Lecture: Tuesday 11 December, at 2:15pm, Faculty Hall, Faculty of Food Technology

IMPROVED STATISTICAL FITTING OF ADSORPTION ISOTHERMS

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Abstract:

Adsorption processes can be studied in food science to understand the proportions of specified bioactive molecules (such as polyphenols) that are adsorbed onto larger molecules present in food, which impact their bioaccessibility. These processes are analyzed with nonlinear mathematical expressions called adsorption isotherms. For given physiological conditions (e.g. temperature, acidity and amount of adsorbent), an adsorption isotherm relates the amount of the bioactive molecules that are adsorbed q_e to the concentration not adsorbed c_e, in equilibrium, for each of several experimentally-specified initial amounts. Traditional fitting of adsorption isotherms by nonlinear regression (minimizing sums of squares of the vertical error at each c_e) suffers from a statistical inconsistency that we overcome. Proper statistical fitting in this setting relates the observed amounts adsorbed to that unique value on the adsorption isotherm that corresponds to the specified initial amount. As we explain, this is a diagonal rather than vertical projection. We explain and illustrate proper fitting with statistical software. Furthermore, a consequence of the nonlinear modeling is a statistical bias in the standard parameter estimates. We show how this bias may be overcome.

Curriculum Vitae:

Andrew R. Barron has served as Professor at Yale University in the Department of Statistics since 1992, including terms as Chair, Director of Undergraduate Studies, and Director of Graduate Studies in the Department. Prior to his tenure at Yale, he was a Professor at the University of Illinois in the Departments of Statistics and Electrical and Computer Engineering. His Bachelor degree is from Rice University in the fields of Mathematical Sciences and Electrical Engineering and his Masters and PhD degrees are from Stanford University (USA) in Electrical Engineering in 1985, with specialization in the role of Information Theory in the fields of Probability and Statistics. He is a Medallion Award winner of the Institute of Mathematical Statistics, a Fellow of the IEEE, and has served several terms on the Board of Governors of the Information Theory Society. He has published more than 80 journal and conference publications, 2 patents, and has provided numerous seminar and conference presentations. He has supervised 19 PhD dissertations. His research interests include entropic central limit theorems, the minimum description length criterion for model selection, analysis of statistical risk of Bayes procedures, optimal rates of function estimation, greedy algorithms, and deep learning networks. His hobby is free-flight aeromodelling, F1A class.