6 Purposes and types of models. M. D. Hanigan*, *Virginia Tech, Blacksburg, VA.*

The principles of mathematical modeling in agricultural sciences are well described by France and Thornley (1984). They categorized models as static or dynamic, empirical or mechanistic, and deterministic or stochastic, although, in practice, they can fall somewhere in the middle of each. In general, our nutrient requirement models are static, empirical, and deterministic; they provide snapshots in time, do not describe the mechanisms underlying responses, and do not consider the inherent variance intrinsic to biological systems. These models are generally easier to derive, and have served the community very well for more than a century. The Molly cow model is dynamic, mechanistic, and deterministic; it predicts responses through time, is based on the underlying driving elements of digestion and metabolism, but does not represent the biological variation underlying predictions. Dynamic models are very useful when one needs to predict changes over time as compared with representing only the new state after the system is given sufficient time to reach steady state. For example, growth and lactation models are typically dynamic, empirical, and deterministic. They capture the effects of slightly greater growth rates on body weight at any point in the growth cycle, or the effect of greater persistency on overall lactational yield. Static nutrient response models only provide the new rate of growth or milk yield after the animal has consumed the diet long enough to reach a new steady state. They cannot predict full lactation yields. Mechanistic models are often used to represent the effects of underlying behavior on higher level performance, e.g., the effects of passage rate on ruminal digestion or the effects of enzymatic activity of a tissue on metabolism. Such representations may provide more precise predictions of higher level performance, although that generally requires that the mechanisms are well defined and provide unbiased estimates. The models are also very useful to assess the relative importance of more basic information. Addition of stochastic elements to mechanistic models can accommodate known variance in the underlying mechanisms and thus provide confidence intervals for predictions.

Key Words: mathematical model, type, review

7 Dynamic deterministic models. T. Hackmann*, *University of Florida, Gainesville, FL.*

This lesson will demonstrate how to construct dynamic deterministic models, which are popular for mechanistic modeling in nutrition research. This type of model represents a biological system as a set of state variables and simulates how these variables change over time. For example, it can represent the rumen system using state variables for fiber, protein, and starch; subsequently, it can simulate the size of these nutrient pools over a feeding cycle. The model is written formally using differential equations, but it can be drawn first as a compartmental model diagram. In this diagram, each state variable is represented by a rectangle (a pool). Arrows leading to and from a pool represents input and output of material. For the rumen, these arrows commonly represent nutrient intake, digestion, and passage. The diagram is then translated into a set of differential equations. These equations define the change of state variables (pools) over time as the difference between inputs and outputs [i.e., d(*state variable*)/d*t* = *inputs* − *outputs*]. These inputs and outputs, in turn, are functions of parameters (e.g., digestion and passage rates) and other state variables. After defining values of parameters, the model is solved and used to generate predictions. A simple model may have an analytical solution, but a more complex model must be solved numerically (e.g., with Euler's method and difference equations). During a demonstration exercise, the speaker will show how to construct a simple (one-pool) model of rumen fermentation by coding difference equations into an Excel spreadsheet. During a hands-on exercise, participants will construct their own, multi-pool model.

Key Words: mathematical model, state variable, differential equation

8 Estimation of parameter values in nutrition models. L. Moraes*, *The Ohio State University, Columbus, OH.*

The use of modeling techniques in animal nutrition relies on the construction of mathematical models determined by a set of parameters. In practice, parameter true values are unknown. Estimators must be obtained with data from designed experiments, observational studies, meta-analysis or another appropriate data generating mechanism. For virtually any type of model, parameter estimates have to be optimal in some sense. For example, linear regression least squares estimates are the minimizers of the squared differences between observations and predictions. In this setting, if model errors are assumed to independent, identically and normally distributed, least squares estimators coincide with maximum likelihood estimators. Maximum likelihood is the standard estimation method for more complex models used in animal nutrition. It seeks parameter values that maximize the likelihood function: a function constructed with the probability density of the observations but as a function of parameters while fixing the data. Nonlinear models are regularly used in the development of mechanistic models as these allow the relationship between variables to be specified by a function that is nonlinear with respect to the parameters. The flexibility of specifying nonlinear functional forms comes with a cost: the function to be optimized is often complex and an analytical solution to the problem is many times not available. Further, several of the mechanistic models used in animal nutrition rely on the use of differential equations that require numerical integration. Parameter estimation in these cases is usually approached by algorithmic optimization of either a likelihood function or a nonlinear least squares cost function. Recently, Bayesian methods have been proposed as estimation approaches for nutrition models as they naturally describe multilevel structures and incorporate prior information in the analysis. This lesson will cover parameter estimation in a variety of models frequently used in animal nutrition as well as demonstration exercises. During a hands-on exercise, workshop participants will estimate parameters in different models using the freely available software R.

Key Words: least squares, likelihood, Bayesian

9 Model evaluation. E. Kebreab*, *University of California, Davis, Davis, CA.*

Statistical measures of model performance commonly compare predictions with observations judged to be reliable. Model evaluation indicates the level of accuracy and precision of model predictions by assessing the credibility or reliability of a model in comparison to real-world observations. Quantitative statistical model evaluation methods can be classified into 3 types including (1) standard regression statistics, which determines strength of linear relationship, (2) error index, which quantifies deviation in observed units, and (3) relative model evaluation that are dimensionless. Within the first category, analysis of residuals