alpha_L L_+ \alpha_a a^*_+ \alpha_b b^*$.
[§] mg kg^{-1}.
[¥] Adjusted correlation coefficient.
[*] Eq. (4).

Table 2
Parameters of multiple linear regression models[#] used to estimate the lycopene concentration using (a^*/b^*), (a^{*2}/b^{*2}) and chroma and their respective statistical results.

Sample	Equipment	α_0[§]	$\alpha_{(a^*/b^*)}$[§]	$\alpha_{(a^{*2}/b^{*2})}$[§]	α_{chroma}[§]	R_a^2[¥]	MPE (%)[*]
Tomato fruit	Minolta	22.238	16.913	–	–	0.201	18.678
		33.913	–	5.931	–	0.214	18.814
		35.940	–	–	0.280	0.236	18.940
	Hunter	14.609	16.907	–	–	0.442	12.853
		28.179	–	5.111	–	0.444	13.020
		29.890	–	–	0.516	0.060	17.057
Tomato juice	Minolta	−92.748	123.488	–	–	0.144	13.853
		−24.223	–	55.559	–	0.132	13.981
		−109.068	–	–	9.628	0.666	10.379
	Hunter	−6.619	37.575	–	–	0.306	12.743
		18.540	–	13.840	–	0.266	13.107
		−7.186	–	–	3.090	0.669	10.939

[#] [Lycopene] = $\alpha_0 + \alpha_{(a*/b*)}(a*/b*)_+ \alpha_{(a^{*2}/b^{*2})}(a^{*2}/b^{*2})_+ \alpha_{chroma}$ chroma.
[§] mg kg^{-1}.
[¥] Adjusted correlation coefficient.
[*] Eq. (4).

In the lab case RBEF model, the lycopene concentration estimated (using the verification sample) showed MPE lower than 0.009 and R_a^2 higher than 0.997 when fresh tomato and tomato juice were measured by both Minolta and Hunter apparatus. In the light of adjusted correlation coefficient and MPE values, all RBEF models were suitable to estimate the lycopene concentration.

Considering now individually the (a^*/b^*), (a^{*2}/b^{*2}) and chroma parameters to perform the RBEF models, the optimized spread constant values and statistical results calculated during the verification processes of these three models are shown in Table 3.

In the R_a^2 terms, these models were comparable to the non-linear model proposed in the Lab case. But accounting MPE values, these models were worse than the aforementioned non-linear model, with the exception of Chroma model of tomato juice using Hunter equipment ($R^2 > 0.999$ and MPE < 0.002%). In any case, in comparison with linear models, the statistical results were improved notably. Thus the lycopene estimation was more reliable. This improvement in the statistical results is expected because the complex mathematical relation between color characteristics of foods and its lycopene concentration can be considered as a non-linear relation.

Table 3
Lycopene concentration estimations by RBEF models using (a^*/b^*), (a^{*2}/b^{*2}) and Chroma parameters using the verification sample.

Sample	Input values	Equipment	Spread constant	R_a^2[¥]	MPE (%)[*]
Tomato fruit	(a^*/b^*)	Minolta	0.01	0.996	1.349
		Hunter	0.10	0.988	3.056
	(a^{*2}/b^{*2})	Minolta	0.01	0.999	0.107
		Hunter	0.01	0.999	0.411
	Chroma	Minolta	0.01	0.996	0.446
		Hunter	0.01	0.995	0.155
Tomato juice	(a^*/b^*)	Minolta	0.11	0.992	0.393
		Hunter	0.11	0.992	0.223
	(a^{*2}/b^{*2})	Minolta	1.00	0.998	1.460
		Hunter	0.10	0.991	1.941
	Chroma	Minolta	0.01	0.995	0.105
		Hunter	0.01	0.999	0.002

[¥] Adjusted correlation coefficient.
[*] Eq. (4).

Linear models ($y = a + b{\cdot}x$) are able to describe only linear relations between dependent (y) and independent (x) variables. Nevertheless, radial basis network models not only are capable to describe non-linear relations between the aforementioned variables, but also given the number of calculation units (neurons), where non-linear calculations are carried out, more complex mathematical relations can be adequately described. Because of this, neural networks can describe more adequately complex mathematical relations than linear models do. On the other hand, in the case of non-linear models the number of parameters used to describe the mathematical relation is higher than in the case of linear model.

Given the statistical results obtained the non-linear models were suitable to estimate the lycopene concentration by the fruit color parameters of fresh tomatoes and tomato juice, obtained by both instruments (Hunter and Minolta).

Once the RBEF models had been optimized, and in order to test the reliability of the non-linear models, external validation process was applied [26].

3.3. Validation of non-linear models

The non-linear models (FM and FH databases) were externally validated using published lycopene concentrations of tomato fruits analyzed by HPLC and their respective color parameters measured both with Hunter and Minolta instruments [17]. This external validation process consisted of comparing the estimation of lycopene content calculated by RBEF models with the real concentration from different samples taken from other source. The databases used in

Table 4
External validation of RBEF models.

Tomato fruit	HPLC* §	Equipment	Estimated (Lab case)§	Estimated (a^*/b^*)§	Estimated (a^{*2}/b^{*2})§	Estimated (Chroma)§
Orange	34.06	Minolta	35.36	31.32	32.44	31.99
		Hunter	35.73	39.3	38.73	39.3
Light red	49.50	Minolta	48.95	45.87	47.07	47.27
		Hunter	47.59	45.55	46.59	47.18

§ Lycopene content in mg kg^{-1}).
* Arias et al. [17].

the learning, verification and validation must be comparable, i.e., these should belong to the same applicability domain [25]. The HPLC lycopene values of tomato fruit [17] and estimated lycopene concentration obtained by the four RBEF models previously optimized are shown in Table 4.

External validation applied confirmed our previous results, the better estimation of lycopene content in tomato fruit was obtained by the RBEF Lab case model (using L^*, a^* and b^* parameters) with independence of the color equipment used.

To conclude, from all the non-linear models applied, the RBEF Lab case model was the best to estimate lycopene content from color parameters (L^*, a^* and b^*) using Minolta or Hunter equipments. This model is a simple non-destructive method for predicting lycopene concentration in tomato fruits and tomato juice, being reproducible and accurate enough to substitute chemical assays, and may be a useful tool for tomato industry with the only requirement of software Matlab version 7.01.24704 (R14) or similar.

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