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Multivariate analysis of the effect of the temperature in NIR diffuse reflectance spectra of an scatterer solution

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ABSTRACT

The results obtained of the multivariate analysis of the NIR diffuse reflectance spectra, collected from intralipid solutions with glucose at different temperatures, shows that, temperature effects over the NIR measurements are quite similar to the caused by the variation in the glucose concentration in the scatterer solution. Also, was possible to calculate a Bias error per Celsius degree of 672.8 mg.dL^{-1} induced by the temperature, when is used a glucose prediction model calibrated at constant temperature.

Introduction

Multivariate data analysis techniques have the advantage to allow the possibility of projecting multivariate data into few dimensions and visualize them in a graphical interface. Multivariate analysis is able to handle large data sets and deal efficiently with real-world multivariate data, taking advantage of previously feared colinearity of spectral data. The most of the multivariate algorithms are based in the Principal Component Analysis method (PCA), which can be considered as the first step in exploratory analysis due to its efficient data-reduction and data-overview capabilities [1,2]. PCA is a mathematical method of reorganizing information in a data set of samples. It can be used when the data set contains information from only a few variables but it becomes more useful when there are large numbers of variables, as in the spectroscopic data. PCA calculates new variables, called "principal components" (PCs), which account for the majority of the variability in the data. This enables us to describe the information with fewer variables than was originally present. The first PC is the direction through the data that explains the most variability in the data. The second and subsequent, PC must be orthogonal to the previous PC and describes the maximum amount of the remaining variability. Once we know the directions of the PCs it is simple geometry that allows us to express the values of individual samples in terms of the PCs as linear summations of the original data multiplied by a coefficient which describes the PC. These new values are known as "scores" and each sample will have a score for each PC [3,4].

Partial least square regression (PLSR) is its counterpart for regression analysis. PLSR is a predictive regression method based on estimated latent variables and applies to the simultaneous analysis of two data sets of the same objects. The purpose of PLSR is to build a linear model that enables prediction of a desired characteristic from a measured spectrum. PLSR is used routinely to correlate spectroscopic data with related chemical/physical data (in this case glucose and temperature) [5]. Both PCA and PLSR are bi-linear methods able to utilize the multivariate advantage when applied to co-linear first order data. They facilitate inference compensation and outlier detection when abnormal or erroneous signals are measured. In addition, multivariate analysis cover methods for spectral variable or interval selection aimed at improving regression models and at developing dedicated fast spectroscopic instruments [6-10].

On the other hand, the on-line non-contact quantification of glucose in a solution o turbid medium is a topic of interest and research in diverse fields, for example; food industry and medical science. The quantification of glucose, using spectroscopic methods in a combination with multivariate methods, has significant advantages because it can be implemented directly in the process line for real time quality monitoring of the continuous stream of raw products in the food industry. In the medical area, the non-invasive glucose quantification in biological fluids like whole blood or serum as a diagnostic and monitoring tool for diabetic patients has been extensively studied for numerous groups and researchers around the world [11-22].

However, the spectroscopic measurements could be affected for diverse external factors, as the scattering characteristics and temperature of the sample. Temperature is a critical parameter for near infrared (NIR) spectroscopic analysis of aqueous-based samples, because alters the extent of hydrogen bonding and causes significant shifts in the NIR band positions [23].

The effect of the temperature over the spectroscopic measurements is well known and reported in the literature [24]. Even, some researchers have reported the calibration of robust glucose prediction models that are insensitive to the temperature effect [25,26]. According to Masatoshi et al, the bias error induced by the temperature effect using a PLS-model calibrated without taken into a count this effect, was of 500 mg dL^{-1} per Celsius degree. Masatoshi carried out a theoretical study using Monte Carlo simulation in order to evaluate that bias error in the glucose prediction due to the temperature effect in a scatterer medium like intralipid using a range of glucose concentration from 0 to 10,000 mg dL^{-1} in the range of 1200 to 1800 nm [25]. Another work in this direction was carried out by Houxin Cui et al., who calculate the effect of the temperature in the absorbance of aqueous glucose in a wavelength from 1200 to 1700 nm [26].

The main purpose of this paper was to analyze the NIR diffuse reflectance spectra, recorded from a scatterer solution with glucose at different concentrations, using multivariate methods like PCA and PLSR as a tool for spectroscopic data analysis, in order to demonstrate and quantify the temperature effect in this kind of spectroscopic measurements. However these methods and methodology could be extended for other cases of study and this paper could serve as a reference for the students which are interested in extract subtle information of spectral data.

Materials and Methods

Methodology

As scatterer medium, a two percent intralipid solution was prepared, using a commercial intralipid solution (lipofundin N 20%) and distilled water, in a volume proportion of 10:90, respectively. One liter of "lipofundin" contains: 200 g of soybean oil; 25 g of glycerol; 12 g of egg lecithin; sodium oleate; 200 mg of a-Tocoferol and distilled water; with an Osmolarity (mOsm/l) of 380 and a pH of 6.5-8.5, [27-29].

Four experiments were carried out independently, and every experiment was divided into three stages. In the first stage, NIR diffuse reflectance spectra of the intralipid at different glucose concentrations ranged from 0 to 5000 mg.dL-1 at a constant temperature of 30ºC, were collected, in order to calibrate a PLS-prediction model.

In the second stage, the temperature of the intralipids of the stage one, for the glucose concentration of 5000 mg dL-1 was increased from 30 to 50ºC and multiple NIR spectra were taken every 2ºC. In the third stage, was predicted the glucose concentration from NIR spectra collected in the stage two using the model calibrated in the stage one, in order to estimate the prediction error caused by the temperature effect. In all stages, the experimental setup remained constant.

First stage: Calibration

In this stage, the goals were; by means of PCA scores and loadings analysis, to identify the spectral regions associated with the increases in glucose concentration, verify that the changes in the NIR spectra was correlated with the variation in the glucose concentration, and using the PLSR method to calibrate a prediction model for the glucose concentration at constant temperature. For this purpose, the glucose concentration in the intralipid was increased from 0 to 5000 mg.dL-1 at increments of 500 mg dL^{-1} at 30±0.1ºC. The high glucose concentration values were chosen only with the purpose to highlight visually the spectral variations due to increase in the glucose concentration. The collected raw spectra were centered and scaled previously to the analysis with PCA and PLSR

Centering and scaling ensure to us, that all results will be interpretable in terms of variation around the mean and each variable get the same variance. For more details of centering and scaling see the next reference [2].

Second stage: Change in temperature

The main objective of this stage was to identify those spectral regions where variations due to increases of temperature are located. For this purpose, the temperature of the intralipid solution of the stage one at 5000 mg dL^{-1} was increased from 30±0.1 to 50±0.1ºC at intervals of 2±0.1ºC. We choose the concentration of 5000 mg dL^{-1} for experimental simplicity. Finally, the recorded spectra were analyzed by PCA and PLSR, in order to verify that the spectral changes were correlated with the variations in temperature.

Third stage: Prediction

The objective in this stage was to calculate the error in the prediction of glucose concentration due to an increase in the temperature of the sample. To do this, we following the next steps: firstly, the glucose concentration was predicted from the NIR spectra collected in the stage two using the PLS-prediction model calibrated in the stage one, for the four experiments. Then, for every temperature measured, we obtain the average of the predicted glucose concentration value. After that, the behavior of the average of predicted values was computed by fitting a polynomial function. Finally the Bias error per Celsius degree was calculated using the data of the fitting. (See figure 1).

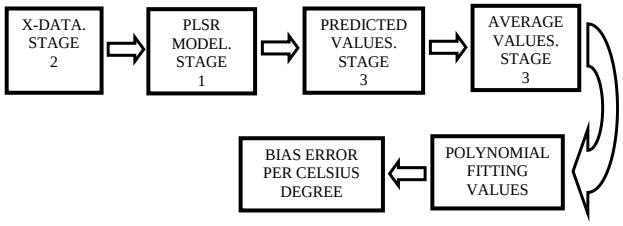

Figure 1. Schematic representation of the procedure followed to calculate the Bias error per Celsius degree caused by the variation of the temperature in the intralipid solution. For the raw data obtained in the stage 2, we applied the prediction model calibrated in the stage 1, then we obtain the average of the glucose prediction values obtained in the stage 3 for different temperatures, and a polynomial function was adjusted to the data, then the Bias error was calculated using the values of the polynomial function.

Experimental Setup

To collect the NIR diffuse reflectance spectra, we using a Tungsten-Halogen lamp (Ocean Optics LS-1, 6.5 W) with a spectral range of 360-2500 nm, with decay rate of ~0.1%/hour after 100 hours burn-in, as a NIR radiation source. The NIR radiation was directed towards the sample using a bifurcate optical fiber (Ocean Optics, R400-7 Vis-NIR) with a stainless steel probe. The NIR spectra were recorded with a NIR spectrometer (Ocean Optics, NIR512) equipped with an air cooled linear array detector of InGaAs (Hamamatsu G9204-512), with a 512 pixel matrix, each one 25 x 500 μm, with a detection range from 850 to 1700 nm, an optical resolution of ~3nm FWHM and a signal to-noise-ratio (SNR) of 4000:1.

Before to collect the spectra, the NIR spectrometer was calibrated, subtracting the dark (electronic contribution) and Reference (light source) signals.

To collect the NIR spectra of intralipid solutions, we followed the next procedure; the 2% intralipid was contained in a glass recipient over a stirrer hot plate with digital display (PC-620D, CORNING), a thermocouple (FLUKE, K-Type thermocouple) was put inside of the intralipid solution to monitoring the sample temperature with a thermometer (FLUKE model 51-2), then the optical fiber probe was put in contact with the glass recipient at a position of 90 degrees, according with the Masatoshi theoretical configuration for incident radiation.

The NIR spectra were collected with an integration time of 2000 ms, for every glucose concentration and temperature, and analyzed in the range from 900 to 1600 nm. Five spectra (replicas) were recorded for every concentration and temperature, in order to characterize the spectral variance. The spectral variance was characterized by analyzing the 100% lines, according with the procedure described by Arnold and Small [30]. The quality of the combination region spectra can be assessed by an analysis of the root-means square (rms) noise of 100% lines. In this analysis, 100% lines were computed for the case of intralipid solution with a glucose concentration of 1000 mg.dL^{-1}. The resulting spectra were converted to absorbance units and fitted to a second-order polynomial. The rms noise was then computed about the polynomial fit over a restricted spectral range. In this study, the average rms noise determined from all samples was 16 μ AU over the 900-1600 nm spectral range.

The data acquisition was realized via OOIBase32 software (version 2.0.0.5, OceanOptics, USA) which also controlled the instrument. Multivariate data analysis and preprocessing as centering and scaling, was realized via UnscramblerTM (version 8.0, CAMO, Norway).

Analysis and Results

Figures 2 depict the NIR diffuse reflectance spectra recorded in the stage one, for an intralipid solution at different glucose concentrations. As can be seen, the absorbance values increases along whole spectral range (900-1600 nm), according with the increase of glucose concentration. This effect could be attributed to a change in the refractive index of the scatterer medium due to the glucose [22].

In order to visualize those spectral regions with the major spectral variations related with the change in glucose concentration, the NIR spectra where superposed, moving horizontally each spectrum at the same absorption intensity value at the wavelength of 900 nm, as is shown in figure 3 (a) and (b). The superposed spectra show noticeable

variations in the absorption band centered in approximately 1445 nm. According with Khalil, this broadband is associated to (2νOH), (νOH + νCH) and (2νCH) overtones [17]. Also, subtle changes in the absorbance can be observed in the region from 900 to 1400 nm, which is assigned to (3νOH), and (3νCH) overtones.

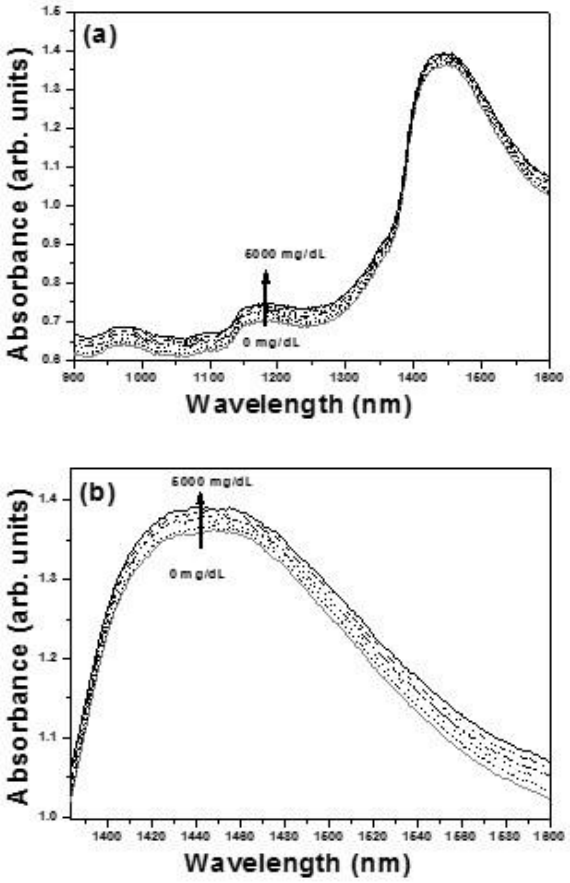

Figure 2. Typical NIR diffuse reflectance spectra of intralipid at different glucose concentrations (0-5000 mg dL-1) in the range of 900 to 1600 nm. (a), and, zoom of the band centered in 1445 nm (b). The arrows indicate the increasing in glucose concentration.

Analyzing the region around 1445 nm, we found a linear behavior between absorbance and glucose concentrations, as is showed in the figure 4. In the table 1 are displayed the absorbance values as function of the glucose concentration. The PCA-Scores plot, suggest that spectral variations are attributed mainly to variations in the glucose concentration, as can be observed in figure 5 (a), where the first component (PC1) explains 100% of the total variance, associated with the increase in glucose concentration for each experiment. The PC1-loading plot in the figure 5 (b), shows the highest loading values around of the 1445 nm, which suggest that the most important changes and influent variables for the PLSR prediction model, due to the variation in the glucose concentration, are located in those wavelengths.

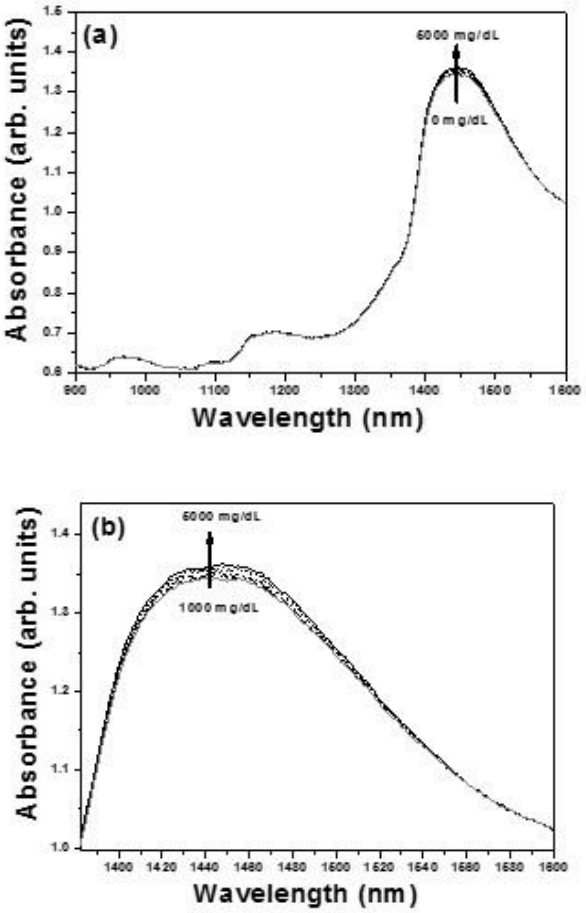

Figure 3. Superposed NIR diffuse reflectance spectra at different glucose concentrations (a). The spectral differences are located in the band centered in 1445 nm. Zoom of the band centered in 1445 nm (b). The increase in the glucose concentration is indicated by the arrows.

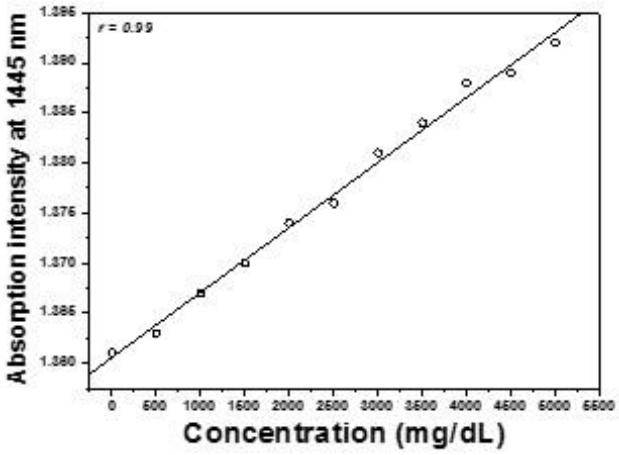

Figure 4. Absorbance values at 1445 nm vs glucose concentration, for the raw NIR spectra. The plot shows a linear behavior with a correlation coefficient (r) of 0.99.

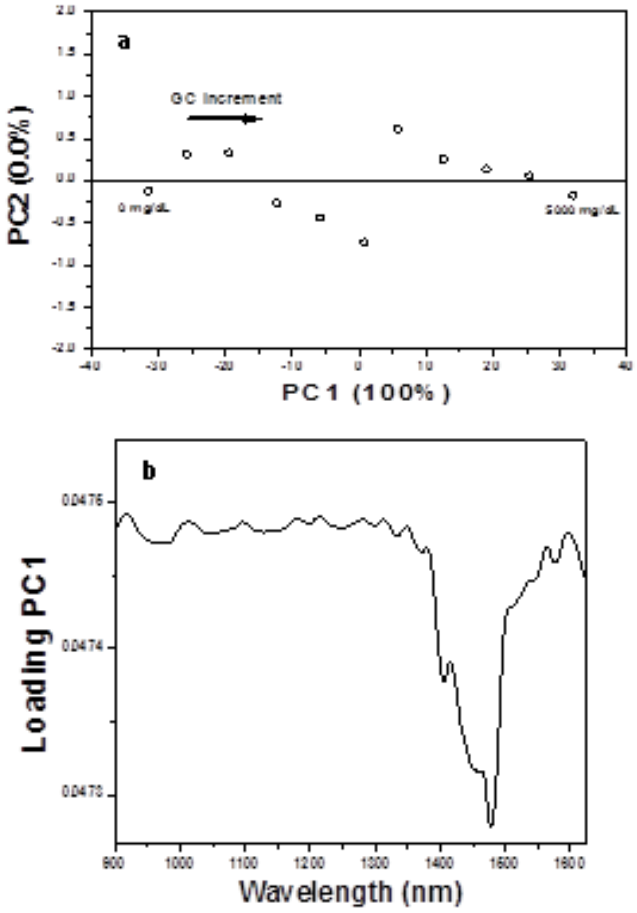

Figure 5. PCA-scores plot for the NIR spectra at glucose concentrations ranged between 0 and 5000 mg.dL-1 (a). The samples are distributed according with the increment in their glucose concentration, along PC1, which explain the 100% of the variance in the data set. PC1-Loading, the highest loading values around 1445 nm, suggest that the most important and influent variables in the PLSR model are located around that wavelength (b).

Table 1. Absorbance intensity at 1445 nm, as function of the glucose concentration, in the range from 0 to 5000 mg.dL^{-1}.

Concentration (mg dL^{-1})	Absorbance intensity at 1445 nm
0	1.361
500	1.363
1000	1.367
1500	1.370
2000	1.374
2500	1.376
3000	1.381
3500	1.384
4000	1.388
4500	1.389
5000	1.392

After PCA analysis, four PLSR models using the full cross validation method and one-PLS factor for the predictions, were calibrated, using the NIR diffuse reflectance spectra at different glucose concentrations. In the table 2 are displayed the r2 and RMSEC values for each calibrated model. The high correlation coefficient and low RMSEC values obtained, indicates that spectral variations recorded are highly correlated with the changes in the glucose concentration. For more details about cross-validation see the next references [2,31].

Table 2. Correlation coefficient values and Root Mean Square Error of Calibration of the four independent PLS-glucose prediction models calibrated in stage one.

Experiment	r^2	RMSEC (mg.dL^{-1})
1	0.99	57.7
2	0.99	33.1
3	0.99	46.4
4	0.99	24.9

NIR spectra collected in the second stage, are depicted in the figure 6. In this figure, can be observed that the spectral variations in the scatterer solution, due to the increase of temperature are located along whole spectral range (900-1600 nm), as happened in the stage one, but we can observe a significant band shift of ~15 nm, in the broad band centered in 1445 nm, due to the temperature effect [23]. By means of analysis of the absorbance intensity values along whole spectral range, we could identify that this band shift causes a linear behavior with negative slope in the region from 1460 to 1600 nm, and a non linear behavior from 1420 to 1460 nm. However in the range of 900 to 1420 nm, remains a linear behavior with positive slope as it happened in the stage one, for changes in the glucose concentration. These behaviors are showed in the figure 7 (a), (b), (c), and their values are displayed in the table 3. These results are in agreement with those reported for Houxin Cui in experimental aqueous solution and Masatoshi Tarumi in their theoretical simulation [25,26]

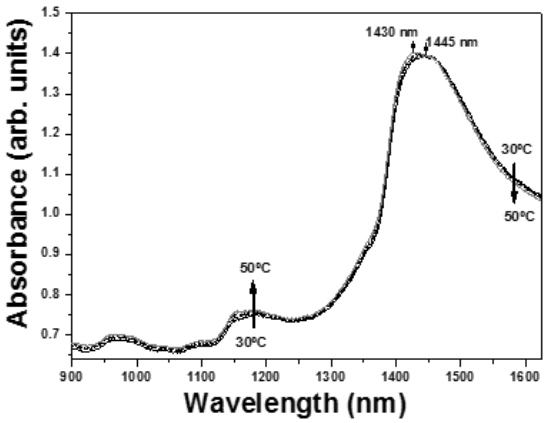

Figure 6. Raw NIR spectra of the intralipid at a glucose concentration of 5000 mg.dL-1 at different temperatures, ranged between 30 to 50ºC on intervals of 2ºC. The arrows show the behavior for the different wavelength regions.

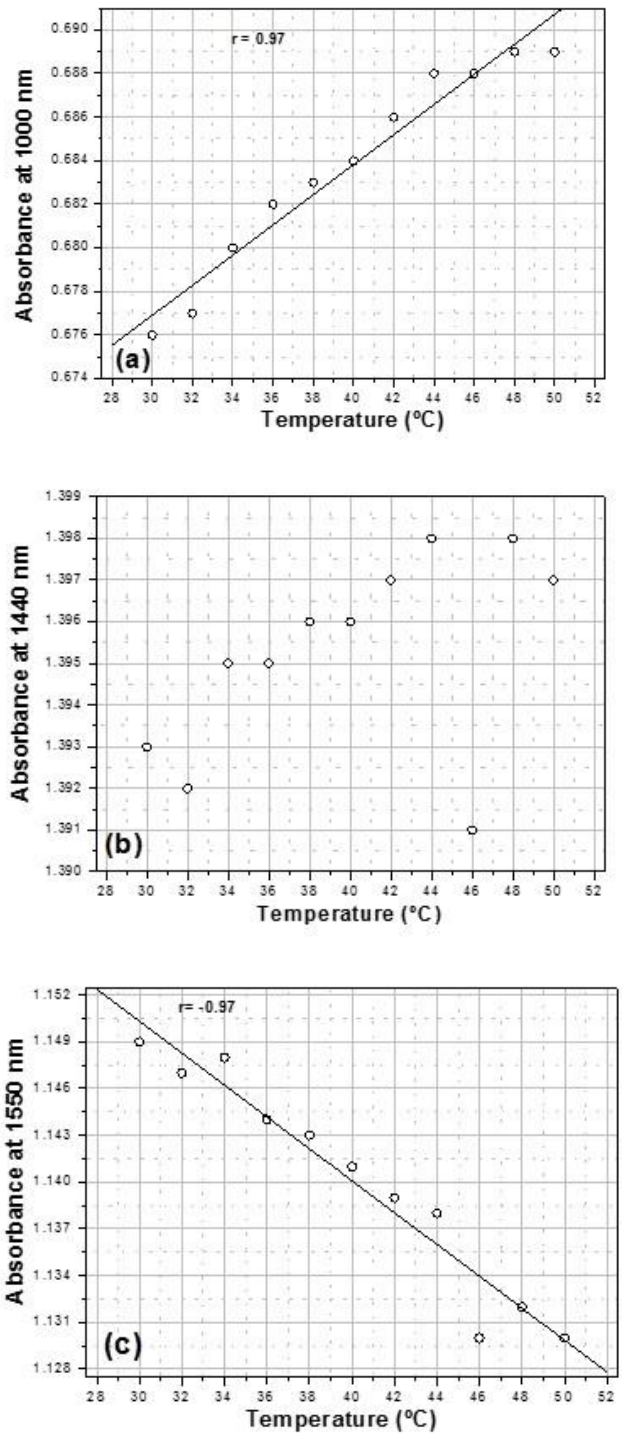

Figure 7. P Absorbance values of raw NIR spectra of stage two at three different wavelengths: 1000 nm (a), 1440 nm (b), and 1550 nm (c), versus temperature.

Figure 8, shows the PCA-Scores plot of PC2 vs PC1 obtained from stage two. These first two components, explains the 99% of the total variance of the spectra; where PC1 explains the spectral variations related with the temperature increase, according with the distribution of the samples along the PC1 direction.

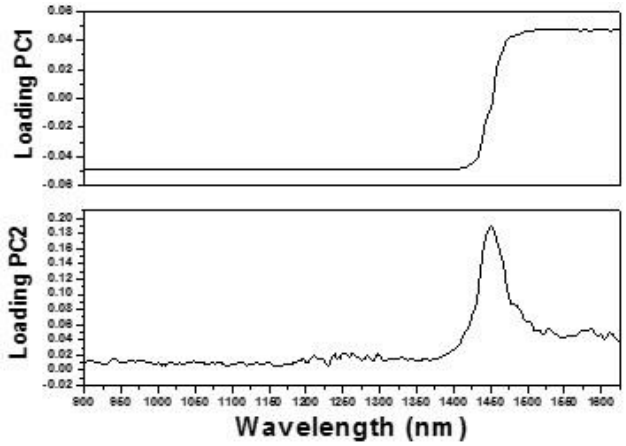

Figure 9. PCA-Loading plots for PC1 and PC2 as wavelength function for the NIR spectra of the stage two.

PC1-loading suggest that the band shift in 1445 nm is the most important effect caused by the temperature in the NIR spectra in the range from 900 to 1600 nm and the linear behavior observed in the range from 900 to 1420 nm, and from 1460 to 1600 nm, means that spectral variations in those variables are constant. However, in the region from 1420 to 1460 nm are located the largest loadings, which correspond to the most important diagnostic variables related with the temperature effect. The PC2-loading plot, show a band centered in approximately 1450 nm, which could be associated to intralipid scattering effects related indirectly with the temperatura.

Table 3. Absorbance intensity at 1000, 1440 and 1550 nm as temperature function.

Temp. (ºC)	*Absorbance at 1000 nm*	*Absorbance at 1440 nm*	*Absorbance at 1550 nm*
30	0.676	1.393	1.149
32	0.677	1.392	1.147
34	0.680	1.395	1.148
36	0.682	1.395	1.144
38	0.683	1.396	1.143
40	0.684	1.396	1.141
42	0.686	1.397	1.139
44	0.688	1.398	1.138
46	0.688	1.391	1.130
48	0.689	1.398	1.132
50	0.689	1.397	1.130

Also, the PC2-loading plot, show a band centered in approximately 1450 nm, which could be associated to intralipid scattering effects related indirectly with the temperature.

In order to obtain the correlation values between the spectral variations and the temperature effect, we using the PLSR method in a full cross validation with two PCs. The r2 and RMSEC values are displayed in the table 4. The high correlation values, indicate that, spectral variations in the

NIR spectra of stage two, are mainly due to the temperature effect.

Table 4. Correlation coefficients and Root mean square error of calibration values of the spectroscopic data of stage two.

Experiment	r^2	RMSEC (ºC)
1	0.99	0.85
2	0.99	0.81
3	0.99	0.51
4	0.99	0.22

In the figure 10, are plotted the glucose prediction values obtained in the stage three, for each experiment, their average value and the fitting values. The data are displayed in the table 5.

Finally, we obtain that, the temperature causes a similar effect, than the caused by the change in the glucose concentration, causing evident changes in the broadband centered at 1445 nm. As consequence, the temperature effect causes a Bias error of 672.8 mg dL^{-1}, in our glucose predictions when the variations due to temperature are no taken into account in the calibration of the glucose prediction model. The Bias error was calculated using the theoretical values obtained of the polynomial fitting (table 5, column 8). The Bias error obtained is in agreement with the theoretical value calculated and reported by Masatoshi et al.

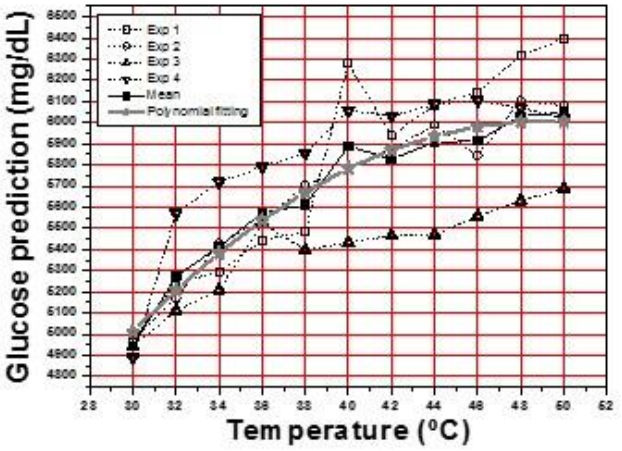

Figure 10. Plot of predicted values obtained for each experiment, their mean predicted values (fill black square + black line) and the calculated values obtained of the polynomial adjust of the mean predicted values (Gray stars + gray line).

Conclusions

Multivariate methods are a powerful tool for the spectral data analysis. In this work we showed the application of multivariate data analysis for the particular study and quantification of the temperature effect over the NIR diffuse reflectance measurements, in order to quantify the glucose concentration in a scatterer medium using a PLSR model.

The temperature variations in the sample cause a similar effect than caused by the variation in the glucose concentration, as is showed in the PCA-loading plots obtained in the stage one and two, where its evident that the band centered at 1445 nm is temperature-sensitive, and show the most important spectral variations for glucose and temperature changes. These effects were analyzed and demonstrated by PCA and PLSR methods. Finally we calculated a Bias error of 672.8 mg dL^{-1} per Celsius degree, induced by the temperature, in the prediction of glucose concentration.

Table 5. Glucose prediction, mean and polynomial fitting values obtained in the stage three and plotted in the figure 10**.**

Temperature (ºC)	Reference (mg/dL)	Prediction (mg/dL) Exp 1	Prediction (mg/dL) Exp 2	Prediction (mg/dL) Exp 3	Prediction (mg/dL) Exp 4	Mean Prediction (mg/dL)	Polynomial fitting (mg/dL)
30	5000	4975	4965	4940	4887	4942	5012
32	5000	5239	5170	5111	5571	5273	5208
34	5000	5297	5431	5210	5720	5414	5384
36	5000	5444	5535	5527	5792	5574	5538
38	5000	5484	5703	5398	5855	5610	5672
40	5000	6280	5786	5432	6057	5889	5784
42	5000	5938	5874	5467	6031	5827	5871
44	5000	6084	5989	5470	6087	5907	5936
46	5000	6144	5845	5558	6105	5913	5981
48	5000	6320	6104	5630	6069	6031	6004
50	5000	6397	6080	5690	6023	6048	6006

Acknowledgments

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