Arabian Journal of Chemistry (2014) xxx, xxx–xxx

King Saud University

Arabian Journal of Chemistry

www.ksu.edu.sa
www.sciencedirect.com

ORIGINAL ARTICLE

The comparison of partial least squares and principal component regression in simultaneous spectrophotometric determination of ascorbic acid, dopamine and uric acid in real samples

Habiboallah Khajehsharifi [a,*], Eslam Pourbasheer [b], Hossein Tavallali [c], Solmaz Sarvi [c], Maasumeh Sadeghi [a]

[a] *Department of Chemistry, Yasouj University, Under Hill, Yasouj, Iran*
[b] *Department of Chemistry, Faculty of Science, University of Qom, Qom, Iran*
[c] *Department of Chemistry, Payame Noor University (PNU), Shiraz, Iran*

Received 17 October 2012; accepted 16 February 2014

KEYWORDS

Partial least squares;
Principal component regression;
Serum;
Urine;
Pharmaceutical formulations

Abstract Partial least squares (PLS1) and principal component regression (PCR) are two multivariate calibration methods that allow simultaneous determination of several analytes in spite of their overlapping spectra. In this research, a spectrophotometric method using PLS1 is proposed for the simultaneous determination of ascorbic acid (AA), dopamine (DA) and uric acid (UA). The linear concentration ranges for AA, DA and UA were 1.76–47.55, 0.57–22.76 and 1.68–28.58 (in μg mL^{-1}), respectively. However, PLS1 and PCR were applied to design calibration set based on absorption spectra in the 250–320 nm range for 36 different mixtures of AA, DA and UA, in all cases, the PLS1 calibration method showed more quantitative prediction ability than PCR method. Cross validation method was used to select the optimum number of principal components (NPC). The NPC for AA, DA and UA was found to be 4 by PLS1 and 5, 12, 8 by PCR. Prediction error sum of squares (PRESS) of AA, DA and UA were 1.2461, 1.1144, 2.3104 for PLS1 and 11.0563, 1.3819, 4.0956 for PCR, respectively. Satisfactory results were achieved for the simultaneous determination of AA, DA and UA in some real samples such as human urine, serum and pharmaceutical formulations.

* Corresponding author. Tel./fax: +98 7412223048.
E-mail addresses: khajeh_h@yahoo.com, haka@yu.ac.ir (H. Khajehsharifi).

Peer review under responsibility of King Saud University.

Production and hosting by Elsevier

1. Introduction

Ascorbic acid (AA), dopamine (DA) and uric acid (UA) are the compounds of great biological and chemical interest that play important roles in the functioning of the human metabolism, central nervous and renal systems (Zare et al., 2006).

1878-5352 © 2014 Production and hosting by Elsevier B.V. on behalf of King Saud University.
http://dx.doi.org/10.1016/j.arabjc.2014.02.006

AA is a soluble vitamin present in many biological systems and in multivitamin preparations which are commonly used to supplement inadequate dietary intake and also as anti-oxidants. The concentration of AA in foodstuffs, beverages and pharmaceuticals can be an index of quality since it changes during production and storage stages (Fox and Cameron, 1989; Yu and Chen, 1997). Ascorbic acid has been used for the prevention and treatment of common colds, mental illnesses, infertility, cancers, and in some clinical manifestations of HIV infections (Arrigori and Tullio, 2002). Similarly, DA is an important neurotransmitter in the brain's neural circuits (Blakely, 2001). It is involved in the functioning of renal, cardiovascular, hormonal and nervous systems. DA is also involved in neurological diseases such as Parkinson (Marceglia et al., 2006), Alzheimer (Kemppainen et al., 2001) and Schizophrenia (Schwieler et al., 2004). Lastly, UA is the final product of purine metabolism in the human body (Simoni et al., 2007) and its excessive accumulation can lead to a type of arthritis known as gout. Also, disorders in purine biosynthesis or purine catabolism can cause hyperuricemia and Lesch–Nyhan syndrome (Cossu et al., 2006). The normal UA level in blood is in the 120–450 μM range whereas in urine it is in the millimolar range (2 mM) (Popa et al., 2000). Therefore, it is essential to develop simple and rapid methods for the determination of these biological molecules in a routine analysis.

Several methods such as electrochemical methods (Argüello et al., 2008; Huang et al., 2008; Liu et al., 2008; Thiagarajan and Chen, 2007; Kang and Lin, 2006; Safavi et al., 2006; Zare et al., 2005; Gao and Huang, 1998), HPLC methods (Ferin et al., 2013) fluorescence (Haloi et al., 2013) and spectrophotometric methods (Rohani Moghadam et al., 2011) have been developed for the quantitation of AA, DA and UA, some of which were difficult to operate and use expensive instruments. Spectrophotometric methods are in general simple, sensitive and suitable for the analysis of analytes in different samples. However, in many cases, the spectral responses of two and sometimes even more components overlap considerably and the analysis is no longer straightforward. Multivariate spectral calibration is now becoming a standard method for quantitative spectral analysis, allowing simultaneous determination of several analytes. Partial least squares (PLS) and principal component regression (PCR) are two full-spectrum and factor analysis based on multivariate calibration methods that have received considerable attention in the chemometrics literatures (Geladi and Kowalski, 1986; Haaland and Thomas, 1988a,b; Haaland and Thomas, 1990; Gerlach et al., 1979; Beebe et al., 1987) and several multicomponent determinations based on the application of these methods to spectrophotometric data have been discussed by several workers (Espinosa-Mansilla et al., 1998; Navalon et al., 1999; Ribone et al., 2000; Al-Degs and Sweileh, 2012; Sarlak and Anizadeh, 2011; Rezaei et al., 2005).

To the best of our knowledge, in the literature, there has been no report on the simultaneous determination of AA, DA and UA by UV–VIS spectrophotometric measurements using multivariate calibration. The present work addresses UV–VIS spectrophotometry which has been applied for quantitative simultaneous determination of AA, DA and UA by PLS regression that performed in the PLS1 and PCR fashion for the calibration and validation of the proposed method and resolve three mixtures of AA, DA and UA in synthetic and real samples.

2. Experimental

2.1. Apparatus

Absorption spectra were recorded on a range of 250–320 nm in a 10 mm quartz cell by a Perkin Elmer Lambda 2 spectrophotometer and software UV-Winlab was used for spectral acquisition and elaboration. The pH measurement was made with a JENWAY/1000 model 3510 using a combined glass electrode. PLS regression and other calculations were performed in the MATLAB (version 7.6.0) environment. The PLS toolbox 2.5 developed by Eigenvector was used for calibration and model validation.

2.2. Chemicals

All chemicals were of analytical grade. Doubly distilled water was used to prepare the solutions. Stock solutions of AA, DA and UA (Merck) were prepared by dissolving appropriate amount of each component in little water and then made up to volume with a buffer (pH = 7.0). These solutions were prepared fresh daily. The buffer solution was made by NaH_2PO_4.

Table 1 Concentration data of the calibration set for three-component system using mixture design.

Mixture	AA ($\mu g\ mL^{-1}$)	DA ($\mu g\ mL^{-1}$)	UA ($\mu g\ mL^{-1}$)
1	1.76	0.57	28.58
2	1.76	3.79	25.22
3	1.76	6.64	21.01
4	1.76	10.43	16.81
5	1.76	13.27	13.45
6	1.76	16.12	9.25
7	1.76	19.91	5.04
8	1.76	22.76	1.68
9	8.81	0.57	25.22
10	8.81	19.91	1.68
11	14.97	0.57	21.01
12	14.97	16.12	1.68
13	14.97	19.91	25.22
14	21.13	0.57	16.81
15	21.13	13.27	1.68
16	21.13	16.12	25.22
17	21.13	19.91	21.01
18	28.18	0.57	13.45
19	28.18	10.43	1.68
20	28.18	13.27	25.22
21	28.18	16.12	21.01
22	28.18	19.91	16.81
23	34.34	0.57	9.25
24	34.34	6.64	1.68
25	34.34	10.43	25.22
26	34.34	13.27	21.01
27	34.34	16.12	16.81
28	34.34	19.91	13.45
29	40.51	0.57	5.04
30	40.51	3.79	1.68
31	40.51	6.64	25.22
32	40.51	10.43	21.01
33	40.51	13.27	16.81
34	40.51	16.12	13.45
35	40.51	19.91	9.25
36	47.55	0.57	1.68

Please cite this article in press as: Khajehsharifi, H. et al., The comparison of partial least squares and principal component regression in simultaneous spectrophotometric determination of ascorbic acid, dopamine and uric acid in real samples. Arabian Journal of Chemistry (2014), http://dx.doi.org/10.1016/j.arabjc.2014.02.006

Table 2 Added and found results of the synthetic mixture of AA, DA and UA for PLS1 and PCR.

PLS	Added ($\mu g\ mL^{-1}$)			Found ($\mu g\ mL^{-1}$)			Recovery (%)		
	AA	DA	UA	AA	DA	UA	AA	DA	UA
Mixture									
1	7.04	0.95	16.81	6.96	0.98	17.78	98.81	103.16	105.75
2	17.61	4.74	6.72	17.29	4.68	6.42	98.18	98.73	95.54
3	36.42	5.69	11.77	36.80	5.40	11.55	101.03	94.90	98.16
4	26.42	10.87	8.40	27.24	11.06	8.95	103.10	101.75	105.51
5	8.81	14.22	20.17	8.58	14.00	20.87	97.39	98.45	103.46
6	21.13	3.79	5.04	21.6	3.77	5.25	102.23	99.47	104.10
7	5.28	17.07	15.13	5.50	18.04	15.83	104.17	105.68	104.63
Mean ± S.D.							100.70 ± 2.62	100.31 ± 3.53	102.45 ± 3.98
PCR	Added ($\mu g\ mL^{-1}$)			Found ($\mu g\ mL^{-1}$)			Recovery (%)		
	AA	DA	UA	AA	DA	UA	AA	DA	UA
1	7.04	0.95	16.81	6.33	1.03	18.06	89.91	108.42	107.44
2	17.61	4.74	6.72	16.01	4.50	7.10	90.91	94.93	105.65
3	36.42	5.69	11.77	38.79	5.13	11.58	106.51	90.16	98.38
4	26.42	10.87	8.40	27.64	11.19	8.87	104.62	102.94	104.60
5	8.81	14.22	20.17	9.68	14.40	20.97	109.88	101.26	103.97
6	21.13	3.79	5.04	21.01	4.18	5.42	99.43	110.29	107.54
7	5.28	17.07	15.13	4.94	16.99	16.32	93.56	99.53	107.86
Mean ± S.D.							99.26 ± 8.00	101.08 ± 7.09	105.06 ± 3.32

2.3. Procedure

A 0.0440 g of AA, 0.047 g of DA and 0.0420 g of UA were dissolved in a little amount of water separately and then diluted with a buffer solution to 25.0 mL. (UA was not soluble in water, so a little of dilute KOH was used to solve it and then diluted with a buffer). The concentrations of each stock solution were 10^{-2} mol L^{-1}. Then they were used to set up the calibration set with concentration established according to the mixture design. An independent prediction set of ternary mixtures, randomly established, was prepared to validate the elaborated multivariate models.

2.4. Multivariate calibration

Multivariate calibration methods, such as PLS and PCR, require a suitable experimental design of a standard belonging to the calibration set in order to provide a good prediction. The first step in the simultaneous determination of the analytes by PLS1 and PCR methodologies involved constructing a calibration mixture for the mixtures of AA, DA and UA. For this purpose, a synthetic set of 43 solutions of mixtures of AA, DA and UA were prepared in the concentration ranges. From these series, 36 solutions were chosen for calibration set according to the mixture design for three component systems (Table 1), and 7 solutions, that were chosen randomly, were used for prediction set (Table 2).

2.5. Real samples' preparation

Human serum and urine, vitamin C tablets (250 mg per tablet) and dopamine injection (200 mg/5 mL) are the real samples which were used. Fresh human serum and urine samples were obtained from clinical laboratories. The serum samples were homogenized. For the deproteinization, 1 mL of 24% w/v trichloroacetic acid was added to 1 mL of serum. After 15 min, the resulting mixture was centrifuged for 15 min at 3000 rpm. Then, NaOH solution was added to the supernatant solution to reach a final pH value of 7.0. Afterwards, an appropriate amount from the stock solution of AA, DA and UA was added to 0.5 mL of the finally prepared serum and then it was completed to the final volume (10 mL volumetric flask) with a buffer solution to obtain the desired concentration in the linear range. The electronic absorption spectrum was recorded in the range of 250–320 nm against a blank solution of universal serum (Khajehsharifi and Pourbasheer, 2008). The urine sample was diluted 1:3 with distilled water. Then, the cell debris and the particulate matter were removed from the urine using low-speed centrifugation (for 5 min at 1500 rpm). Afterwards, NaOH solution was added to the supernatant solution until its final pH value amounted to 7.0. Moreover, appropriate amounts from the stock solution of AA, DA and UA were added to 0.5 mL of the finally prepared urine and completed to the final volume (10 mL volumetric flask) with a buffer solution to get the desired concentration in the linear range (Khajehsharifi and Pourbasheer, 2008). The sample of vitamin C was obtained initially from dissolution of tablets in water. The solution was filtered, then diluted and used to determine AA in the sample (Babaei et al., 2008). In order to verify the reliability of the method for analysis of DA in pharmaceutical product, PLS1 model was also applied to determine DA in dopamine injection. For the assay of DA, the sample must have been diluted appropriately within the linear range of the determination of DA. The ampoules we used were 5 mL, containing 200 mg dopamine (Wei et al., 2007).

3. Results and discussion

3.1. Spectroscopic measurements

Fig. 1 shows the absorption spectra in aqueous solution of ascorbic acid, dopamine and uric acid separately at

Please cite this article in press as: Khajehsharifi, H. et al., The comparison of partial least squares and principal component regression in simultaneous spectrophotometric determination of ascorbic acid, dopamine and uric acid in real samples. Arabian Journal of Chemistry (2014), http://dx.doi.org/10.1016/j.arabjc.2014.02.006

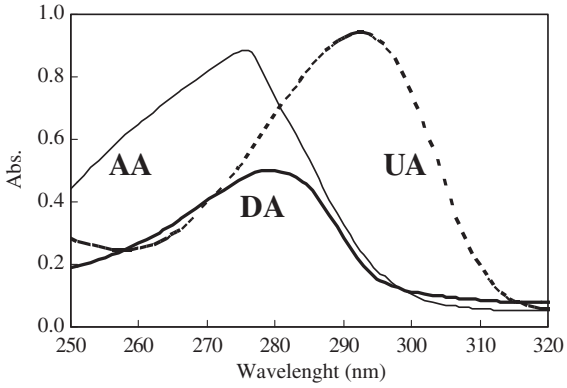

Figure 1 Absorption spectra of AA (21.13 μg mL^{-1}), DA (10.75 μg mL^{-1}), and UA (15.13 μg mL^{-1}) in pH = 7.0, at 25 °C.

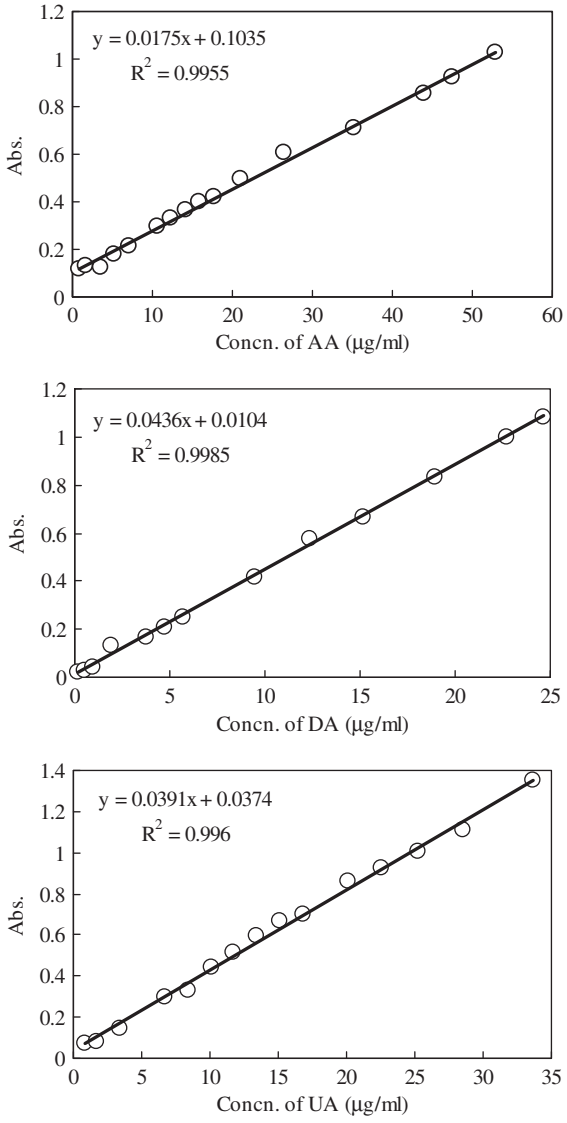

Figure 2 Analytical curve for univariate determination of AA, DA and UA.

pH = 7.0. The simultaneous determination of AA, DA and UA in mixtures by common spectrophotometric methods is hindered by spectral overlap throughout the wavelength range. Such a determination could theoretically be facilitated by some of chemometrics methods.

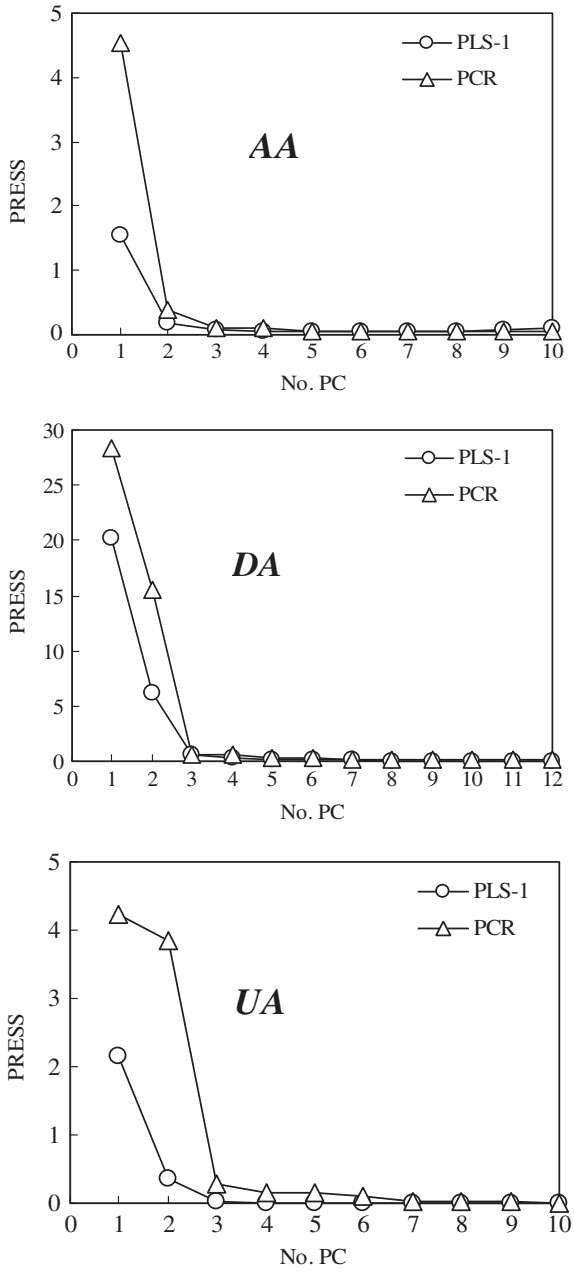

Figure 3 Plots of PRESS vs. No. of PC by PLS1 and PCR for AA, DA and UA.

3.2. Partial least squares and principal component regression

Principal component regression and partial least squares regression are two related families of methods that are often used in chemometrics. Both involve selecting a subspace of the column space of X on which to project the response vector Y. The use of PLS method for chemical applications was initiated by Joreskog and Wold (Joreskog and Wold, 1982). PLS is a quantitative spectral decomposition technique that is closely related to principal component regression (PCR). However, in

Please cite this article in press as: Khajehsharifi, H. et al., The comparison of partial least squares and principal component regression in simultaneous spectrophotometric determination of ascorbic acid, dopamine and uric acid in real samples. Arabian Journal of Chemistry (2014), http://dx.doi.org/10.1016/j.arabjc.2014.02.006

Table 3 Statistical parameters of the PLS1 and PCR models.

		AA	DA	UA
PLS1	LV[a]	4	4	4
	PRESS[b]	1.2461	1.1144	2.3104
	RMSEP[c]	0.4219	0.3990	0.5745
	SEC[d]	0.2005	0.1896	0.2730
PCR	LV	5	12	8
	PRESS	11.0563	1.3819	4.0956
	RMSEP	1.2568	0.4443	0.7649
	SEC[d]	0.6071	0.2451	0.3895

[a] Latent variable.
[b] Prediction error sum of square.
[c] Root mean square error of prediction.
[d] Standard error of calibration.

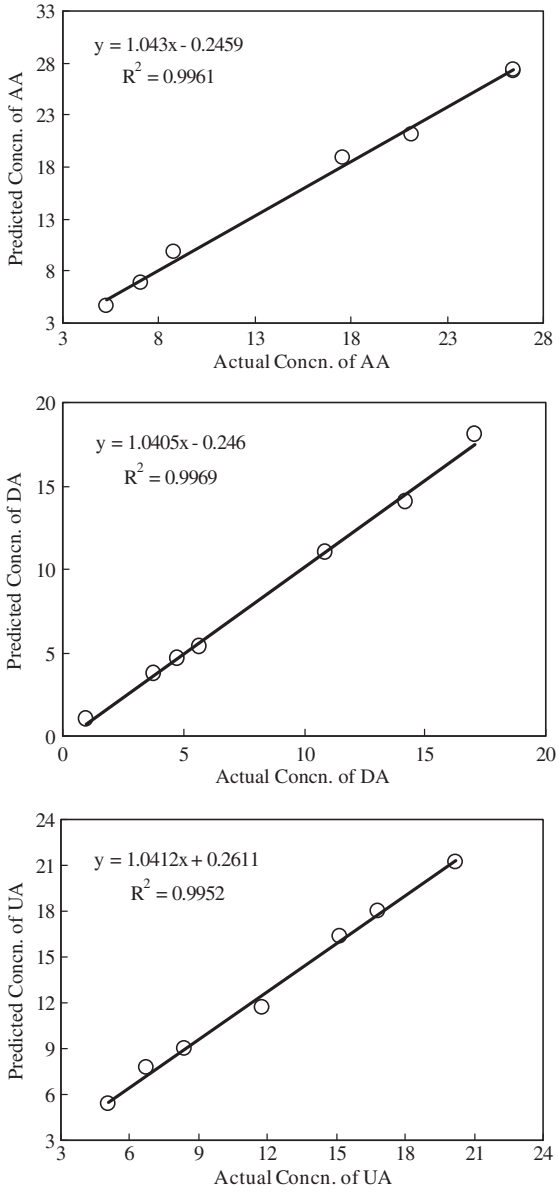

Figure 4 Plots of predicted concentration vs. actual concentration for AA, DA and UA by PLS1.

PLS the decomposition is performed in a slightly different fashion. Instead of first decomposing the spectral matrix into a set of scores and loadings, and regress for them against the concentrations as a separate step, PLS actually uses the concentration information during the decomposition process. Thus, the scores and loadings, calculated using PLS, is quite different from those of PCR. The main idea of PLS is to get as much concentration information as possible into the first few loading vectors. There are actually two versions of the PLS algorithm, PLS1 and PLS2.

The PLS1 corresponds to the case where there is only one dependent variable but the PLS2 corresponds to the case where there are several dependent variables. The differences between these methods are subtle but have very important effects on the results. In PLS1, a separate set of scores and loading vectors is calculated for each constituent of interest. In this case, the separate set of scores and loading vectors are specifically tuned for each constituent, and therefore, should give more accurate predictions than PCR or PLS2 (Khajehsharifi et al., 2004). An important feature of PLS is that it takes into account errors in both the concentration estimates and the spectra. A method such as PCR assumes that the concentration estimates are error free (Brereton, 2003).

3.3. Univariate calibration

The temperature has no appreciable effect on the spectra of the analytes, so 25 °C was chosen as a suitable temperature in this study. Furthermore, pH = 7.0 was selected to obtain sufficient data points in biological conditions. The individual calibration curves for each analyte have been determined by plotting the absorbencies at the corresponding λ_{max} versus the analytes' concentration in the linear range for AA, DA, and UA (Fig. 2). Line equations and R^2 are also shown in Fig. 2. The concentration ranges for AA, DA and UA were 1.76–47.55, 0.57–22.76 and 1.68–28.58 (in μg mL^{-1}), respectively. The λ_{max} that recorded for AA, DA and UA were 276.0, 280.0 and 292.0 nm respectively.

3.4. Selection of the optimum number of factors

Selecting the number of loading vectors (or alternatively, the number of scores or factors), allows to model as much of the complexity of the system without over-fitting the concentration data. To accomplish this goal, leave-one-out cross-validation was used and then PLS and PCR calibrations were used for the remaining standard spectra (Stone, 1974; Martens and Naes, 1991). By using this calibration, the concentration of the sample left out was predicted. This process was repeated until each standard had been left out once. The concentration predicted for each sample is then compared with the known concentration of this reference sample. The sum of the squared concentration prediction errors for all calibration samples (prediction error sum of squares or PRESS) is a measure of how well, a particular PLS1 and PCR model fits the concentration data, which is defined as follows:

$$\mathrm{PRESS} = \sum_{i=1}^{n} (\hat{c}_i - c_i)^2$$

where c_i is the added concentration of the analyte and $\hat{c}_i$ represents the found concentration of the analyte in sample

Please cite this article in press as: Khajehsharifi, H. et al., The comparison of partial least squares and principal component regression in simultaneous spectrophotometric determination of ascorbic acid, dopamine and uric acid in real samples. Arabian Journal of Chemistry (2014), http://dx.doi.org/10.1016/j.arabjc.2014.02.006

i. PRESS is calculated in the same manner each time a new factor is added to the models. One reasonable choice for the optimum number of factors would be the number that yielded the minimum PRESS. Since, there is a finite number of samples in the training set, in many cases the minimum PRESS value causes over-fitting for unknown samples that were not included in the model. A solution to this problem has been suggested by Haaland and Thomas (1988a,b), (1990). In all cases, the number of factors for the first PRESS values whose F-ratio probability drops to below 0.75 was selected as the optimum. Fig. 3 shows the PRESS obtained by optimizing the calibration matrix of the absorption spectra with PCR and PLS1 methods.

3.5. Statistical analysis

Prediction capability of the chemometric calibrations was evaluated by the standard error of calibration (SEC) and the root mean standard error of prediction (RMSEP) as follows (Kramer, 1998):

$$\mathrm{SEC} = (\mathrm{PRESS}/n_c - f - 1)^{1/2}$$
$$\mathrm{RMSEP} = (\mathrm{PRESS}/n_p)^{1/2}$$

where n_c is the total number of samples in calibration set, f is the number of factors and n_p is the total number of samples in prediction set. The value of these statistical parameters and number of factors in the optimum number of factors calculated for AA, DA and UA concentration by PLS1 and PCR are reported in Table 3.

3.6. Synthetic mixtures and real sample analysis

The predictive ability of the method was determined by using 7 three-component mixtures (their compositions are given in Table 2). The results, by applying PLS1 and PCR algorithm to seven synthetic samples, are listed in Table 2, which also shows the recovery for the synthetic series of AA, DA and UA mixtures. As it can be seen, the recovery was also acceptable. The plots of the predicted concentration versus actual values by the PLS1 method for AA, DA and UA are shown in Fig. 4. According to the results, PLS1 model is capable of predict the concentrations of AA, DA and UA in the mixtures. The good recoveries of the mixture samples indicate the successful applicability of the proposed method for the simultaneous determination of AA, DA, and UA.

In addition, we tested the real applicability of the method for the determination of AA in commercially available vitamin C tablets, DA in dopamine hydrochloride injection, and DA plus UA plus AA in spiked serum and urine samples. The data presented are the average of three determinations (Table 4).

4. Conclusion

The most important aspect of this paper is the spectrophotometry simultaneous determination of ascorbic acid, dopamine and uric acid in spite of their overlapping spectra. PLS1 and PCR were applied for the resolution of the three-component mixture of AA, DA and UA. Based on the results of the present research, it was shown that the best recovery values were obtained by the application of PLS1 model to the absorbance spectra of AA, DA and UA. In addition, in comparison with the other methods such as electrochemical [12–19], the proposed work is superior, in view of simplicity, low cost, and satisfactory recoveries.

Moreover, the results obtained from the application of the proposed method for determining AA, DA, and UA in real samples such as urine, serum and pharmaceutical samples confirmed the good accuracy and precision of our proposed method.

Table 4 Recovery of the assay measured in a human urine, serum and pharmaceutical preparations.

Real sample	Analytes	Added	Found[a]	Recovery (%)
Urine	AA	0	ND	
	AA	10.0	9.2(±3.5)	92
	DA	0	ND[b]	–
	DA	10.0	9.8(±1.1)	98
	UA	0	9.5(±1.8)	–
	UA	10.0	19.7(±0.9)	102
Serum	AA	0	ND	
	AA	20.0	19.6(±3.3)	98
	DA	0	ND	
	DA	20.0	20.3(±1.7)	101.5
	UA	0	2.4(±1.0)	
	UA	10.0	13.1(±1.9)	107
Vitamin C tablet[c]	AA	–	18.2(±3.7)	
	AA	10.0	27.7(±2.8)	95
Dopamine[d]	DA	–	19.3(±4.2)	
	DA	20.0	38.7(±3.1)	97

[a] Mean value ± standard deviation (n = 3).
[b] No detected.
[c] Vitamin C tablet: (label amount: 250 mg/tablet), Osveh pharmaceutical Co. (Tehran, Iran).
[d] Dopamine hydrochloride injection, 200 mg/5 mL, Caspian Tameen pharmaceutical Co. (Rasht, Iran).

Please cite this article in press as: Khajehsharifi, H. et al., The comparison of partial least squares and principal component regression in simultaneous spectrophotometric determination of ascorbic acid, dopamine and uric acid in real samples. Arabian Journal of Chemistry (2014), http://dx.doi.org/10.1016/j.arabjc.2014.02.006

5. Conflict of interest

There is no conflict of interest to declare.

Acknowledgment

This work was supported by the Shiraz Payame Noor University Research Council.

References

Al-Degs, Y.S., Sweileh, J.A., 2012. Simultaneous determination of five commercial cationic dyes in stream waters using diatomite solid-phase extractant and multivariate calibration. Arabian J. Chem. 5, 219–224.

Argüello, J., Leidens, V.L., Magosso, H.A., Ramos, R.R., Gushikem, Y., 2008. Simultaneous voltammetric determination of ascorbic acid, dopamine and uric acid by methylene blue adsorbed on a phosphorylated zirconia–silica composite electrode. Electrochim. Acta 54, 560–565.

Arrigori, O., Tullio, C.D., 2002. Ascorbic acid: much more than just an antioxidant. Biochim. Biophys. Acta 1569, 1–3.

Babaei, A., Zendehdel, M., Khalilzadeh, B., Taheri, A., 2008. Simultaneous determination of tryptophan, uric acid and ascorbic acid at iron (III) doped zeolite modified carbon paste electrode. Colloids Surf. B 66, 226–232.

Beebe, K.R., Kowalski, B.R., Wold, H., 1987. An introduction to multivariate calibration and analysis. Anal. Chem. 59, 1007A–1017A.

Blakely, R.D., 2001. Dopamine's reversal of fortune. Science 293, 2407–2409.

Brereton, R.G., 2003. Chemometrics, Data Analysis for the Laboratory and Chemical Plant. John Wily and Sons Ltd., England.

Cossu, A., Orru, S., Jacomelli, G., Carcassi, C., Contu, L., Sestini, M.R., Pompucci, G., Carcassi, A., Micheli, V., 2006. HPRTSardinia: a new point mutation causing HPRT deficiency without Lesch-Nyhan disease. Biochim. Biophys. Acta 1762, 29–33.

Espinosa-Mansilla, A., Duran-Meras, I., Salinas, F.J., 1998. Simultaneous determination of pteridines in multicomponent mixtures using derivative spectrophotometry and partial least-squares calibration. Pharm. Biomed. Anal. 17, 1325–1334.

Ferin, R., Leonor Pavão, M., Baptista, J., 2013. Rapid, sensitive and simultaneous determination of ascorbic and uric acids in human plasma by ion-exclusion HPLC-UV. Clin. Biochem. 46, 665–669.

Fox BA, Cameron AG. 1989. Food Science, Nutrition and Health, E. Arnold (Ed.), Electrocatalytic oxidation and determination of ascorbic acid at poly (glutamic acid) chemically modified electrode. CRC Press, London, p. 261.

Gao, Z.Q., Huang, H., 1998. Simultaneous determination of dopamine, uric acid and ascorbic acid at an ultrathin film modified gold electrode. Chem. Commun. 19, 2107–2108.

Geladi, P., Kowalski, B.R., 1986. Partial least-squares regression. A tutorial. Anal. Chim. Acta 185, 1–18.

Gerlach, R.W., Kowalski, B.R., Wold, H., 1979. Partial least-squares path modeling with latent variables. Anal. Chim. Acta 112, 417–421.

Haaland, D.M., Thomas, E.V., 1988a. Partial least-squares methods for spectral analyses, Relation to other quantitative calibration methods and the extraction of qualitative information. Anal. Chem. 60, 1193–1202.

Haaland, D.M., Thomas, E.V., 1988b. Partial least-squares methods for spectralanalyses, application to simulated and glass spectral data. Anal. Chem. 60, 1202–1208.

Haaland, D.M., Thomas, E.V., 1990. Comparison of multivariate calibration methods for quantitative spectral analysis. Anal. Chem. 62, 1091–1099.

Haloi, S., Goswami, P., Kumar, Das.D., 2013. Differentiating response of 2,7-dichlorofluorescein intercalated CTAB modified Na-MMT clay matrix towards dopamine and ascorbic acid investigated by electronic, fluorescence spectroscopy and electrochemistry. Appl. Clay Sci. 77, 79–82.

Huang, J., Liu, Y., Hou, H., You, T., 2008. Simultaneous electrochemical determination of dopamine, uric acid and ascorbic acid using palladium nanoparticle-loaded carbon nanofibers modified electrode. Biosens. Bioelect. 24, 632–637.

Joreskog, K.G., Wold, H., 1982. System Under Indirect Observations. North Holand, Amsterdam, The Netherlands.

Kang, G.F., Lin, X.Q., 2006. RNA modified electrodes for simultaneous determination of dopamine and uric acid in the presence of high amounts of ascorbic acid. Electroanaysis 18, 2458–2466.

Kemppainen, N., Marjamaki, P., Roytta, M., Rinne, J., 2001. Different pattern of reduction of striatal dopamine reuptake sites in Alzheimer's disease and ageing. J. Neura Transm. 108, 827–836.

Khajehsharifi, H., Pourbasheer, E., 2008. Genetic- algorithm- based wavelength selection in multicomponent spectrophotometric determination by PLS: application on ascorbic acid and uric acid mixture. J. Chin. Chem. Soc. 55, 163–170.

Khajehsharifi, H., Mousavi, M.F., Ghasemi, J., Shamsipur, M., 2004. Kinetic spectrophotometric method for simultaneous determination of selenium and tellurium using partial least squares calibration. Anal. Chim. Acta 512, 369–373.

Kramer, R., 1998. Chemometric Techniques for Quantitative Analysis. Marcel Dekker, New York.

Liu, Y., Huang, J., Hou, H., You, T., 2008. Simultaneous determination of dopamine, ascorbic acid and uric acid with electrospun carbon nanofibers modified electrode. Electrochem. Commun. 10, 1431–1434.

Marceglia, S., Foffani, G., Bianchi, A., Baselli, G., Tamma, F., Egidi, M., Priori, A., 2006. Dopamine-dependent non-linear correlation between subthalamic rhythms in Parkinson's disease. J. Physio. 571, 579–591.

Martens, H., Naes, T., 1991. Multivariate Calibration. John Wiley, New York.

Navalon, A., Blanc, R., del Olmo, M., Vilchez, J.L., 1999. Simultaneous determination of naproxen, salicylic acid and acetylsalicylic acid by spectrofluorimetry using partial least-squares (PLS) multivariate calibration. Talanta 48, 469–475.

Popa, E., Kubota, Y., Tryk, D.A., Fijishima, A., 2000. Voltammetric and amperometric detection of uric acid with oxidized diamond film electrodes. Anal. Chem. 72, 1724–1727.

Rezaei, Z., Hemmateenejad, B., Khabnadideh, S., Gorgin, M., 2005. Simultaneous spectrophotometric determination of carbamazepine and phenytoin in serum by PLS regression and comparison with HPLC. Talanta 65, 21–28.

Ribone, M.E., Pagani, A.P., Olivieri, A.C., 2000. Determination of the minor component bromhexine in cotrimoxazole-containing tablets by absorption spectrophotometry and partial least-squares (PLS-1) multivariate calibration. J. Pharm. Biomed. Anal. 23, 591–595.

Rohani Moghadam, M., Dadfarnia, S., Haji Shabani, A.M., Shahbazikhah, P., 2011. Chemometric-assisted kinetic–spectrophotometric method for simultaneous determination of ascorbic acid, uric acid, and dopamine. Anal. Biochem. 410, 289–295.

Safavi, A., Maleki, N., Moradlou, O., Tajabadi, F., 2006. Simultaneous determination of dopamine, ascorbic acid, and uric acid using carbon ionic liquid electrode. Anal. Biochem. 359, 224–229.

Sarlak, N., Anizadeh, M., 2011. Simultaneous kinetic spectrophotometric determination of sulfide and sulfite ions by using an optode and the partial least squares (PLS) regression. Sensor. Actuat. B-Chem. 160, 644–649.

Schwieler, L., Engberg, G., Erhardt, S., 2004. Clozapine modulates midbrain dopamine neuron firing via interaction with the NMDA receptor complex. Synapse 52, 114–122.

Simoni, R.E., Ferreira, L.N.L., Scalco, F.B., Oliveria, C.P.H., Aquino, F.R., Oliveria, M.L.C., 2007. Uric acid changes in urine and

plasma: an effective tool in screening for purine inborn errors of metabolism and other pathological conditions. J. Inherit. Metab. Dis. 30, 295–309.

Stone, M., 1974. Cross-validatory choice and assessment of statistical predictions (with discussion). J. Roy. Statist. Soc. 36, 111–147.

Thiagarajan, S., Chen, M., 2007. Preparation and characterization of PtAu hybrid film modified electrodes and their use in simultaneous determination of dopamine, ascorbic acid and uric acid. Talanta 74, 212–222.

Wei, W., Wang, H.J., Jiang, C.Q., 2007. Spectrofluriometric determination of dopamine using 1,5-bis (4,6-dicholro-1,3,5-triazinylamino) naphthalene. Luminescence 22, 581–587.

Yu, A.M., Chen, H.Y., 1997. Electrocatalytic oxidation and determination of ascorbic acid at poly (glutamic acid) chemically modified electrode. Anal. Chim. Acta 344, 181–185.

Zare, H.R., Nasirizadeh, N., Ardakani, M.M., 2005. Voltammetric studies of an oracet blue modified glassy carbon electrode and its application for the simultaneous determination of dopamine, ascorbic acid and uric acid. J. Electroanal. Chem. 577, 25–33.

Zare, H.R., Rajabzade, N., Nasirizadeh, N., Ardakani, M.M., 2006. Voltammetric studies of an oracet blue modified glassy carbon electrode and its application for the simultaneous determination of dopamine, ascorbic acid and uric acid. J. Electroanal. Chem. 589, 60–69.

Please cite this article in press as: Khajehsharifi, H. et al., The comparison of partial least squares and principal component regression in simultaneous spectrophotometric determination of ascorbic acid, dopamine and uric acid in real samples. Arabian Journal of Chemistry (2014), http://dx.doi.org/10.1016/j.arabjc.2014.02.006