2016 ACC Workshop Description

Nonlinear Regression Modeling: Techniques and Enabling Design of Experiments

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Topics:

This full-day workshop will be a practical guide for nonlinear regression modeling. Although theoretical analysis behind techniques will be revealed, the takeaway will be the participant's ability to:

- Choose appropriate concepts for defining the regression objective,
- Choose an optimization approach and criteria for convergence,
- Apply both data-based and logical criteria for model validation and model discrimination,
- Design experiments for data generation that support model validation,
- Select an appropriate model design considering both order/complexity and utility in use, and
- Estimate model uncertainty based on data variability.

Participants will receive a copy of a new textbook, which will be used as the workshop notes (or, the author's manuscript, if the publication is delayed). Exercises and code can be implemented in any environment, but Excel/VBA will used as in-workshop examples and exercises. The author's software will be provided (Leapfrogging as an optimizer, steady-state as stopping criteria, bootstrapping for estimating model uncertainty) along with several case-study data sets for revealing course concepts. Participants are invited to bring a laptop with Excel version 2010 or higher for in-class applications.

Rational:

Models based on data are often central for model-based control, forecasting, training simulators, analysis and diagnosis, mechanism validation, design scale-up, and supervisory optimization. For many of these applications nonlinear models are preferred in order to capture the process/device behavior. Regression is the procedure of fitting models to data, and nonlinear regression means that the adjustable model coefficients do not appear linearly within the model; and, even for seemingly linear models, a variable delay introduces a nonlinear model coefficient, and which is also constrained to integer values.

Workshop topics will include equation structures, optimization of parameter values in the presence of constraints and local traps, choosing optimization convergence criteria based on model properties, data preprocessing and post-processing, data-based model validation, discrimination between models, design of experiments that support validation outcomes, propagation of uncertainty, and model utility evaluation.

This is not the standard linear regression approach to develop response surface model structures, and classic experimental designs such as Latin Square, Box, and Star plans. This workshop will focus on techniques for nonlinear regression and enabling design of experiments.

Prerequisite skills

Any undergraduate engineering or mathematics program should have provided an adequate experience with topics in calculus, analytical geometry, linear algebra, vector/matrix notation, statistics, and computer programming. The short course will review essential topics that are commonly un-remembered from undergraduate courses.

Format:

One full-day. I will need a projector and screen for my presentation from my laptop computer. For in-class explanations, I'll need black/white board or flipchart. Participants should have tables for their laptops and their course notes. Instructor and participants need electrical power for laptops.

Presenter:

R. Russell Rhinehart – see bio at the end.

Workshop Schedule:

AM – Session 1 Introductory Concepts Model Types Regression Target – Objective Function Constraints Break

AM – Session 2 The Distortion of Linearizing Transforms Optimization Algorithms Multiple Optima Lunch

PM – Session 1 Regression Stopping Criterion Undesired Model Characteristics and Effects Data Pre- and Post-processing Break

PM – Session 2 Model & Experimental Validation Design of Experiments Propagation of Uncertainty Utility vs. Perfection End

Intended Audience:

The intended audience is engineering employees, students, and faculty who use regression modeling techniques to develop and validate models. This is a practical guide on the use of best practices from conventional methods, with examples to illustrate the choices and techniques. Supporting theory will be addressed, but the takeaway will be the ability to specify regression criteria, include constraints, select an appropriate optimizer, validate models, design experiments for relevant data generation, and to estimate uncertainty of the resulting models.

Expected Enrollment:

I suspect there will be about 15 participants, roughly 1/3 students, 1/3 faculty, and 1/3 from industry. This short-course is based partly on an interdisciplinary engineering graduate course (the most popular one at the

university), and on experience in applying the techniques in the undergraduate unit operations laboratory.

To complement the ACC publicity, I plan on doing my own marketing to professional and university groups in the Boston area.

Completeness:

I'd like to include more topics, but it's only a one-day workshop. I believe that with the basic concepts from the workshop, individuals will have the ability to understand the more advanced techniques. There are next generation optimizers, there are build-on techniques for the objective functions. Hopefully I can provide the grounding so that participants can independently move in the other directions. The book as part of the course materials will cover many of the additional topics.

Context:

At the 2015 and 2014 ACCs, I presented workshops on optimization. Although there are similarities, because regression uses optimization, this workshop will return to the content I offered at the 2012 and 2013 ACCs, which has a focus on model development, model validation, and design of experiments.

Presenter Bio:

This workshop will be presented by Russ Rhinehart.

Dr. R. Russell Rhinehart, professor in the School of Chemical Engineering at Oklahoma State University, holds the BP Endowed Chair, and has experience in both industry (13 years) and academe. He was Head of the School from 1997 to 2008, and again from 2011 to 2012. Russ is Past President of the American Automatic Control Council, and was Editor-in-Chief of ISA



Transactions from 1998 to 2012). He is a Fellow of ISA, a CONTROL Automation Hall of Fame inductee, and received the 2009 ISA

Distinguished Service Award, the 2013 Fray International Sustainability Award, and numerous teaching excellence recognitions.

His 1968 B.S. in Chemical Engineering and subsequent M.S. in Nuclear Engineering are both from the University of Maryland. His 1985 Ph.D. in Chemical Engineering is from North Carolina State University.

Russ is the author of the book that will be used for this course, <u>Nonlinear Regression Modeling for Engineering Applications: Modeling,</u> <u>Model Validation, and Enabling Design of Experiments</u>, a Wiley publication anticipated in 2016. He is also coauthor of the Dekker textbook, <u>Applied</u> <u>Engineering Statistics</u>, and has a contract with Wiley for a book on <u>Optimization Applications</u>. He authored six handbook chapters on modeling, uncertainty, process control, and optimization.

Russ teaches modeling, optimization, and process control courses; and has developed short courses for industrial participants offered through ISA or directly to companies related to statistical process control, instrument and control systems, modeling, and model-based control. Much of the material in this short course has been tested in the unit operations laboratory course, and in his nonlinear control research using pilot-scale process equipment.