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**Research tutorial (ResT)**

# [Computational] TensorLab (CTLab)
## Part I: 3D-surfaces and 2D-contours in OmniMetricS

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**Mother Nature**
**Creator/ preserver/ assimilator of knowledge/ Information/ Data systems (Kids)**

## Conspectus

*Background:Tensorial representation of numerical (integer, floating point) values, also called m-way data, is the basic input in data-information-knowledge cycle. Graphical output of primary data as scatter diagrams to model fitting, residual trend exploitation for better explanation are not only coveted visual appreciation tools, but explore misfits, unexplained/unexplored information etc. The reliable software no doubt result in parameters/ statistics of model mostly in the traditional mode or in limited cases with expert system (ES) driven inferences.*

*3D-surfaces and 2D-contours: The profiles of linear, full quadratic, polynomial, exponential, transcendental functions in two variables as 3D-surfaces, 2D-contours with gradients, rotating view angle (i.e. keeping one of the variable constant ) such that surface reduces to 2D- plots are detailed.The depth and breadth of the response surface modelling strategy is highlighted.The popular graphics of data sets in vector/ matrix form using today's state-of-art-profiles are incorporated in appendices.*

*m-Way data generation:Zero to third order instruments, variation of influential experimental variables and external environmental factors in the interacting as well as non-interacting chemical systems generate one- to multi-way through 5-way data tensors. They are usually modelled with multi-variate methods in the unfolded modeor as they are. The possible unfolding modes and ill effect on end results are discussed. The nomenclature of numerical data under different heads like vector, matrices, tensors, multi-ways are brought under the same roof.*

*Applications in Omnimetrics:The role of multi-dimensional graphics of raw experimental data in exploratory data analysis and in various phases of multi-variate-multi-response-linear-nonlinear parametric-/non-parametric-/ free-variable models in prime disciplines viz. environment, foodomics, medical diagnosis, pharma industry, physical chemistry reported during last two years are incorporated. The typical case studies incorporated in this research tutorial (HOT Ice: hands on tutorial for intelligent*

*chemical education) include applications in quality of natural water (streams, estuaries etc.)/ artificial water reservoirs, water quality tap water, potable watertreatment,waste water treatment plants, aerosols, metabolic profiling, pollutants like PAHs, adulterants in lime fruits/fruit juices, wine discrimination andclinical analysis of urine. The DOM (dissolved organic matter) in different phases of environment drew attention of multi-variate methods and graphics. The estimation of rate/ equilibrium constants of metal ligand systems and outersphere/ innersphere complexes are improved by multivariate chemometric methods and contour diagrams. The excitation-emission fluorescence spectroscopy, 2D-NMR, HPLC-DAD etc. are prime second order hyphenated instrumental techniques employed in these studies.The 3D surfaces and corresponding contour diagrams in basic and inter-disciplinary chemical research are reproduced from research literature in the appendices.*

*A brief note of a few multi-way chemometric methods are incorporated with a tinge of knowledge base/necessary conditions /failure instances and remedial measures. The statistical/fuzzy distributions, chaotic series, multiple global functions not discussed here will be described in a separate communication.*

**Keywords:**3D-surface, 2D-contour, Tensorial data, Local/global extrema, iso-surfaces/contours, Kriging, Neural networks, Interpolation, omnimetrics, experimental design, Environment, Dietetometrics, physical chemistry, chemical physics, chemical biology.

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