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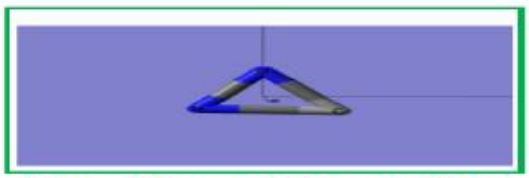
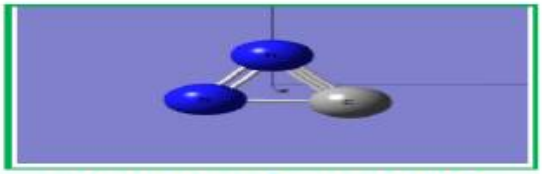
New Chemistry News

$^{-}N=C=N^{-}$



New News of Chem (NNC)



ChemNewsNew (CNN)

4-way data in

Quantitation & Curve resolution

Information Source (is)
ACS.org
Sciencedirect.com

Reviews

"Second- and third-order multivariate calibration: data, algorithms and applications	TrAC Trends in Analytical Chemistry, 26(7)2007, 752-765 doi.org/10.1016/j.trac.2007.04.006
Graciela M. Escandar and Alejandro C. Olivieri and Nicholaas (Klaas) M. Faber and Héctor C. Goicoechea and Arsenio Muñoz de la Peña and Ronei J. Poppi	

Second- and higher-order data generation and calibration: A tutorial	Analytica Chimica Acta, 806 (2014) 8– 26
Graciela M. Escandar, Héctor C. Goicoechea, Arsenio Munoz de la Pena, Alejandro C. Olivieri	

Factor Analysis/Multivariate Curve Resolution	Encyclopedia of Analytical Science, 3rd Edition, 2018, doi.org/10.1016/B978-0-12-409547-2.14043-0
Jamile Mohammad Jafari, Anna de Juan, Roma Tauler	

Quadrilinear decomposition-based blind Signal detection for polarization Sensitive uniform square array	Progress In Electromagnetics Research, PIER 87 (2008) 263–278
Y. Shi and X. Zhang	

	Infinte-way data 4-way data 3-way data
Analytical Advantages of Multivariate Data Processing. One, Two, Three, Infinity	Anal. Chem. , 80 (2008) 5713–5720
Alejandro C. Olivieri	

Part-per-Trillion Determination of Pharmaceuticals, Pesticides, and Related Organic Contaminants in River Water by Solid-Phase Extraction Followed by Comprehensive Two-Dimensional Gas Chromatography Time-of-Flight Mass Spectrometry	Anal. Chem., 82 (2010) 699–706

Review on Multiway Analysis in Chemistry—2000–2005	Critical Reviews in Analytical Chemistry, 36 (2006) 279–293
Rasmus Bro	

Multi-way chromatographic calibration—A review	ournal of Chromatography A, Volume 1587, 2019,2-13 doi.org/10.1016/j.chroma.2019.01.012
Graciela M.EscandarAlejandro C.Olivieri	

A review on second- and third-order multivariate calibration applied to chromatographic data	J. Chromatography B, 910 (2012) 22-30
Juan A. Arancibia, Patricia C. Damiani, Graciela M. Escandar, Gabriela A. Ibanez, Alejandro C. Olivieri	

Instru.Hyphenated:	Methods.MathStat:	Food processes/analysis
o HPLC- DAD o LC or GC–MS-spectrometry,	MCR o Unknown interferents	✓ Authentication ✓ Adulteration ✓ Interpretation

Chapter 6 - Multivariate Curve Resolution Methods for Food Chemistry"	editor = "Federico Marini", series = "Data Handling in Science and Technology", publisher = "Elsevier", 28,2013,235-263
Anna de Juan and Sílvia Mas	

Instrument	Complexity. Data.Instum.Chromat	Data.Sets
o Chromatography	▪ Overlapping among chromatographic peaks ▪ correction of unintended effects ▪ Baseline artifacts ▪ Peak shifts	o Biological o Food o Environmental

Chapter 21 - Data analysis; Liquid Chromatography (Second Edition)	editor = "Salvatore Fanali and Paul R. Haddad and Colin F. Poole and Marja-Liisa Riekkola", Elsevier",,2017,515-531 doi.org/10.1016/B978-0-12-805393-5.00021-X
"Alejandro C. Olivieri and Pablo L. Pisano and Arsenio Muñoz de la Peña and Héctor C. Goicoechea	

Software MatLab

Software. 4wayData.MV_MCAnalysis:	Methods.MathStat:	
Graphical user interface o MVC3_GUI in MATLAB	QLD models	Non-QLD models
	o PLS Reg o Resid. trilinearization	o Extended MCR-ALS o Augmented PARAFAC o PARAFAC2

MVC3_GUI: A MATLAB graphical user interface for third-order multivariate calibration. An upgrade including new multi-way models	Chemometrics and Intelligent Laboratory Systems, 173(2017)21-29 doi.org/10.1016/j.chemolab.2017.12.012
Sarmento J. Mazivila, Santiago A. Bortolato, Alejandro C. Olivieri	

Order Advantage

Second-Order Advantage Achieved with Four-Way Fluorescence Excitation-Emission-Kinetic Data Processed by Parallel Factor Analysis and Trilinear Least-Squares. Determination of Methotrexate and Leucovorin in Human Urine	Anal. Chem., 76 (2004) 5657-5666
Alejandro C. Olivieri, Juan A. Arancibia, Arsenio Munoz de la Pena, Isabel Duran-Meras, and Anunciacion Espinosa Mansilla	

Discussion on the superiority of third-order advantage: Analytical application for four-way data in complex system	Microchemical Journal, 145 (2019) 1078–1085
Xiao-Hua Zhang, Xiang-Dong Qing, Hai-Long Wu	

Figure of Merit (FoM)

	4-way data 3-way data 2-way data
Analytical Figures of Merit: From Univariate to Multiway Calibration	Chem. Rev , 114 (2014) 5358-5378
Alejandro C. Olivieri	

Figures of Merit in Multiway Calibration	Data Handling in Science and Technology, 29 (2016) 541-575
Alejandro C. Olivieri, Santiago Bortolato and Franco Allegrini	

Biomolecules

Chem.Syst:

- o l-phenylalanine, l-tyrosine, l-tryptophan in human plasma
  AND
- \- Unknown, uncalibrated interferent

Quantitation

- 4-Way Calibration

Order advantage

Third-order advantage

- \+ Higher resolving power
- \+ Sensitive, accurate, efficient

Mathemaatical separation

- \+ Fast
- \+ environmentally friendly (Green) compared to analytical separations

Direct quantitative analysis of aromatic aminoacids in human plasma by four-way calibration using intrinsic fluorescence:Exploration of third-order advantages	Talanta, 122(2014) 293–301
Chao Kang,Hai-LongWu n, Li-XiaXie,Shou-XiaXiang,Ru-QinYu	

Chem.Syst:

Tyrosine (Tyr) ;
Levodopa (Lev);

Sample.RealLife.ClinicalLab

Human plasma

4-way Data Tensor:

[kinetic time] x Ex.Em.Fl] x [#samples]

Complexity. Data

- Unknown spectral interferents

→Serious collinearity problems

Methods.MathStat:

Alternating quadrilinear decomposition (AQLD):	Calibration method. Third-order

Simultaneous determination of tyrosine and levodopa in human plasma using enzyme-induced excitation-emission-kinetic third-order calibration method

Chemometrics and Intelligent Laboratory Systems, 148,2015,9-19

Li-Xia Xie and Hai-Long Wu and Yu Fang and Chao Kang and Shou-Xia Xiang and Li Zhu and Xiao-Li Yin and Hui-Wen Gu and Zhi Liu and Ru-Qin Yu

Chem.Syst:

Active ingredients of Schisandra chinensis "Schizandrol A, Schizandrol B in DMEM"

4-way Data Tensor:

[Ex.Em.Fl] x [Solvent] x [#samples]

Complexity. Data

- Serious collinearity
- High background interference

Methods.MathStat:

- 🕮 Four-way self-weighted alternating normalized residue fitting algorithm (SWANRF)
- 🕮 four-way PARAFAC
- ✓ Satisfactory results

order [Instrument/variable/both] advantage: both

- Third-order advantage Exploited

Exploiting third-order advantage using four-way calibration method for direct quantitative analysis of active ingredients of Schisandra chinensis in DMEM by processing four-way excitation–emission-solvent fluorescence data

Chemometrics and Intelligent Laboratory Systems , 155 (2016) 46–53

Xiao-Hua Zhang, Hai-Long Wu, Xiao-Li Yin, Yong Li, Xiang-Dong Qing, Hui-Wen Gu, Chao Kang, Ru-Qin Yu

Chem.Syst:

Analytes: Levodopa (LD), carbidopa (CD), methyldopa (MD), acetaminophen (AC), tramadol (TRA), lidocaine (LC), tolperisone (TOP), ofloxacin (OF), levofloxacin (LOF), and norfloxacin (NOF)
uncalibrated interferents: benserazide (BA), dopamine (DP), ciprofloxacin (COF

Task: Quantitation: Simultaneous

Instrument(s)

Differential Pulse Voltammetry (DPV)
multi-walled carbon nanotubes modified glassy carbon electrode (MWCNTs/GCE)

Data

3-way Data Tensor:

- DPV response of each sample was recorded thirty-six times. Six current-potential matrices were recorded at six different pulse durations. Each matrix consists of six vectors which have been recorded at six different pulse heights. The three-way data array obtained for the calibration set (cali_3w)and for each of the test samples (Test_#)

4-way Data Tensor:

[kinetic time] x [Ex.Em.Fl] x [#samples]

Joined ((cali_3w)and for each of the test samples (Test_#)) into a single four-way data tensor

Complexity. Data

- Four-way data array was nonlinear

Third-order advantage Exploited

Methods.MathStat:

- Potential shift correction for non-linearities
  Correlation-optimized warping (COW)
- Third-order multivariate calibration algorithms.
  - Unfolded-partial least squares/residual trilinearization (U-Pls/Rtl)
  - Multi-way-PLS/RTL (N-PLS/RTL)

Multidimensional voltammetry: Four-way multivariate calibration with third-order differential pulse voltammetric data for multi-analyte quantification in the presence of uncalibrated interferences

Chemomet. Intel. Lab. Systems 148 (2015) 60–71

Ali R. Jalalvand a,b, Mohammad-Bagher Gholivand a, Hector C. Goicoechea.

Data.Chem

- Electroanalytical data

Data.Order

- Second-order
- Third-order

Review

Complexity. Data. voltammetric

- ! Alterations in baselines
- ! Sample-to-sample potential shifts
  - Surmounting limitations: Preprocessing

Applications and challenges of multi-way calibration in electrochemical analysis

TrAC Trends in Analytical Chemistry 87(2017) 32-48

Ali R. Jalalvand and Hector C. Goicoechea and Douglas N. Rutledge.

Data	
Data. Simulated ▪ Chromatograms ! Different degrees of overlapping ! Misalignment among the chromatographic peaks	Data. Experimental data ▪ Olive oil samples
▪ Creating augmented three-way array: [elution time direction, containing data for the calibration sample set and for each of the test samples]	Four-way data ▪ Third order: [high-performance LC ; [matrix excitation–emission SP (fluorescence detection)] - Non-quadrilinear
Chemometric analysis	
Methods.MathStat: ▪ Augmented PARAFAC	Comparison with ❖ MCR-AL S
Novel augmented parallel factor model for four-way calibration of high-performance liquid chromatography–fluorescence excitation–emission data	Chemometrics and Intelligent Laboratory Systems, 141,2015,1-11
Santiago A. Bortolato and Valeria A. Lozano and Arsenio Muñoz de la Peña and Alejandro C. Olivieri	

Chem.Syst:	Chemists' taks
+ Multiple analytes + + Unknown uncalibrated interferents	▶ Direct quantitative analysis of analytes

Experiments
Hyphenated instruments
Multi- (2, 3, 4-) way Data

Data Processing
Pre-processing
Calibration models

Chemometric advantages
+ Second-order advantage
✓ Third-order advantage

Figures of Merit
Higher sensitivity

Chapter 4 - Practical Analytical Applications of Multiway Calibration Methods Based on Alternating Multilinear Decomposition	Data Handling in Science and Technology, Elsevier, 29,2015,167-246 doi.org/10.1016/B978-0-444-63527-3.00004-7",
editor = "Arsenio Muñoz de la Peña and Héctor C. Goicoechea and Graciela M. Escandar and Alejandro C. Olivieri	

Enzymes

Chem.Syst:	Process
Metabolic oenzymes o Reduced nicotinamide adenine dinucleotide (NADH) o Flavin adenine dinucleotide (FAD	Formation reaction of FAD in human plasma - Uncalibrated interferent

Instrument(s)	Complexity. Data	3way Data
Ex-Em_Fl	- Highly collinear systems	[Ex.EM] [kinetic time]

Quantitative fluorescence kinetic analysis of NADH and FAD in human plasma using three- and four-way calibration methods capable of providing the second-order advantage	Analytica Chimica Acta, 910(2016) 36-44 doi.org/10.1016/j.aca.2015.12.047
Chao Kang, Hai-Long Wu, Chang Zhou, Shou-Xia Xiang, Xiao-Hua Zhang, Yong-Jie Yu, Ru-Qin Yu	

Drugs

Chem.Syst:	Sample.RealLife.Environment
o Hydrolysis of irinotecan, a drug,	Human plasma in complex dynamic samples

Methods.MathStat:

Three-way calibration	Four-way calibration
o Alternating normalization-weighted error (ANWE) o Alternating penalty trilinear decomposition (APTLD)	o Alternating weighted residual constraint quadrilinear decomposition (AWRCQLD) o Alternating penalty quadrilinear decomposition (APQLD)

Inference:

✓ Three-way as well as four-way calibration models achieve real-time quantitative analysis of the hydrolysis of CPT-11 in human plasma

Comparison of three-way and four-way calibration for the real-time quantitative analysis of drug hydrolysis in complex dynamic samples by excitation-emission matrix fluorescence	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 192 (2018) 437–445
Xiao-Li Yin, Hui-Wen Gu, Xiao-Lu Liu, Shan-Hui Zhang, Hai-Long Wu	

Chem.Syst:

- Anticancer drugs

Reaction: kinetics

Oxidation of leucovorin and metotrexate with potassium permanganate → Highly fluorescent compounds

Methods.MathStat:

- ✓ Trilinear least-squares (TLLS) coupled to residual trilinearization (RTL)
- ✓ SVD-least-squares (SVD-LS) [also called bilinear least-squares] + residual bilinearization (RBL)

OutPut Comparison with

- PARAFAC
- Unfolded PLS with RTL

Insrrum.second-order.advantage in third-order calibdration (TO.Calib)

+ Estimation of analyte concentrations in presence of uncalibrated components

"Trilinear least-squares and unfolded-PLS coupled to residual trilinearization: New chemometric tools for the analysis of four-way instrumental data

Chemometrics and Intelligent Laboratory Systems, 80(1),2006,77-86doi.org/10.1016/j.chemolab.2005.08.002

Juan A. Arancibia and Alejandro C. Olivieri and Diego Bohoyo Gil and Anunciación Espinosa Mansilla and Isabel Durán-Merás and Arsenio Muñoz de la Peña

Multiway Partial Least-Squares Coupled to Residual trilinearization: A Genuine Multidimensional Tool for the Study of Third-Order Data. Simultaneous Analysis of Procaine and Its Metabolite p-Aminobenzoic Acid in Equine Serum

Anal. Chem. 79, (2007) 6949-6958

Patricia C. Damiani, Isabel Duran-Meras, Alejandro Garcıa-Reiriz, Ana Jimenez-Giron, Arsenio Munoz de la Pena, and Alejandro C. Olivieri

Chem.Syst:

- Folic acid, Methotrexate

Sample.RealLife.Environment

- Human serum

DataSets

Four-way data

Process.Chem

- Oxidation of analytes with potassium permanganate, in slightly acidic medium; (7minutes)

Monitoring begin

- Fast-scanning spectrofluorimeter, (recording each complete EEM in 12s). This allows the acquisition of 10 successive EEMs, at different reaction times

End monitoring

Methods.MathStat:

- ✓ Unfolded-PLS,
- ✓ Residual trilinearization

Evaluation of unfolded-partial least-squares coupled to residual trilinearization for four-way calibration of folic acid and methotrexate in human serum samples	Talanta, 72(4), 2007,1261 - 1268", doi.org/10.1016/j.talanta.2007.01.018
A. Muñoz de la Peña and I. Durán Merás and A. Jiménez Girón and H.C. Goicoechea	

Chem.Syst:
- Thiamine

Sample.RealLife.Environment
Multivitamin complex, local market

Instrument
- [Ex-Enm-Fl]

Method. Chemometric
- Standard addition

Methods.MathStat:
PARAFAC

Insrrum.Second_order.advantages

- Estimation of analyte concentrations even in the presence of unknown fluorescent interferences
  - Does not prevent matrix effects or interferences affecting the reaction mechanism or kinetic properties
  - Remedy: standard addition

Chemometric modeling of kinetic-fluorescent third-order data for thiamine determination in multivitamin complexes	Microchemical Journal, 128 (2016) 42–46
Wallace D. Fragoso, Alejandro C. Olivieri	

Chem.Syst:
- Tetracycline +
- Quenching matrix effect

Sample.RealLife.Environment
- Tea

Complexity. Data
- ✓ Quenching effect in fluorescent measurements
  - ✓ Quencher multiplicative effect made on the tetracycline signal
  - ✓ Impossibility of resolution with (SO) Second order)-Calib (ration) model
  - ✓ Wayout: arranging the experimental data in a four-way tensor

Methods.MathStat:
- ✓ PARAFAC
- ✓ Four-way PLS better

Fluorescence quantification of tetracycline in the presence of quenching matrix effect by means of a four-way model	Talanta, 77(3)(2009)1129-1136 doi.org/10.1016/j.talanta.2008.08.023
Shao-Hua Zhu and Hai-Long Wu and A-Lin Xia and Jin-Fang Nie and Ying-Chao Bian and Chen-Bo Cai and Ru-Qin Yu	

Chem.Syst:

- Folic acid
- Its two main metabolites

Sample.RealLife.Environment

- Serum

Methods.MathStat:

- ✓ U-PLS
- ✓ N-PLS/residual trilinearization (RTL)

Data. Fourth Order Tensor (FO.T).Aquisition

Four-way data

- On line irradiation of compounds with a UV lamp
- Data of photochemical reaction recorded
- Fast scanning spectrofluorimeter: Excitation–emission matrices (EEMs) were recorded as a function of the irradiation time
- Consequences → Selectivity:
  - arises due to different rates of formation and degradation of photoproducts of the folic acid derivatives

On line photochemically induced excitation–emission-kinetic four-way data: Analytical application for the determination of folic acid and its two main metabolites in serum by U-PLS and N-PLS/residual trilinearization (RTL) calibration

Analytica Chimica Acta622,2008,94-103
doi.org/10.1016/j.aca.2008.05.079

A. Jiménez Girón and I. Durán-Merás and A. Espinosa-Mansilla and A. Muñoz de la Peña and F. Cañada Cañada and A.C. Olivieri

Chem.Syst:

- Carbendazim, thiabendazole, fuberidazole, carbofuran, carbaryl and 1-naphtol

Sample.RealLife. Dietetometrics

Fruit juice

Data.aquisition

Sample → HPLC→ fractions at different elution times
At each t , measure Ex_EM Fl absorance 2-way data tensor
→ 3way- Sec order data

Methods.MathStat:

- PARAFAC,
- U-PLS/RTL
- MCR-ALS

Best Result.Algorithm

U-PLS/RTL

Order advantage

SecondOrder.Advantage

- \+ Samples containing uncalibrated components

Third.Order.Advantage

Figures of merit

- \+ Second- to third-order data
- \+ LODs obtained were ranged between 0.02 and 2.4μgL−1

i

Spray drying formulation of albendazole microspheres by experimental design. In vitro–in vivo studies

Drug Dev Ind Pharm, Early Online, (2015) 1–9

Agustina Garcia, Darıo Leonardi, Gisela N. Piccirilli, Maria E. Mamprin, Alejandro C. Olivieri, and Marı´a C. Lamas

Pesticides

Highly sensitive quantitation of pesticides in fruit juice samples by modeling four-way data gathered with high-performance liquid chromatography with fluorescence excitation-emission detection	Talanta 154(2016) 208–218 doi.org/10.1016/j.talanta.2016.03.078
M. Montemurro, L. Pinto, G. Véras, A. de Araújo Gomes, M.J. Culzoni, M.C. Ugulino de Araújo, H.C. Goicoechea	

	4-way data
Four-Way Data Coupled to Parallel Factor Model Applied to Environmental Analysis: Determination of 2,3,7,8-Tetrachloro-dibenzo-para-dioxin in Highly Contaminated Waters by Solid-Liquid Extraction Laser-Excited Time-Resolved Shpol'skii Spectroscopy	Anal. Chem. , 77 (2005) 2608-2616
Hector C. Goicoechea, Shenjiang Yu, Alejandro C. Olivieri, and Andres D. Campiglia	

Chem.Syst:

- Carbamate pesticides (carbaryl and carbendazim)
- Degradation product of carbaryl (1-naphthol)

Sample.RealLife.Environment

- Iceberg lettuce

3rd Oder (4-way) Data Tensor:

- [Ex.Em.Fl]
  +
- [Different dilutions of the extract from iceberg lettuce as a fourth way]

Complexity. Data.Instum.Chromat

- Matrix interferences
- High fluorescent overlapping existed between the three analytes and fluorophores of the matrix

Method. Chemometric

- Standard addition method

Data Analysis

- Step 1: Four-way model: The identification of two fluorescent matrix constituents enabled to know matrix contribution in each dilution of the extract.
- Step 2: This contribution was subtracted from the previous signals
- Step 3: Three-way model: performed with tensors corresponding to each dilution. PARAFAC decomposition of these resulting tensors showed a CORCONDIA index equal to 99%

Standard addition method based on four-way PARAFAC decomposition to solve the matrix interferences in the determination of carbamate pesticides in lettuce using excitation–emission fluorescence data	Talanta, 138,2015,86-99 doi.org/10.1016/j.talanta.2015.01.042
L. Rubio and L.A. Sarabia and M.C. Ortiz	

PAHs

Chem.Syst:

PAHs
- Acenaphthene (ANA),
- Naphthalene (NAP)
- Fluorene (FLU)

Sample.RealLife.Environment

Polluted water

4-way Data Tensor:

4way.data: [Excitation-emission fluorescence matrixes (EEMs)] x [different volumes of fulvic acid

Complexity.Data

- Fulvic acid affects PAHs determination seriously in real-world situation,
- Remedy: It is simulated as an interfering agent

Methods.MathStat

Alternating weighted residue constraint Quadrilinear decomposition	AWRCQLD
Quadrilinear parallel factor analysis	4-PARAFAC
Alternate penalty quadrilinear decomposition	APQLD
Alternate penalty trilinear decomposition	APTLD

Figure of Merit

- Higher accuracy
- Better predictive ability compared to second-order data

Comparison of several third-order correction algorithms applied to fluorescence excitation–emission-sample data array: Interference-free determination of PAHs in water pollution

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 205(2018) 381390
doi.org/10.1016/j.saa.2018.07.045

Xiao-Li Yin, Hui-Wen Gu, Xiao-Lu Liu, Shan-Hui Zhang, Hai-Long Wu

Chem.Syst:

PAHs
- Acenaphthene (ANA)
- Naphthalene (NAP)

Task.Cem.

Environmental
- Qualitative
- Quantitative

4-way Data Tensor:

Four-dimensional data
- [Ex-Em-Fl] x [samples (of different concentration PAHs)] x [Three solvents: methanol, ethanol and Ultra-pure water]

Preprocessing

Wavelet transform
- To solve the redundant information of the three-dimensional fluorescence spectral data
- Compress data

Methods.MathStat:

- AWRCQLD model (alternating weighted residue constraint quadrilinear decomposition)

Four-dimensional data coupled to alternating weighted residue constraint quadrilinear decomposition model applied to environmental analysis: Determination of polycyclic aromatic hydrocarbons

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 193,2018,1386-1425
doi.org/10.1016/j.saa.2017.12.003

Tingting Liu and Ling Zhang and Shutao Wang and Yaoyao Cui and Yutian Wang and Lingfei Liu and Zhe Yang

Chem.Syst:

- Polycyclic aromatic hydrocarbons (Phenanthrene, pyrene, anthracene and fluorene) +
- Humic acid (a fluorescent quencher)

Sample.RealLife.Environment

River water

OutPut

Four loading matrices correspond to

- relative concentration, excitation spectra, emission spectra ; fluorescence quantum yield

Methods.MathStat:

- Four-way PARFAC

Determination of polycyclic aromatic hydrocarbons by four-way parallel factor analysis in presence of humic acid

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy,152,2016,384-390
doi.org/10.1016/j.saa.2015.07.094

Ruifang Yang and Nanjing Zhao and Xue Xiao and Shaohui Yu and Jianguo Liu and Wenqing Liu

Chem.Syst:

PAHs:

- Phenanthrene, naphthalene; acenaphthene

Sample.RealLife.Environment

Beverages: Tea

4-way Data Tensor:

[[Ex-Em-Fl] x [Temperature] x [#samples]

Methods.MathStat:

- Four-way PARAFAC
- \+ .4-four-way PARAFAC >> 3-way

Figures of merit

- LOD: [0.026 to 0.14] μg L−1

Determination of three polycyclic aromatic hydrocarbons in tea using four-way fluorescence data coupled with third-order calibration method

Microchemical Journal, 146,2019,957-964

Fengkai Shang, Yutian Wang, Junzhu Wang, Ling Zhang, Shutao Wang

Chem.Syst:

- Catechin
- Epicatechin

Sample.RealLife.Environment

To compare grape water extracts

- ✓ Of two consecutive sampling dates
- ✓ Corresponding with two maturation stages
- ✓ And subjected to full irrigation and non-irrigation

Instrument

- Front-face excitation-emission fluorescence spectroscopy

4-way Data Tensor:

[3-way] + [diethyl ether extraction]

- \+ Differentiate between irrigated and non-irrigated samples with the same assayed algorithms

Methods.MathStat:

LDA + PARAFAC
LDA + unfolding (U-PLS)
+ Allowed to discriminate between the first and the second maturation stages

Opinion:

- Authors opine it to the first time report the use of four-way data arrays for classification

Combination of fluorescence excitation emission matrices in polar and non-polar solvents to obtain three- and four- way arrays for classification of Tempranillo grapes according to maturation stage and hydric status

Talanta, 1999,2019,652-661

Manuel Cabrera-Bañegil, Esperanza Valdés-Sánchez, Arsenio Muñoz de la Peña, Isabel Durán-Merás

Chem.Syst:

Heavy- PAHs
- Fluoranthene, pyrene, benz[a]anthracene,
- chrysene, benzo[b]fluoranthene,
- benzo[k]fluoranthene, benzo[a]pyrene,
- dibenz[a,h]anthracene

Calibration.MV_MC

- ✓ Third-order
- ✓ Simultaneous quantitation

Instrument

- LC-EEFM

Methods.MathStat:

- Four-way PARAFAC

Order.advantages ([Instrum [LC: 1 ; ExEmFl: 2]])

Insrrum.second-order.advantage	Data.Third-order advantage
Second-order advantage + Quantification of the analytes in interfering media	Third-order advantage + Resolution of the system of a high degree of collinearity + Increased sensitivity, LOD range 0.4–2.9 ngmL−1

On-line generation of third-order liquid chromatography–excitation-emission fluorescence matrix data. Quantitation of heavy-polycyclic aromatic hydrocarbons

Journal of Chromatography A, 1527,(2017),61-69

Maira D. Carabajal, Juan A. Arancibia, and Graciela M. Escandar

Chem.Syst:

Heavy- PAHs
- Benzo[a]pyrene,
- dibenz[a,h]anthracene,
- benzo[b]fluoranthene,
- benzo[k]fluoranthene
- benz[a]anthracene

Process.dynamics (kinetic evolution)

- ✓ Fenton degradation

Instrument

- Excitation-emission fluorescence matrix- for each sample
- kinetic data (different reaction times)

Order.advantages ([Instrum (2) ; Kinetic time (1)])

Insrrum.second-order.advantage	Data.Third-order advantage
Analyte concentrations in the presence of an uncalibrated fluorescent background	+ Sensivity

Excitation-emission fluorescence-kinetic data obtained by Fenton degradation. Determination of heavy-polycyclic aromatic hydrocarbons by four-way parallel factor analysis	Talanta 165 (2017) 52–63., doi.org/10.1016/j.chemolab.2014.11.013
Maira D. Carabajal, Juan A. Arancibia, Graciela M. Escandar	

Chem.Syst:

PAHs
- Benz[a]anthracene, chrysene, benzo[b]fluoranthene, and benzo[a]pyrene

Instrument
- LC-EEFM

Calibration.MV_MC
- ✓ Third-order;4-way

Task.Chemical
- ✓ Simultaneous quantitation

Complexity.Model
- Two mutually dependent instrumental modes, namely elution time and excitation wavelength modes

Model.Data
- Non-quadrilinear type 4

Methods.MathStat:
- MCurveResolu-ALS

Figure of Merit
- LOD: 1.0–1.4 ng mL–1 of PH

Multivariate curve resolution strategy for nonquadrilinear type 4 third-order/four way liquid chromatography–excitation-emission fluorescence matrix data	Talanta, 189(2018)509-516 doi.org/10.1016/j.talanta.2018.07.017
Maira D. Carabajal, Juan A. Arancibia, Graciela M.Escandar	

Environmetrics - water

Chem.Syst:
- Carbaryl

Sample.RealLife.Environment
- Spiked tap water samples

Processing
- Hydrolysis kinetics of carbaryl

Data.
- Room-temperature phosphorescence data +
- Uncalibrated phosphorescence background

Complexity. Data(4way)
- ✓ Spectral background drift produced in measured dataset
- ✓ Overcome by: modeling the drift as an additional component in the mathematical model

Methods.MathStat:

- PARAFAC
- Alternating weighted residue constraint quadrilinear decomposition (AWRCQLD)
- Alternating quadrilinear decomposition (AQLD) (third-order calibration algorithm;quadrilinear model)
  - Direct extension of alternating trilinear decomposition for quadrilinear data
    - ✓ Constructed in pseudo-fully stretched matrix

Development of a novel alternating quadrilinear decomposition algorithm for the kinetic analysis of four-way room-temperature phosphorescence data

Chemometrics and Intelligent Laboratory Systems, 132(2014)8-17

Xiang-Dong Qing and Hai-Long Wu and Xiu-Fang Yan and Yong Li and Li-Qun Ouyang and Chong-Chong Nie and Ru-Qin Yu

Chem.Syst:

- Carbaryl

Sample.RealLife.Environment

- Effluent water

Process.Chem

- hydrolysis

Data. Fourth Order Tensor (FO.T)

- kinetic evolution of excitation-emission matrix fluorescence (ExEmFl]

Methods.MathStat:

- ✓ □ Quadrilinear PARAFAC

Insrrum.second-order.advantage in third-order calibdration (TO.Calib)

+ Estimation of analyte concentrations in presence of an uncalibrated fluorescent background

Excitation-emission-kinetic fluorescence coupled with third-order calibration for quantifying carbaryl and investigating the hydrolysis in effluent water

Talanta, 77(5)(2009)1640-1646 doi.org/10.1016/j.talanta.2008.09.052

Shao-Hua Zhu and Hai-Long Wu and A-Lin Xia and Jin-Fang Nie and Ying-Chao Bian and Chen-Bo Cai and Ru-Qin Yu

Chem.Syst:

Pesticides

- Carbaryl;
- 1-naphthol

Sample.RealLife.Environment

- Water samples +
- Fluorescent interferents

Data. Fourth Order Tensor (FO.T).Aquisition

Four-way data

- kinetic-excitation-emission fluorescence

Process.Chem

- Kinetics of alkaline hydrolysis of carbaryl → 1-naphthol
- Consequence → Data complexity
- Introduces strong linear dependencies and multi-linearity losses

Complexity. Data

Water samples contain

- ✓ Uncalibrated interferences, (agrochemicals) +
- ✓ Naturally occurring background signal

Methods.MathStat:
✓ Unfolded PLS + residual trilinearization (U-PLS/RTL)
✓ PARAFAC (suitably initialized and restricted)
✓ U-PLS/RTL provides similar FOM

Insrrum.order.advantage
+ Second-order advantage

Four-way kinetic-excitation-emission fluorescence data processed by multi-way algorithms. Determination of carbaryl and 1-naphthol in water samples in the presence of fluorescent interferents	Analytica Chimica Acta,677(2)(2010)97-107 doi.org/10.1016/j.aca.2010.07.045
Rubén M. Maggio and Patricia C. Damiani and Alejandro C. Olivieri	

Chem.Syst:	Sample.RealLife.Environment
o Fluoroquinolones	▪ Tap water samples

Instru.Hyphenated:	Order.Instru
o [fast-HPLC] + o [Ex.Em.Fl	One Two
Total order	Three per sample

Complexity. Data
- Occurrence of temporal shift → leads to loss of quadrilinearity
✓ Wayout: MCR-ALS

Methods.MathStat:
o PARAFAC,
o U-PLS/RTL
o MCR-ALS

Order.advantages	
Insrrum.second-order.advantage	Data.Third-order advantage
+ Samples containing uncalibrated interferences	+ Enhancement of FOM from second to third order data + Relative error of prediction (REP%) + 9.9% for ofloxacin + 14.0% for ciprofloxacin

Modeling four and three-way fast high-performance liquid chromatography with fluorescence detection data for quantitation of fluoroquinolones in water samples	Analytica Chimica Acta 809,2014,37-46
Mirta Raquel Alcaráz and Gabriel G. Siano and María Julia Culzoni and Arsenio Muñoz de la Peña and Héctor C. Goicoechea	

Online Third-Order Liquid Chromatographic Data with Native and Photoinduced Fluorescence Detection for the Quantitation of Organic Pollutants in Environmental Water	ACS Omega, 2018, 3, 15771−15779
Rocío B. Pellegrino Vidal, Alejandro C. Olivieri, Gabriela A. Ibañez, and Graciela M. Escandar	

Sample.RealLife.Environment

- Crude oil
- ! Petrochemical industry refinery inferences

Task.Industry.Oil

- ! Calibration
- ! Prediction. Property

Instrument

- GC × GC-TOFMS

Data.Order

- Third-order

Methods.MathStat:

- N-way N-PLS

Comprehensive and multidimensional tools for crude oil property prediction and petrochemical industry refinery inferences

Fuel ,223,2018,188-197
doi.org/10.1016/j.fuel.2018.01.109

Ariana P. Pagani, Gabriela A. Ibañez

GC_GC_MS

Instrument

- [GC-GC] [MS]

Complexity. Data.Instum.Chromat

- Noise, elution time shifts in both chromatographic dimensions
- Peak overlap

Remedy: Interferences are considered as the main artifacts

Data

- Simulated

Figures of merit

Multivariate AFOMs including

- Analytical SEN (γ),
- Selectivity (SEL)
- LOD extended to GC×GC–MS
- Variance-covariance matrix of residuals to estimate the noise level

Methods.MathStat:

- MCR-ALS
- PARAFAC

Multivariate analytical figures of merit as a metric for evaluation of quantitative measurements using comprehensive two-dimensional gas chromatography–mass spectrometry

Journal of Chromatography A, 1466,2016,155-165
doi.org/10.1016/j.chroma.2016.09.016

Ali Eftekhari and Hadi Parastar

Slicing alternating quadrilinear decomposition (SAQLD): It is a generalization of ATLD to four-way case with third order advantage.

Alg. SAQLD

Iterate alternately the updates of four underlying matrices

- Operation of extracting diagonal elements is adopted,
- which makes SAQLD focus on extracting the quadrilinear part in data, leading to a significant decrease in the loss function

until convergence is reached

- ✓ High-performance computing strategy for SAQLD, i.e., fast convergence

Advantages.SAQLD

- + With the present specific optimization approach, it recovers parameter matrices faster compared with other quadrilinear decomposition algorithms
- + Even if number of chemical components used in calculation is more than actual number, it gives quantitative results
- + Robust to inaccurate number of inputs of chemical components

Slicing" data array in quadrilinear component model: An alternative quadrilinear decomposition algorithm for third-order calibration method	Chemometrics and Intelligent Laboratory Systems, 167 (2017) 12–22
Li-Xia Xie, Hai-Long Wu, Xiao-Hua Zhang, Tong Wang, Li Zhu, Shou-Xia Xiang, Zhi Liu, Ru-Qin Yu	

A novel quadrilinear decomposition method for four-way data arrays analysis based on algorithms combination strategy: Comparison	Chemometrics and Intelligent Laboratory Systems, 185 (2019) 92–104
Tong Wang, Hai-Long Wu, Li-Xia Xie, Wan-Jun Long, Li Cheng, Ru-Qin Yu	

Chemical rank

Task.Chemometric

- o Number of chemical components in four-way data from mixture of analytes and interferents

DataSets

- Simulated: two
- Real four-way: two

Methods.MathStat:

1) Core consistency diagnostic (CORCONDIA) test
2) ADD-ONE-UP truncating and fitting method (ADD-ONE-UP)
3) Factor indicator function (IND)
4) Alternating weighted quadrilinear decomposition incorporating Monte Carlo simulation (AWQLD-MCS): An extension of self-weighted alternating trilinear decomposition incorporating Monte Carlo simulation

Figure of Merit

- o AWQLD-MCS >>1), 2) and 3)
- o Fast analytical speed
- o Strong ability of anti-noise-interference
- o Anticollinearity

A new method to determine the number of chemical components of four-way data from mixtures	Microchemical Journal,135 (2017) 114 - 121 doi: 10.1016/j.microc.2017.08.011
Xiang-Dong Qing, Yong Li, Jin Wen, Xiang-Zhong Shen, Chun-Yan Li, Xiao-Lin Liu, Jing Xie	

Mathematical rank

Task. Rank of Tensor(order,way,Variables)

! # mathematical component

Data:Tensor

Three-way trilinear tensor

Review

Order.Advantage

✓ Second-order advantage

Disciplines.Applications

- Pharmaceuticals
- Biological matrices
- Environmental matrices

Multi-way chemometric methodologies and applications: A central summary of our research work

Analytica Chimica Acta,650(1)(2009)131-142
doi.org/10.1016/j.aca.2009.05.041

Hai-Long Wu and Jin-Fang Nie and Yong-Jie Yu and Ru-Qin Yu

Task.

! # mathematical components (PCAs, PLSCs etc.

! Chemical Rank

Methods.MathStat:

- PCA
- MCR
- PARAFAC (4-way)
- ADLS
  - (Angle Distribution of Loading Subspace)

Methods.MathStat.#components. Classical

- Scree plot
- Cross-validation in PCA

Methods.MathStat. .#components.advanced

Chemical rank (number of chemical components) for four-way real-life data tensors

- Core consistency diagnostics (CORCONDIA) in PARAFAC)
  - Fails for datasets with high coherence

ADLS for number of components

+ Chemical rank (of four-way data) by ADLS >> CORCONDIA /split-half analysis [in precision; information]

✓ ADLS performed better when estimating the chemical rank for MCR analysis, compared with scree plots

- biased results and CORCONDIA / split-half analysis provided relatively unstable results

✓ Improved ADLS in multi-way analysis (three- and four-way PARAFAC) by calculating the loading subspace in advance using the Khatri-Rao product.

+ Correct result for the simulated three-way fluorescence datasets of high complexity

! Unevenly distributed coherence at different dimension

Angle Distribution of Loading Subspace (ADLS) for estimating chemical rank in multivariate analysis: Applications in spectroscopy and chromatography

Talanta, 194 (2019) 90–97

Ya-Juan Liu, Geert Postma, Hai-Long Wu, Hui-Wen Gu, Chao Kang, Jeroen Jansen, Ludovic Duponchel

Chem.Syst:
- o Dye mixtures

Instrument
- LC-EEM
- + Measurements in the order of tens of milliseconds

Methods.MathStat:
- PARAFAC

Multiway analysis through direct excitation-emission matrix imaging)

Analytica Chimica Acta 1032,2018,32-39
doi.org/10.1016/j.aca.2018.07.069

"Mirta R. Alcaraz and Ezequiel Morzán and Cecilia Sorbello and Héctor C. Goicoechea and Roberto Etchenique

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Data
- + Third-order data

Inst.Order
- o {LC] {Ex.Em Fl]

Chem.Syst:
- o Three analytes

Complexity. Data.Instum.Chromat
- Data is Non-quadrilinear

Methods.MathStat:
- Augmented PARAFAC
- MCR-ALS

Third order chromatographic-excitation–emission fluorescence data: Advances, challenges and prospects in analytical applications

TrAC Trends in Analytical Chemistry 93, 2017,119-1
doi.org/10.1016/j.trac.2017.05.01133

Ariana P. Pagani and Gabriela A. Ibañez

Four-way calibration applied to the processing of pH-modulated fluorescence excitation-emission matrices. Analysis of fluoroquinolones in the presence of significant spectral overlapping

Microchemical Journal, 132 (2017) 211–218

Ariana P. Pagani, Gabriela A. Ibañez

Chem.Syst:
- o Quinolones
- o Pipemidic acid,
- o Enoxacin
- o Marbofloxacin
- o Enrofloxacin

Sample.RealLife.Environment
- Edible animal tissues
- Bovine kidney, chicken
- Porcine meat samples, fortified at various concentration levels

Task.Cem.
- Simultaneous determination

3rd Oder (4-way) Data Tensor:
- [excitation–emission fluorescence] [modulated by pH gradient]

Process
- o Generated in situ through hydrolysis of glucono delta–lactone

Complexity. Data.Instum.Chromat	Method. Chemometric
▪ Strongly overlapped spectra within the analytes ▪ Highly complex tissue matrix	o (Unfolded –PLS/RTL). + o Residual trilinearization
Analytical approach for the simultaneous determination of quinolones in edible animal products. Modeling pH–modulated fluorescence excitation–emission matrices four–way arrays	Talanta, 192, 2019, 52-60 doi.org/10.1016/j.talanta.2018.09.015
Milagros Montemurro and Gabriel G. Siano and Mirta R. Alcaráz and Héctor C. Goicoechea	

Chem.Syst:	Sample.RealLife.Environment
o Chlorophylls a and b o Pheophytins a and b + o Interfering fluorescent compounds	▪ Olive oil
Method. Chemometric	**Instru.Hyphenated:** / **Order.Instru**
+ Direct analysis + No previous sample treatment	o [ultra-HPLC] + o [Ex.Em.Fl] — One / Two Total order — Three per sample
Data.Aquisition.Instum.Chromat	**Methods.MathStat:**
Eight times, in sequential mode ▪ Each sample was injected into the chromatograph Each time emission spectra were recorded along the full chromatogram using a fast scanning fluorescence detector, exciting at a different wavelength across the excitation spectra of compounds of interest ▪ End each End eight	MV.MC,Calib Four-way o PARAFAC o Unfolded PLS with residual trilinearization (U-PLS/RTL) o Multi-way PLS with residual trilinearization (N-PLS/RTL)
4-Way Data Tensor	**Quality of Output:**
✓ Input: three-way ETM data for the calibration sample set and for each of the test samples were joined into a single tensor ✓ Output: 4-way data tensor	▪ Best results were found when either U-PLS/RTL or N-PLS/RTL algorithms were used to perform the multivariate calibration
Four-way multivariate calibration using ultra-fast high-performance liquid chromatography with fluorescence excitation–emission detection. Application to the direct analysis of chlorophylls a and b and pheophytins a and b in olive oils	Chemometrics and Intelligent Laboratory Systems, 125,2013,121-131 doi.org/10.1016/j.chemolab.2013.04.005
Valeria A. Lozano and Arsenio Muñoz de la Peña and Isabel Durán-Merás and Anunciación Espinosa Mansilla and Graciela M. Escandar	

DataSsets .

- Simulated data
- Four-way fluorescence excitation–emission–pH data,

Methods.MathStat: 4wayData.MV_MComp.Calib:

- Regularized self-weighted alternating quadrilinear decomposition (RSWAQLD)
- Basis: Least-squares scheme + two extra terms are added to each loss function
- Philosophy of self-weighting operation (from SWATLD)
  - + Quite stable; flexible
  - + Insensitive to the excess estimated number factors (as long as it is no less than the true number of factors)
  - + Higher-order advantage
    - + Provide a satisfying result even in high collinear systems RSWAQLD, Four-way PARAFAC

An alternative quadrilinear decomposition algorithm for four-way calibration with application to analysis of four-way fluorescence excitation–emission–pH data array	Analytica Chimica Acta 758,2013,45-57 doi.org/10.1016/j.aca.2012.10.056

Chao Kang and Hai-Long Wu and Yong-Jie Yu and Ya-Juan Liu and Shu-Rong Zhang and Xiao-Hua Zhang and Ru-Qin Yu

Chem.Syst:

- Adrenaline ;
- Noradrenaline;
- catecholamine mixtures

Sample.RealLife.Environment

- Urine from healthy subjects

Data. Fourth Order Tensor (FO.T)

- Two component

Process.Chem

- Formation of fluorescing 3,5,6-trihydroxyindole derivatives (lutines) of the catecholamines
- Degradation for adrenaline ;noradrenaline.
- Selectivity: Because of different reaction rates

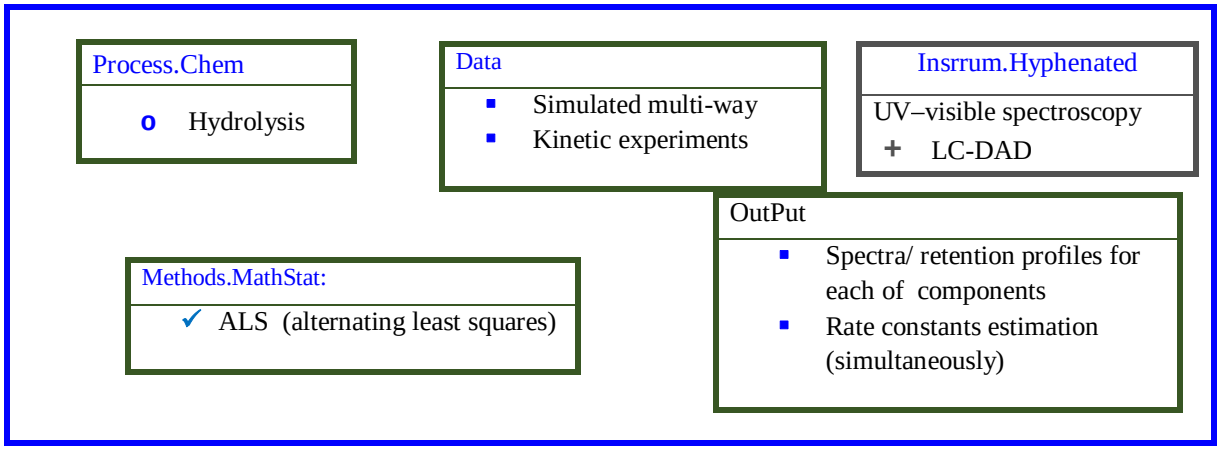
Methods.MathStat:

Two-components

- ✓ Four-way PARAFAC
- ✓ Multilinear-PLSR
- ✓ Similar RMSECV

Quantifying catecholamines using multi-way kinetic modelling	Analytica Chimica Acta,475(1),203,137-150 doi.org/10.1016/S0003-2670(02)01256-4

Rikke P.H Nikolajsen and Karl S Booksh and Åse M Hansen and Rasmus Bro



Analysis of three- and four-way data using multivariate curve resolution-alternating least squares with global multi-way kinetic fitting	Chemometrics and Intelligent Laboratory Systems, 81(1)2006,82-93 doi.org/10.1016/j.chemolab.2005.10.005
Ernst Bezemer and Sarah C. Rutan	

DataSets: ▪ Three-way ▪ four-way	Tasks ▪ Exploratory analysis ▪ Curve resolution, ▪ calibration
3D - Review of Chemometrics Applied to Spectroscopy: Multiway Analysis"	The Handbook of Organic Compounds, Academic Press, 2001,339-352doi.org/10.1016/B978-012763560-6/50033-7
Jerry Workman	

ACS.org ; sciencedirect.com : Information Source

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