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Chemometrics and Intelligent Laboratory Systems 81 (2006) 202 – 208

Chemometrics and intelligent laboratory systems

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Chemometrics in Iran

Bahram Hemmateenejad *

Chemistry Department, Shiraz University, Shiraz 71454, Iran
Medicinal and Natural Products Chemistry Research Center, Shiraz University of Medical Sciences, Shiraz, Iran

Received 8 December 2005; accepted 8 December 2005
Available online 19 January 2006

Abstract

To represent the activity of the Iranian chemometrics community, a list of the publication of the Iranian scientists in the chemometrics was collected from the ISI web of science database. This article will review these publications to increase the awareness about the studies of chemometrics in Iran. A rapid growth is observed in the chemometrics publication in Iran and up to June 2005, some 200 scientific papers have been published in this context, in all fields of chemometrics.

Keywords: Iran; Chemometrics; Multivariate methods; Principal component analysis; Artificial intelligence; QSAR; QSPR

1. Introduction

The advent of chemometrics research in Iran is thought to be 1997. The first published report in the area has appeared in the literature in 1998 [1]. With the rapid growth of chemometrics in the world, the Iranian analytical chemists have increasingly used chemometrics methods in their researches since 1998. In spite of a long delay (more than 10 years), chemometrics grew rapidly in Iran so that up to now some 200 scientific papers (Fig. 1) have been published by Iranian chemometricians and more than 8 active chemometrics research groups are now existing in this country. This sudden motivation in the chemometrics publications can be attributed to two main factors. First, it is attributed to the increased rate of scientific publications in different scientific areas in Iran, in recent years [2] and, second to the presence of several interested young academic staff and graduate students who work hard to learn and to perform chemometrics research. Chemometrics courses are now being taught in some Iranian Universities for graduate students. As a result, many of them have received their MS or PhD degrees in chemometrics. The Iranian Chemometrics Society was established as a major branch of the Iranian Chemical Society in 2000. Annual Iranian Chemometrics workshops have been organized from 2001 to train more interested young scientists in the area by both Iranian and international experts.

The primary goal of this article is to increase the awareness about the studies of chemometrics in Iran and to review the published works of the major Iranian research groups and their achievements. The review is limited to the publications that are cited by the ISI web of science up to June 2005. It should be also noted that those which are solely computational in nature have not been considered.

Iranian chemometricians are now using almost all of the chemometrics techniques including experimental design, factor analysis and principal component analysis, multivariate calibration, multivariate curve resolution analysis and artificial intelligence (neural networks and genetic algorithms) in their research work. In addition, chemometrics techniques have widely been applied to quantitative structure–activity/property relationship (QSPR/QSAR) studies, drug design and bioinformatics. The relative frequency of the published papers in each field is represented in Fig. 2. As seen, QSAR/QSPR studies, multivariate calibration (MVC) methods and artificial intelligence (AI) are the most widely used chemometrics methods by Iranian chemists; while, FA/PCA, multivariate curve resolution (MCR) and experimental design (ED) have received less attention. It should be noted that PCA-based multivariate calibration methods are classified in the MCV and not in FA/PCA category. Indeed, one may notice that sum of the percentages in Fig. 2 is larger than 100. This is due to the some multi-subject

* Tel.: +98 711 2284822; fax: +98 711 2286008.
E-mail address: hemmatb@sums.ac.ir.

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doi:10.1016/j.chemolab.2005.12.004

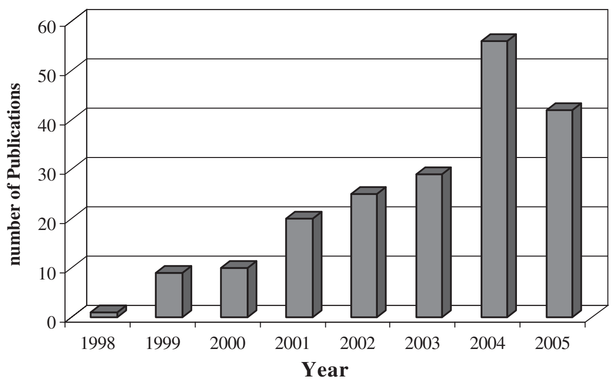

Fig. 1. Chemometrics publications in Iran.

papers, in fact some papers have used the artificial intelligence in QSAR studies or MVC studies and these papers have been classified in both categories.

Organization of the paper is based on the explanation of the type of chemometrics techniques used and the published results by different research groups located at different Iranian universities in alphabetic order.

2. Institute of Advanced Studies in Basic Sciences (IASBS)

This group, which was founded by Abdollahi in 2000, is one of the most active chemometrics research group in the country especially in chemometrics teaching. The annual Iranian chemometrics workshops are organized by this institute. Abdollahi started his chemometrics research by application of PCR and PLS regression for simultaneous determination of metal ions [3,4] and use of spectral peak deconvolution methods for characterization of weak association equilibria [5,6]. Then he got interested in the H-point standard addition method (HPSAM) for simultaneous determination of two analytes using spectrophotometric, kinetic and electrochemical methods [7–11]. In the last two years, he and his graduate students have applied genetic algorithm-based wavelength region selection-PLS regression to the spectrophotometric data obtained after cloud-point or solid-phase extraction to enhance the detection limits of the multicomponent analyses [12,13]. A method for spectral curve deconvolution has also been developed by Abdollahi and coworkers [14,15]. The technique was based on combination of H-point curve isolation method for extracting the pure spectra and HPSAM for calculation of the equilibrium concentrations. Application of PCA for differentiation between bovine and porcine gelatins is one of the interesting works performed by the Abdollahi research work [16]. They also reported the use for rank annihilation factor analysis for spectrophotometric study of complex formation equilibria [17]. In their continuous work on the use of factor analysis method, they developed a nonlinear iterative target transformation factor analysis method for simultaneous mixture analysis in the case of nonlinear spectrophotometric data and highly overlapping spectra [18].

Kompany-Zareh's research group at IASBS involves in working on different field of chemometrics at IASBS. Kompany-Zareh in his first chemometrics trials employed MLR, PCR, PLS and artificial neural networks (ANN) for simultaneous mixture analysis of metal cations [19–24]. Then, he used multivariate calibration methods for processing of the hand scanner data for individual or simultaneous analyses [25–27]. Kompany-Zareh is also interested in optimization methods and, therefore, he runs different projects to use genetic algorithms for the determination of optimum conditions or the best wavelength region in the multicomponent analysis [26–28]. Indeed, he and his coworkers applied ANN (feed forward and radial basis function) to kinetic and thermodynamic–spectrophotometric multicomponent analyses [29,30]. One of the most interesting papers of this group, in my opinion, is the use of PCA to select the best wavelength pairs in the ternary HPSAM (t-HPSAM) for simultaneous determination of Cu(II) and Zn(II) in the case of nonlinear spectral signals [31]. He is also interested in QSPR/QSAR studies and has published some papers in this context [32,33].

3. Isfahan University of Technology (IUT)

Khayamian and Ensafi founded this group in 1998. I was the first MS student who graduated from this research group. We started chemometrics by experimental design in optimization of FIA parameters using factorial design and MLR modeling [34]. We also wrote a singular value decomposition (SVD)-based PLS program and used it for simultaneous spectrophotometric determination of cobalt, nickel and copper [35].

Khayamian, Ensafi and their graduate students then employed factorial design optimization in different electroanalytical methods [36,37]. They also used ANN and PC-ANN methods in the processing of electrochemical data (especially differential pulse voltammetry) for simultaneous mixture analysis and for extending the linear dynamic range in individual analysis [38–40]. They are also interested in signal processing and used Fourier filtering to enhance the signal to noise ratio of electrochemical data [41]. Very recently, Khayamian has become interested in wavelet transformation and QSPR studies and has subsequently published some interesting papers in which he and his coworkers used a wavelet neural network in predicting the solubility of polycyclic aromatic hydrocarbons in super critical carbon dioxide [42] and in predicting the critical micelle concentration of Gemini

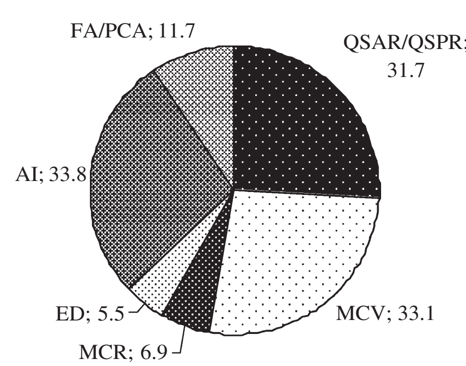

Fig. 2. Distribution of the types of Chemometrics publications in Iran.

surfactants [43]. In a very recent chemometrics paper, they proposed a principal component–wavelet neural network as a new multivariate calibration method and used it for simultaneous determination of metal ions [44].

4. Mazandaran University (MU)

Fatemi is the head of the chemometrics research group at MU. He received his PhD degree from Sharif Universiry of Technology under the supervision of professor Jalali-Heravi and continued his research work at MU. His basic research area is application of artificial neural network modeling in QSPR studies. He mainly focuses his researches on the modeling of retention behavior in micellar electrokinetic chromatography, electrophoretic mobility and super critical chromatography [45–50]. Among his works is the modeling and prediction of migration indices of 53 benzene derivatives and heterocyclic compounds in microemulsion electrokinetic chromatography [45].

5. Razi University (RU)

Shamsipur, the famous Iranian chemist who has the largest number of publications in Iran, began chemometrics in his multidisciplinary research group. Shamsipur's research group is spread in some different geographical points of Iran. Shamsipur was interested on chemometrics when I started my PhD thesis in his group at Shiraz University. Shamsipur and his chemometrician coworkers are now working in different chemometrics areas such as multicomponent analysis, multivariate curve resolution, QSAR/QSPR studies and application of TFA in linear solvation free energy relationships [51–66]. They proposed an ANN modeling method for processing of the derivative absorbance data in simultaneous determination of three phenothiazine drugs [51]. Processing of nonlinear relationship between the potential/pH of solution at different added volumes of titrant and the initial concentration of mixtures of analytes by PC-ANN method was developed in Shamsipur research group for the first time [52,53]. Application of GA for selection of factors in PC-ANN modeling was also proposed in this research group for the first time [54]. Shamsipur et al. defined some new topological indices based on the combination of distance sum and connectivity approaches. These topological indices, called Sh indices, were successfully applied to predict different properties of alkanes and in predicting log *P* and liquid density of extensive set of organic molecules [55,56]. Shamsipur and his coworkers processed the ^{1}H NMR spectral data for simultaneous determination of theophiline and caffeine [67]. Three chemometrics PhD students have been graduated from this group and some of the current PhD students are working on the development of different feature selection methods for use in multivariate calibrations and QSAR/QSPR studies.

Another chemometrics research group at RU is managed by Ghasemi. The main research area of Ghasemi was the study of the kinetics and thermodynamics of metal-ligand complexation. However, when chemometrics research was started in Iran, his interests were shifted to the use of chemometrics in his studies. Ghasemi and his graduate students focused on the two chemometrics methods namely, multicomponent analysis and multivariate curve resolution (MCR). They first extensively employed PLS regression to develop analytical methods for simultaneous determination of diverse set of chemicals [68–79]. They applied PLS to both the kinetic and thermodynamic spectrophotometric data. The uses of beta-correction and orthogonal signal correction as a preprocessing method for partial least squares have also been reported by this research group [80,81]. Among the multicomponent analysis methods proposed by Ghasemi et al. I would like to mention their paper about the application of two- and three-way chemometrics methods (PLS and parallel factor analysis; PARAFAK) for spectrophotometric determination of lorazepam in pharmaceutical and biological fluid [82]. In the case of MCR, Ghasemi in collaboration with Kubista proposed a new algorithm for characterization of the dimerization equilibria [83]. Then they determined the protolytic constants of PAR indicator in some binary organic-water solvents [84,85].

6. Sharif University of Technology (SUT)

The first chemometrics research group in Iran was established by Jalali-Heravi at SUT. I would like to call him as the father of chemometrics in Iran. As a computational chemist in origin, he started some QSAR/QSPR studies since 1993 and published valuable papers regarding the use of QSPR studies in the chromatographic sciences [1,86–93]. During the past decade, he has trained a number of MS and PhD students in the area of chemometrics. Jalali-Heravi and his graduate students developed QSPR models to predict the critical micelle concentration of surfactants [94–96] and to simulate the mass spectra or ^{13}C NMR of organic molecules [97,98]. The main modeling methods used in Jalali-Heravi's research group are MLR, GA, and ANN. They developed comprehensive descriptors for modeling of retention behavior in chromatographic methods [87]. Also, they propose self-training ANN for use in QSPR modeling of the gas chromatographic retention time [89]. This model was converged much faster and used much less parameters in comparison with conventional feed-forward ANN method. Jalali-Heravi indicated, by many comparative studies, the superiority of ANN modeling method over MLR analysis [99]. They also extended QSPR studies to the biological systems and performed comprehensive studies on the electrophoretic motilities of peptides in capillary zone electrophoresis [100–104]. In their efforts, this research group published two valuable papers in the journal of chemical information and computer sciences. In one paper, they used artificial neural networks in QSAR study of anti-HIV activity for a large set of HEPT derivatives [105] and in another one a hybrid method consisting of PCA, MLR and ANN has been developed for predicting the retention time of 149 C_3–C_{12} volatile organic compounds [106]. PCA and MLR were used as feature selecting tools for ANN. In recent years, Jalali-Heravi has been interested in multivariate data analysis methods. He used windows factor analysis (WFA), a MCR technique, for characterization and determination of fatty acids in fish oil by GS–MS [107]. In another interesting work, Jalali-Heravi and Vosough used a generalized rank annihilation method (GRAM) for screening, resolving and determining triazines in the presence of coeluting interferences by GC–selected ion mass spectrometry [108].

7. Groups in Shiraz University (SU)

The chemistry department of Shiraz University can be considered as the most active one in chemometrics research. Almost all of the analytical research groups at this department use chemometrics methods in their research works. In the multidisciplinary research group of Safavi, chemometrics was began from 1999 and since then one PhD and some MS students have been graduated from this group in the field of analytical chemometrics. Safavi is mainly interested in multicomponent analysis. She and her graduate students have proposed different methods for simultaneous determination of two or more analytes by the kinetic and catalytic methods [7,109–117]. They used H-point standard addition method and artificial neural networks in the multicomponent determinations. Also, they have applied PLS to thermodynamic spectrophotometric data for simultaneous determination of metal ions [3,4,118,119]. They have used ANN as a technique for interference removal in the kinetic spectrophotometric determination of Se(IV) [117]. The use of multivariate calibration methods for the speciation of Fe(II)–Fe(III) [111] and sulfite–sulfide [109] are examples of the works reported by this group. In an interesting paper, Safavi et al. employed a CCD camera imaging method for single-step calibration, prediction and real samples data acquisition by taking a single image from the solutions of Al(III)–Fe(III)–chrome azurol S, and then applied ANN to the image data for simultaneous determination of the cations [120]. Indeed, tensammetric analysis for simultaneous determination of four Brijes non-ionic surfactants by ANN was another interesting paper [121]. Absalan has also published some papers in collaboration with Safavi [115–117] and is now performing chemometrics researches in his group [122–124].

Abbaspour has recently used chemometrics in his research works as well. Abbaspour and coworkers have applied PLS, HPSAM and artificial neural network for multicomponent analysis of pharmaceutics or metal ions [125–129]. A chemometrics method for simultaneous determination of V(V) and Al(III) was developed in this research group by application of ANN to the beta-corrected spectra [127]. Abbaspour and Kamyabi employed MCR-alternative least squares to study the complexation equilibria of Cu(II)-L-histidine as a function of pH of solution [130].

The interest of Hemmateenejad on chemometrics started in his MS course in research group of Ensafi and Khayamian with MLR-based factor design optimization [34] and multivariate calibration based on PLS regression [35]. In the PhD course, he was interested in QSAR/QSPR studies and MCR analysis methods other than multicomponent analysis [55–60]. He performed multicomponent acid-base titration by using principal component–artificial neural network and PLS methods [52,53,61]. In the case of QSAR studies, he first applied genetic algorithm for feature selection in QSAR analysis based on PLS regression [58] and then used this to select the PCs in PC-ANN and proposed a new QSAR algorithm called PC-GA-ANN [54]. By the use of different MCR analysis methods, he and coworkers monitored photo-degradation kinetics of nifedipine [62], studied the behavior of iodine in mixture of cyclohexane with dioxane and tetrahydrofuran [63] and analyzed the spectro-electrochemistry of 9,10-anthraquinone reduction [64]. After receiving his PhD degree, he joined the Medicinal and Natural Products Chemistry Research Center (MNCRC) of the Shiraz University of medical sciences and mainly focused on the QSAR studies and drug design and published some papers in these areas [43,56,63,131–138]. He and his coworkers used ab initio-derived electronic feature for use in QSAR studies. Hemmateenejad proposed a correlation ranking procedure for factor selection in PC-ANN modeling and also developed a correlation ranking-based PCR for use in QSAR/QSPR studies [139–142]. The results have been published in Chemometrics and Intelligent Laboratory Systems, Journal of Chemometrics and Journal of Chemical Information and Computer Sciences. He also worked in the field of multicomponent analysis and more or less used PLS, ANN and net analyte signal (NAS) calculations in the simultaneous determination of analytes [66,143,144]. Hemmateenejad and coworkers proposed a simple and efficient nonlinear multicomponent analysis algorithm based on the use of NAS and ANN [144]. Hemmateenejad has been a member of the Chemistry Department of Shiraz University since last year. Other than QSAR/QSPR studies and multivariate calibrations, he has used chemometrics methods in analysis of solution chemistry and biological systems. Hemmateenejad, in collaboration with Shamsipur, used an unmodified carbon paste electrode and ANN for simultaneous determination of metal ions by potentiometric titration. Their proposed procedure for simultaneous determination of phenol and its mono nitro isomers were highlighted in the "Chemometrics Word" home page. Hemmateenejad had a major contribution in the paper concerning the use of MCR analysis to study of the chemical denaturation of RNase A [145].

8. Other chemometrics research in Iran

There are some chemometrics papers published by Iranian chemists whose major contribution is not chemometrics and therefore it is difficult to classify them as distinct chemometrics research groups. In this section, I will summarize these papers.

Iranian chemists are familiar with experimental design and there are some literature reports about using this technique in optimization of different chemical systems such as solid phase extraction [146], synthesis [147–149], fluorimetric analyses [150,151], micellar liquid chromatography [152–154], electrodialysis separation [155–157], microwave-assisted extraction [158,159], industrial analysis [160], and industrial production [161]. The chemometrics methods used for experimental design include mixed level orthogonal array designs [146], factorial designs [147,161], Taguchi designs [148,149,156,157,160,162], and face centered cube response surfaces [152–154]. Multicomponent analyses based on PLS [162–174] and ANN

[175,176] for determination of metal ions and pharmaceuticals have also been reported. For these determinations different analytical methods such as UV/Vis and FT-IR spectrophotometry and voltammetric methods have been used. Iranian chemists have also employed PCA and FA methods in analysis of airborne geophysical data [177], determination of citric acid in fermentation media [178], determination of elemental associates in a regional stream–sediment geochemical exploration [179] and in the processing systems [180]. There are also some literature reports on QSPR/QSAR analysis methods by Iranian chemists. Use of QSPR methods to model the electrophoretic mobility in capillary zone electrophoresis [181], QSAR study of the binding affinity of adenosine deaminase toward several adenine nucleosides [182], QSPR study on corrosion inhibition of mild steel by some Schiff base compounds [183,184], prediction of solvent effects on the rate constant of cycloaddition reaction [185] and prediction of the normalized polarity parameter in binary mixed solvent systems by ANN, are examples of these publications. Finally, I would like to mention the modified evolving widows factor analysis method that is developed by Setarehdan for process monitoring [186].

Acknowledgment

Financial support of the work by the Iran National Science Foundation (INSF) is acknowledged. I thank all Iranian chemometricians, especially Professors Shamsipur, Safavi and Jalali-Heravi, for their help and guidance through the preparation of this article. Especial thanks are due to Professor Hibbert for final editing of the manuscript.

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