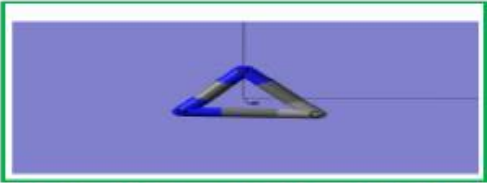
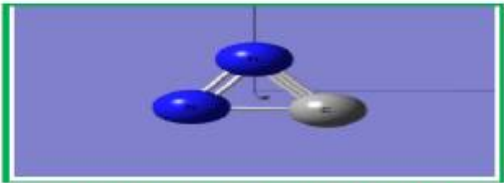




New Chemistry News
N=C=N



New News of Chem (NNC)



ChemNewsNew (CNN)

Support vector machines (SVM) in Omni_metrics (Om)

Reviews & Tutorials`

Twin Support Vector Machine: A review from 2007 to 2014

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Automation of SVM

Automated support vector regression

J. Chemometrics, 31(2017)xxx
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[super SVR: bootstrapped Latin partitions (BLPs) embedded into calibration → opt value of cost fns [Gauss, Laplace, and Huber] >>
[Super PLS]; Data[linear data with uniformly distributed noise; outliers; real life samples]

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[no cost function ; no slack variables to optimize] ;
[NMR spectra obtained from 12 tea sample extracts.] ;
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Chemometrics and Intelligent Laboratory
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31

[SVM;PLS-DA; LASSO; Sparse PLS]; [sparse regularization + subsampling]

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Robust variable selection based on bagging classification tree for support vector machine in metabonomic data analysis

J. Chemometrics, (2018), xxx
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[bagging classification tree-SVM];

Chen, Shu-Fang and Gu, Hui and Tu, Meng-Ying and Zhou, Yan-Ping and Cui, Yan-Fang

Robust variable selection based on bagging classification tree for support vector machine in metabonomic data analysis

J. Chemometrics,
doi = {10.1002/cem.2921},

[metabonomic Data; Probe: ¹HNMR ; subjects: Lung cancer vs healthy controls]

[bagging + classification tree (CT) {variable selection ; measuring variable importance }] →
{robustly selecting the informative variables}}

[BaG_CT_SVM]

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The prediction of food additives in the fruit juice based on electronic nose with chemometrics Food Chemistry 230 (2017) 208–214

[PLSR, SVM;ELM;RF] [monitoring benzoic acid and chitosan in fruit juices]

Shanshan Qiu, Jun Wanga,

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[LS-SVM]; [Extreme Learning Machines (ELM); Kernel ELM; K-NN]

Ayşegül Uçar, Recep Özalp,

Efficient android electronic nose design for recognition and perception of fruit odors using Kernel Extreme Learning Machines, Chemometrics and Intelligent Laboratory Systems, Volume 166, 15 July 2017, 69-80,

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[VW-SVM:variable-weighted support vector machine; PSO]

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[SVM; RF; Cubist, Gaussian process (GP), and Boosting];
[1830 drug compounds [NSGA-II;PLS] ; [Williams plot and scaffold analyses]

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Sujie Xue, Xuefeng Yan,

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[SVM; Naive Bayes; C4.5 Decision Tree; Random Forest];
[SOM]; [601 601 noncongeneric PLK1 inhibitors]

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[SVM; Probabilistic_NN; k-NN]

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[deep learning] >> [SVM; NNs]

Tian, Shengwei and Yan, Yilin and Yu, Long and Qian, Jin and Ye, Feiyue

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Detection of unexpected frauds: Screening and quantification of maleic acid in cassava starch by Fourier transform near-infrared spectroscopy
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[PSL1; LS-SVM; Standard normal variate transform]

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Comparing the analytical performances of Micro-NIR and FT-NIR spectrometers in the evaluation of acerola fruit quality, using PLS and SVM regression algorithms	Talanta 165 (2017) 112–116
[miniature dispersion NIR spectrometer (weight < 60 g); FT-NIR]; [PLSR; E-SVR (epsilon SVR)] Cristina Malegoria, Emanuel José Nascimento Marques, Sergio Tonetto de Freitas, Maria Fernanda Pimentel, Celio Pasquinie, Ernestina Casiraghia	
Application of terahertz spectroscopy imaging for discrimination of transgenic rice seeds with chemometrics	Food Chemistry 210 (2016) 415–421
[Ls-SVM;PCA;RF;MLP-BP]; [misclassification of nontransgenic rice seeds as transgenic rice and vice versa] Wei Liu, Changhong Liu, Xiaohua Hu, Jianbo Yang, Lei Zheng	
Quantitative determination of aflatoxin B1 concentration in acetonitrile by chemometric methods using terahertz spectroscopy	Food Chemistry 209 (2016) 286–292
[PLS; PCR 1–50 lg/ml] ; [SVM (RBF kernel) ; GA-SVM 1–50 lg/l] Hongyi Ge, Yuying Jiang, Feiyu Lian, Yuan Zhang, Shanhong Xia	
Combining the genetic algorithm and successive projection algorithm for the selection of feature wavelengths to evaluate exudative characteristics in frozen–thawed fish muscle	Food Chemistry 197 (2016) 855–863
[GA–SPA–LS-SVM; SPA–LS-SVM; GA–LS-SVM] [SPA: successive projections algorithm] Jun-Hu Cheng, Da-Wen Sun, Hongbin Pu	
How to predict the sugariness and hardness of melons: A near-infrared hyperspectral imaging method	Food Chemistry 218 (2017) 413–421
[SVM; PCA;NN;PLSR] Meijun Sun, Dong Zhang, Li Liu, Zheng Wang	
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[LS-SVM] Jiang-Lin Li, Da-Wen Sun, Hongbin Pu, Digvir S. Jayas	
Unravelling effects of flavanols and their derivatives on acrylamide formation via support vector machine modelling	Food Chemistry 221 (2017) 178–186
[SVR; MLR] Mengmeng Huang, Qiao Wang, Xinyu Chen, Yu Zhang	

One input-class and two input-class classifications for differentiating olive oil from other edible vegetable oils by use of the normal-phase liquid chromatography fingerprint of the methyl-transesterified fraction Food Chemistry 221 (2017) 1784–1791
 Ana M. Jiménez-Carvelo, Estefanía Pérez-Castaño, Antonio González-Casado, Luis Cuadros-Rodríguez

Comparison of different CCD detectors and chemometrics for predicting total anthocyanin content and antioxidant activity of mulberry fruit using visible and near infrared hyperspectral imaging technique Food Chemistry 224 (2017) 1–10
 [LS-SVM; PLSR] [SPA;UVA;CARS: for wavelength selection]
 UVE : uninformative variable elimination
 CARS : competitive adaptive reweighted sampling
 SPA : successive projections algorithm
 Lingxia Huang, Yibin Zhou, Liuwei Meng, Di Wuc, Yong He d

Determining the geographical origin of *Sechium edule* fruits by multielement analysis and advanced chemometric techniques Food Chemistry 210 (2016) 228–234
 [SVM;PCA; LDA; kNN; pLS-DA]
 Melisa J. Hidalgo, Diana C. Fechner, Eduardo J. Marchevsky, Roberto G. Pellerano

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 [SVM; PLSR]
 Fei Maa, Hao Qin, Kefu Shi, Cunliu Zhou, Conggui Chen, Xiaohua Huc, Lei Zheng

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 Rocío Ríos-Rein, Saioa Elcoroaristizaba, Juan A. Ocaña-González, Diego L. García-González, José M. Amigo, Raquel M. Callejón

Development of predictive models for total phenolics and free p-coumaric acid contents in barley grain by near-infrared spectroscopy Food Chemistry 227 (2017) 342–348
 [PLS; SVM]; [90 Barleysamples]
 Zhigang Han, Shengguan Cai, Xuelei Zhang, Qiufeng Qian, Yuqing Huang, Fei Dai, Guoping Zhang

Ion mobility spectrometry fingerprints: A rapid detection technology for adulteration of sesame oil Food Chemistry 192 (2016) 60–66
 [recursive_SVM; PCA, RF]; [Pareto scaling]
 Liangxiao Zhang, Qian Shuai, Peiwu Li, Qi Zhang, Fei Maa, Wen Zhang, Xiaoxia Ding

Multivariate adulteration detection for sesame oil Chemometrics and Intelligent Laboratory Systems, Volume 161, 15 February 2017, 147-150,
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 Liangxiao Zhang, Xiaorong Huang, Peiwu Li, Wei Na, Jun Jiang, Jin Mao, Xiaoxia Ding, Qi Zhang,

- Nonlinear classification of commercial Mexican tequilas
 [SVM, Counter propagation NNs; PLS_DA; Kernel-PLS; QDA]
 {GA; SRI index; variable selection}
 Andrade, Jose Manuel and Ballabio, Davide and Gómez-Carracedo, Maria Paz and Pérez-Caballero, Guadalupe
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 [SVM; Synergy interval PLS; PCA]
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- Potential of multispectral imaging for real-time determination of colour change and moisture distribution in carrot slices during hot air dehydration
 [LS-SVM-RBFKernel; PLS; MLP-BP]
 Changhong Liu, Wei Liu, Xuzhong Lu, Wei Chen, Jianbo Yang, Lei Zheng
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- Parsimonious model development for real-time monitoring of moisture in red meat using hyperspectral imaging
 Mohammed Kamruzzaman, Yoshio Makino, Seiichi Oshita
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- LS-SVM-Simplex opt with LOO-CV
 Active learning algorithm can establish classifier of blueberry damage with very small training dataset using hyperspectral transmittance data
 [SVM ; SOM; classifier based on estimated error reduction]
 Meng-Han Hu, Yu Zhao, Guang-Tao Zhai,
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- Global metabolite profiling and diagnostic ion filtering strategy by LC-QTOF MS for rapid identification of raw and processed pieces of *Rheum palmatum* L.
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 Ying Liu, Li Li, Yong-Qing Xiao, Jia-Qi Yao, Peng-Yuan Li, Ding-Rong Yu, Yin-Lian Ma
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 Luigi Portinale, Giorgio Leonardi, Marco Arlorio, Jean Daniel Coisson, Fabiano Travaglia, Monica Locatelli,
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Chemometrics and Intelligent Laboratory Systems, Volume 164, 15 May 2017, 8-15

[SVM];

[Preprocessing: multiplicative scatter correction; Savitzky-Golay smoothing; first derivative and wavelet transform]

[multivariate curve resolution alternating least squares (MCR-ALS)]

Xin Zhang, Shaohua Lu, Yi Liao, Zhuoyong Zhang,

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[SIMCA: soft independent modeling of class analogies) ; PLS-DA]

Biancolillo A, Bucci R, Magrì AL, Magrì AD, Marini F

2-DE combined with two-layer feature selection accurately establishes the origin of oolong tea

Food Chemistry 211 (2016) 392–399

[Two layer feature selection]

Han-Ju Chien, Yen-Wei Chu, Chi-Wei Chen, Yu-Min Juang, Min-Wei Chien, Chih-Wei Liu,
Chia-Chang Wu, Jason T.C. Tzen, Chien-Chen Lai

Binary mixtures of waxy wheat and conventional wheat as measured by NIR reflectance

Talanta146(2016)496–506

[SVM; PCA;PLS; LR];

Stephen R. Delwiche, Robert A. Graybosch

Pharmacometrics

Performance of NIR handheld spectrometers for the detection of counterfeit tablets
[SVM_RBF; LDA; QDA; kNN] [PCA]

Aurélie Guillemain, Klara Dégardin, Yves Roggo

Talanta 165 (2017) 632–640

Development of particle swarm optimization–support vector regression (PSO-SVR) coupled with microwave plasma torch–atomic emission spectrometry for quality control of ginseng

[PSO-SVR;PLSR]

Ying, Yangwei and Jin, Wei and Yu, Haixiang and Yu, Bingwen and Shan, Jin and Lv, Shaowu and Zhu, Dan and Jin, Qinhan and Mu, Ying

J. Chemometrics, 31(1)(2017), xxx
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Environmetrics

Calibration of UV/Vis spectrophotometers: A review and comparison of different methods to estimate TSS and total and dissolved COD concentrations in sewers, WWTPs and rivers
[SVM; MLR; EVOLUTIONARY algorithm; PLS]

Mathieu Lepot, Andres Torres, Thomas Hofer, Nicolas Caradot, Günter Gruber, Jean-Baptiste Aubin, Jean-Luc Bertrand-Krajewski

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Industry- Melt index

A real-time model based on optimized least squares support vector machine for industrial polypropylene melt index prediction

[LS_SVM]; [Hyb_ACO_DE_LSSVM, DE-LS_SVM]

Zhang, Miao and Liu, Xinggao

J. Chemometrics, 30(6)(2016)324-331

Industry- Steel

Steel surface defects recognition based on multi-type statistical features and enhanced twin support vector machine

Maoxiang Chu, Rongfen Gong, Song Gao, Jie Zhao,

Chemometrics and Intelligent Laboratory Systems, Volume 171, 15 December 2017, 140-150

Steel surface defect classification using multiple hyper-spheres support vector machine with additional information

[multiple hyper-spheres-SVM]

Rongfen Gong, Chengdong Wu, Maoxiang Chu,

Chemomet. Intel. Lab. Syst., 172, 15
January 2018, 109-117

Prediction of pitting corrosion status of EN 1.4404 stainless steel by using a 2-stage procedure based on support vector machines

[automatic model]; [ROC]

Jiménez-Come, María Jesús and Turias Domínguez, Ignacio José and Matres, Victoria

J. Chemometrics, 31(12)(2017)
doi = {10.1002/cem.2936},

Determination of carbon and sulfur content in coal by laser induced breakdown spectroscopy combined with kernel-based extreme learning machine Chemometrics and Intelligent Laboratory Systems, Volume 167, 15 August 2017, 226-231

[LS-SVM]; MLP-BP] < [kernel-based extreme learning machine (K-ELM)]
 Chunhua Yan, Juan Qi, Junxiu Ma, Hongsheng Tang, Tianlong Zhang, Hua Li,

Ensemble deep kernel learning with application to quality prediction in industrial polymerization processes , Chemomet. Intel. Lab. Syst., 174, 15 March 2018, 15-21

[SVR:PLS];
 [data-rich-but-information-poor task;
 ensemble deep kernel learning model ; deep brief network]
 Yi Liu, Chao Yang, Zengliang Gao, Yuan Yao,

Biochemistry

Prediction subcellular localization of Gram-negative bacterial proteins by support vector machine using wavelet denoising and Chou's pseudo amino acid composition Chemometrics and Intelligent Laboratory Systems, Volume 167, 15 August 2017, 102-112

Bin Yu, Shan Li, Cheng Chen, Jiameng Xu, Wenying Qiu, Xue Wu, Ruixin Chen,

A novel nucleic acid sequence encoding strategy for high-performance aptamer identification and the aid of sequence design and optimization Chemometrics and Intelligent Laboratory Systems, Volume 170, 15 November 2017, 32-37

Qin Yang, Sui-Ping Wang, Xin-Liang Yu, Xiao-Hai Yang, Qiu-Ping Guo, Li-Juan Tang, Jian-Hui Jiang, Ru-Qin Yu

Diagnostics

Development of diagnostic models for canine osteoarthritis based on serum and joint fluid mid-infrared spectral data using five different discrimination and classification methods J. Chemometrics, 30(11)(2016)663-681

[SVM]; [PCA-DA; MLR; PLS_DA; mult.logistic.Reg.; Regularized_LDA]
 Hou, Siyuan

Headspace-programmed temperature vaporizer-massspectrometry and pattern recognition techniques for the analysis of volatiles in saliva samples Talanta160(2016)21-27

[Cancer patients vs control group]
 [SVM;Mahalanobis Dist;PCA; kNN; SIMCA]
 Ana PérezAntón, MigueldelNogalSánchez, ÁngelPedroCrisolinoPozas, José LuisPérezPavón, BernardoMorenoCordero

Support vector regression coupled with wavelength selection as a robust analytical method, Chemomet. Intel. Lab. Syst., 172, 15 January 2018, 167-17

[SVR-RFE;] [Probe: NIR]
 interval PLS; backward interval PLS; synergy interval PLS;
 recursive feature elimination (RFE)
 Felipe Soares, Michel J. Anzanello,

ChemBCPP: A freely available web server for calculating commonly used physicochemical properties, [aqueous solubility, octanol-water partition coefficient; BP; density, flash point; viscosity, surface tension; vapor pressure; melting point]	Chemometrics and Intelligent Laboratory Systems, Volume 171, 15 December 2017, 65-73
Jie Dong, Ning-Ning Wang, Ke-Yi Liu, Min-Feng Zhu, Yong-Huan Yun, Wen-Bin Zeng, Alex F. Chen, Dong-Sheng Cao,	
NIR hyperspectral imaging spectroscopy and chemometrics for the discrimination of roots and crop residues extracted from soil samples	J. Chemometrics, 32(1)(2018), xxx doi = {10.1002/cem.2982}
[SVR; PLS] [wheat roots]	
Eylenbosch, Damien and Bodson, Bernard and Baeten, Vincent and Fernández Pierna, Juan Antonio	
Application of near-infrared spectroscopy combined with chemometrics for online monitoring of Moluodan extraction	J. Chemometrics, (2018), xxx doi = {10.1002/cem.2979},
[PSO_LS_SVM + SPXY_Cars] ; {PLS}; [Paeoniflorin online quantitation] [set partitioning based on joint X-Y distances algorithm (SPXY) ; competitive adaptive reweighted sampling (Cars)];	
Tao, Lingyan and Li, Wenjing and Jin, Ye and Yang, Yue and Wu, Yongjiang and Liu, Xuesong	
Authentication and inference of seal stamps on Chinese traditional painting by using multivariate classification and near-infrared spectroscopy	Chemometrics and Intelligent Laboratory Systems, Volume 171, 15 December 2017, 226-233
[NL-SVM; PLS-DA;HCA] [1, 2.5% noise in NIR] [Mahalanobis distances]	
Zewei Chen, An Gu, Xin Zhang, Zhuoyong Zhang,	
Artificially generated near-infrared spectral data for classification purposes	Chemomet. Intel. Lab. Syst., 172, 15 January 2018, 100-108
[class-imbalanced classification problem] [SVM; LDA; classification trees;]	
Vilma Sem, Jana Kolar, Lara Lusa	
Identifying animal species in NIR hyperspectral images of processed animal proteins (PAPs): Comparison of multivariate techniques	Chemomet. Intel. Lab. Syst., 172, 15 January 2018, 139-149
{SVM; PLS-DA; Subspace Discriminant}	
Cecilia Riccioli, Dolores Pérez-Marín, Ana Garrido-Varo,	
Estimating nitrogen status of rice canopy using hyperspectral reflectance combined with BPSO-SVR in cold region	Chemomet. Intel. Lab. Syst., 172, 15 January 2018, 68-79
[Binary-PSO-SVR]; [PLSR; PCR; GA-MLP-BP]	
Kezhu Tan, Shuwen Wang, Yuzhu Song, Yao Liu, Zhenping Gong,	
Comparing unfolded and two-dimensional discriminant analysis and support vector machines for classification of EEM data	Chemometrics and Intelligent Laboratory Systems, Volume 170, 15 November 2017, 1-12,
[modified 2D-PCA-SVM ; 2D-PCA-LDA; 2D-PCA-QDA;] [3-way data] [unfolding ; folding]	

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Ewa Szyman´ska, Jan Gerretzen, Jasper Engel, Brigitte Geurts, Lionel Blanchet,
 Lutgarde M.C. Buydens

One-dimensional convolutional neural networks for spectroscopic signal regression [SVM; 1D CNN +PSO; Gaussian process regression] *J. Chemometrics*, (2018) xxx doi = {10.1002/cem.2977},
 Malek, Salim and Melgani, Farid and Bazi, Yakoub

sciedirect.com (SD): Information Source (is)

Hybrid SVM (Support vector machine)

Binary hybrid SVM

\$\$_	SVM
PSO	SVM
Super	SVM
Twin	SVM
Variable weighted	SVM
GA	SVM
Recursive	SVM
One-class	SVM
Simplex	SVM
multiple hyper-spheres	SVM
NL	SVM
PSO (Binary)	SVM
PCA(2D-)	SVM
Automated	SVR
ε-	SVR
Fuzzy entropy	SVR
Probability distribution`	SVR
Recursive feature elimination	SVR

Ternary hybrid SVM

SS1	\$\$2	SVM
Bagging	Classification tree	SVM
ACO	Differential evolution	LSSVM
GA	Successive Projection Algorithm	LS-SVM

Abbreviation		Acronym
\$\$1	\$\$2	
	Bag	Bagging
	C 4.5	
	CT	classification tree
	Decision trees	Decision trees
	DeepLrn	Deep Learning
	ELM	Extreme learning machine
Kernel	ELM	Kernel ELM
	Evolv.alg	Evolutionary algorithm
	k-NN	k-nearest neighbors
	LASSO	
	LDA	Linear discriminate analysis
Mult.logistic.Reg.; Regularized_	LDA	
	MLP	Multi layer perceptron
	MLR	Multiple linear regression
	Neocognitron	Neocognitron
	NN	Neural network
probabilistic	NN	
Deep	NN	
	NSGA-II	
	SOM	Self organizing map

Abbreviation		Acronym
\$\$1	\$\$2	
	PCA	Principal component analysis
	PCR	Principal component regression
Super	PCR	Super PCR
	PLS	Partial Least squares
Super	PLS	
Sparse	PLS	
Ortho	PLS	
Interval	PLS	
	PLS1	PLS with one response variable
	PLS2	PLS with more than one response variable
	PLSR	PLS regression
Logistic	R	Logistic regression
Gaussian process	regres	
	regres	Regresson
	RF	Random forest
	RF	Random Forest
	SIMCA	Soft independent modeling of class analogies