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Joint Event

David A Vaccari, Chemistry and Biomedicine 2018, Volume 8
DOI: 10.4066/2249-622X-C4-012

8th World Congress on

Chemistry and Organic Chemistry

&

International Conference on

Biomedicine & Pharmacotherapy

October 22-23, 2018 | Frankfurt, Germany

Multivariate polynomial regression for response surface analysis – A new tool for empirical data discovery

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A novel approach is described for empirically modeling multivariate response surfaces, either timeseries or nontime series. Potential applications in chemistry include structure-property relationships and physicochemical property correlations, among many others. The approach uses multivariate polynomial regression (MPR) with a step-wise algorithm to select terms. The approach includes advantages of multilinear regression such as simplicity and transparency. It also has the advantages of more complex modeling approaches such as artificial neural networks (ANNs) in its ability to model complex response surfaces, including high degree curvilinear interactions. Furthermore, MPR has advantages over ANNs in its transparency, tractability, parsimony and resistance to overfitting. These advantages are illustrated by an example and a freely-available online tool for fitting these models is described. Two applications are described. The first is a non-time-series material property correlation using eight independent variables to predict the strength of a concrete mixture. The second is a vector autoregression (VAR) model to describe tungsten flow in the U.S. economy.

Speaker Biography

David Vaccari is a professor of environmental engineering at Stevens Institute of Technology in Hoboken, NJ. He has a masters and PhD in environmental science and a master's in chemical engineering, all from Rutgers University. Originally focused on waste water treatment and water pollution, he now specializes in modeling global phosphorus resource flows and in nonlinear statistical modeling in general. The specialization in phosphorus grew from involvement in planning bioregenerative life support for long-term space missions for NASA, from research for a textbook in Environmental Biology published by John Wiley, and from work on models of phosphorus pollution in streams. He is a licensed professional engineer, a Board-Certified Environmental Engineer, and is listed in the Who's Who in Environmental Engineering and Science.

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