Methods and Tools for Eevaluating Uncertainty in Ecological Models: a Survey

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EPA United States Environmental Protection Agency

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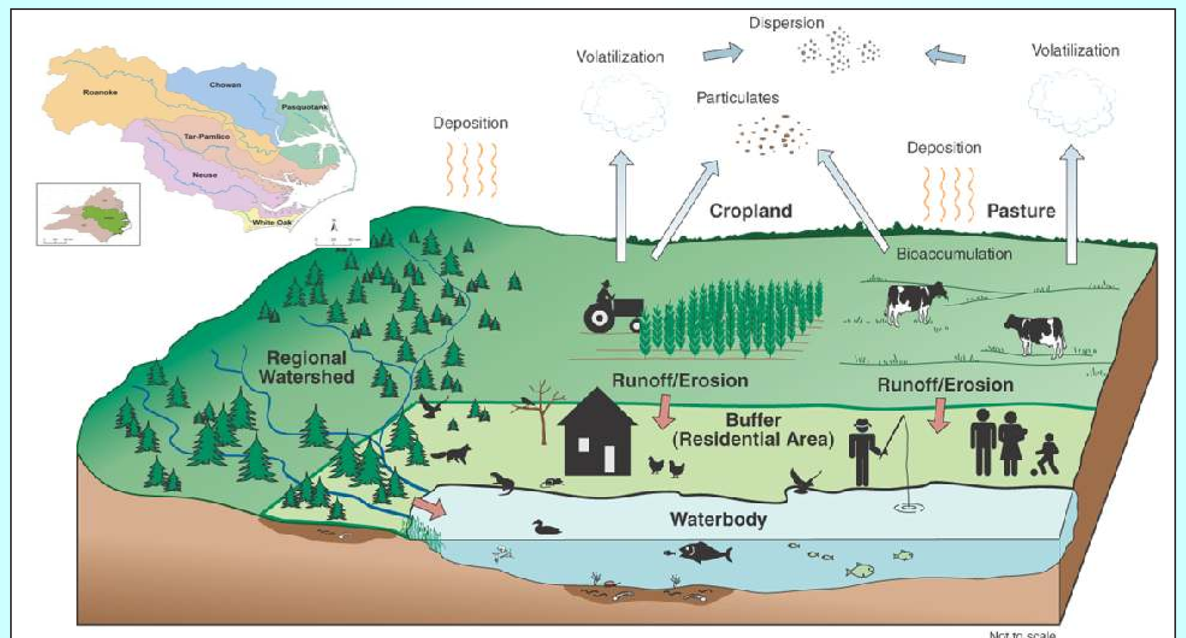
Google "EPA Model Evaluation" or http://www.epa.gov/athens/research/modeling/modelevaluation/index.html

Introduction

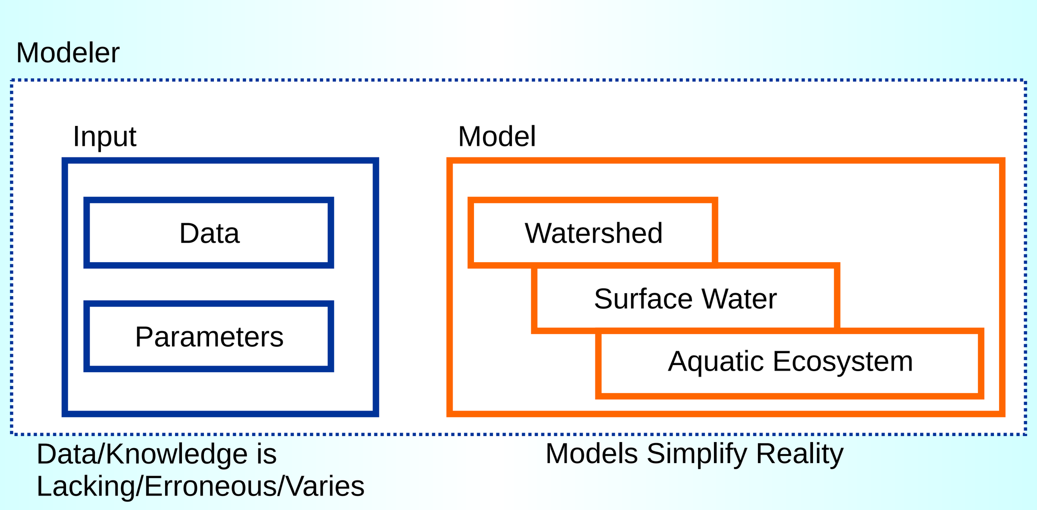
Integrated environmental models have emerged as useful tools supporting research, policy analysis, and decision-making. In this regard, model integration often utilizes an underlying framework, a set of consistent, interdependent, and compatible science components (i.e., models, data, and assessment methods) presented in a context of organizing principles, standards, infrastructure, and software. Besides facilitating model integration, many frameworks provide model-independent tools, additional software codes that supplement the capabilities of the linked components. A variety of tools support model selection and evaluation, the process of determining model usefulness and estimating the range or likelihood of various interesting outcomes. Integrating and evaluating these types of models is challenging in many respects, but such activity can yield a solid foundation for environmental assessment.



This project was motivated by the complexities of integrating process-based numerical models to develop a regional assessment of several ecosystem services (primarily water quantity, water quality, and fish productivity) in the Albermarle-Pamlico Estuary System (APES) in Virginia and North Carolina. Our group has developed an integrated modeling system to estimate ecosystem services in the APES and to simulate the consequences of altered stressor scenarios (changes in nitrogen and mercury loadings, land use and global climate) on the production of these services. The system is primarily composed of four interacting models: SWAT for watershed dynamics and loadings of various contaminants; WASP for surface water routing and water quality; BASS for aquatic community modeling; and HSI, a model of fish habitat suitability. These four are set within a software framework (FRAMES) that allows for the models to communicate with each other, access shared data resources, and run model-independent components for model evaluation purposes.

Concepts and Tools

This poster summarizes available tools for model evaluation; emphasizing approaches that characterize, quantify, or propagate uncertainty. To provide some context, we review sources and types of uncertainty and categorize methods of model evaluation. We then present a tabulation of model evaluation tools; published algorithms or software codes that implement evaluation methods in a model-independent manner, along with a functionality matrix for identifying and comparing tool capabilities. Such a compendium is inherently subjective, and deserving tools may have been left out. The functionality matrix has been translated into a publicly accessible Web site hosted by the USEPA.



Three primary sources of uncertainty include modeler, input, and model. The modeler is responsible for determining and assembling both an input vector (X) and the model (f(X)) operating on an input vector to simulate output. Different modelers may make different decisions about the form and content of X and f(X). Input uncertainty is associated with quantities in the input and output vectors; these can be subdivided into input data, response data, and model parameters. Model uncertainty reflects the inability of a model, even when provided with perfect (i.e., certain or purely irreducible) input, to generate output indistinguishable from corresponding real-world observations.

Ecologists are familiar with a variety of uncertainty techniques, particularly in the intersection of maximum likelihood parameter estimation and Monte Carlo analysis techniques, as well as a recent increase in Bayesian applications. This poster reviews evaluation concepts for integrated environmental modeling and surveys relevant software-based tools, some from areas of model evaluation and uncertainty analysis rarely visited by ecologists. A simplified taxonomy consisting of seven thematic model evaluation methods is used to present a software survey that identified 65 different model evaluation tools. These tools are accessible in the form of a companion web-site containing download links for the identified tools. The survey also reviews strategies for tool interoperability and offers guidance for both ecological practitioners and tool developers.

Model Evaluation Methods

Model evaluation is motivated by a desire to minimize the possibility of making a "wrong" decision about a potentially adverse environmental outcome. Central to such activity is the need to characterize, quantify and propagate uncertainty, while recognizing that both quantitative and qualitative components are present. The desire to be comprehensive has yielded a broad variety of model evaluation methods and packaged software tools. Numerous uncertainty taxonomies and classification systems have been advocated. In some cases, different systems assign different meanings to the same terms; in others, different systems reflect alternative perspectives. This intrinsic vagueness is an example of "linguistic uncertainty" and can cause significant confusion. Seven subjective categories of methods for quantitative model evaluation were identified (Table 1). The identified categories reflect common terminology used in the literature when describing the purpose of a given model evaluation tool or algorithm. Assigning tools to a particular method was occasionally difficult and necessarily subjective, as there is a certain degree of overlap. Ideally, core model evaluation activities performed for decision support should include (1) data analysis to characterize any available input and response data, (2) sensitivity analysis to determine the most important set of inputs, and (3) uncertainty analysis to establish the range or likelihood of predicted outcomes. If sufficient response data is available, identifiability analysis and parameter estimation. If sufficient expertise is available, Bayesian networks may be helpful. Given adequate resources and knowledge base, several alternative models should be developed and subjected to multimodel analysis.

Discussion

The list presented on the right illustrates the wide variety of tools covering all aspects of model evaluation. Integrating these tools would facilitate routine and comprehensive model evaluations within the environmental modeling community. owever, there are numerous barriers to achieving such integration. Many different programming languages, compilers, and development platforms have been used, leaving largely incompatible source codes.

The review portion of this work is intended to serve as a springboard for identifying and understanding relevant concepts, methods, and issues. An extensive tool catalog has been compiled, which can facilitate selection and acquisition of necessary tools for comprehensive model evaluation, and also hopefully minimize redundant tool development in the future. The assembled list of tools contains a considerable amount of overlapping functionality. This redundancy confounds selecting the best tool for the job.

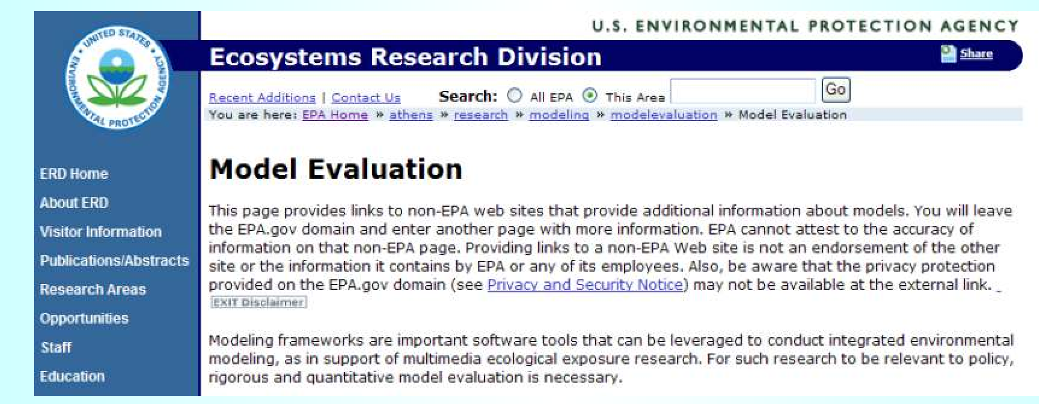
Ultimately, we anticipate robust community support for only a small number of de facto frameworks within different regulatory and application modeling domains. Ongoing multi-institutional efforts will then establish consistent standards across these frameworks. Such advancements will send a clear message to developers: tools that adhere to interoperability standards will have broader support, greater usage, and more impact. In this way, standards and frameworks will encourage enhanced tool interoperability and facilitate a much more comprehensive model evaluation paradigm.

Table 1. Quantitative Methods of Model Evaluation

Method	Purpose of the Method	Subclassifications
Data analysis (DA)	to evaluate or summarize input, response, or model output data	time series, population, geospatial
Identifiability analysis (IA)	to expose inadequacies in the data or suggest improvements in the model structure	temporal, behavioral, spatial
Parameter estimation (PE)	to quantify uncertain model parameters using model simulations and available response data	single solution, multiple solution
Uncertainty analysis (UA)	to quantify output uncertainty by propagating sources of uncertainty through the model	sampling methods, approximation methods
Sensitivity analysis (SA)	to determine which inputs are most significant	screening, local, global
Multimodel analysis (MMA)	to evaluate model uncertainty or generate ensemble predictions via consideration of multiple plausible models	quantitative, qualitative
Bayesian networks (BN)	to combine prior distributions of uncertainty with general knowledge and site-specific data to yield an updated (posterior) set of distributions	hierarchical Bayesian,Bayesian decision networks

Tool Compilation and Web Site

Sixty-five tools were identified and included on the web site. Using the seven model evaluation methods previously discussed, the overall tool coverage consisted of: data analysis (5 tools), identifiability analysis (10 tools), parameter estimation (32 tools), uncertainty analysis (26 tools), sensitivity analysis (33 tools), multimodel analysis (6 tools), Bayesian networks (5 tools). Direct links to tools are provided, some are available for download as standalone executables, complete with user manual; some are provided as source code on request from a designated contact; and others are available only as published algorithm descriptions. Although free and open source tools are better fits for integrated modeling, some popular proprietary tools are also included in the catalog.



Snapshot of tools- A to D

Tool Name	DA[a]	IA[b]	PE[c]	UA[d]	SA[e]	MM[f]	BN[g]	CIT	AV[h]	DIS[i]
ACE (Alternating Conditional Expectation)		2						2	2	1
ACUARS (Automatic Calibration and Uncertainty Assessment using Response Surfaces)			4	3	1			2	1	3
AMALGAM (A Multi-ALgorithm Genetically Adaptive Multiobjective method)			3					5	2	2
BaRE (Bayesian Recursive Estimation)			4	3	1			75	1	3
BATEA (BAyesian Total Error Analysis)			5	3	1			34	2	1
BFL (Bayesian Filtering Library)		1						1	2-3	1
BFS (Bayesian Forecasting System)							1	68	1	3
BMC (Bayesian Monte Carlo)			4	3	1			39	1	3
BMElib (Bayesian Maximum Entropy - library)							2	54	2-4	1
BUGS (Bayesian inference Using Gibbs Sampling (plus extensions))							1	576	2-4	1
CANOPI (Confidence ANalysis Of Physical Inputs)				3				4	1	3
DAKOTA (Design Analysis Kit for Optimization and Terascale Applications)			1-3	1-2,4	2			72	2-4	1
DBM (Data-based Mechanistic modeling)		2						187	2-4	1
DDS, DDS-AU (Dynamically Dimensioned Search, DDS for Approximation of			2,4	3	1			2	2,4	1

[a]NA means not applicable; tool for surrogate-based modeling.
[b]DA, data analysis; 1, population data; 2, geospatial data; 3, time series data.
[c]IA, identifiability analysis; 1, temporal; 2, behavioral; 3, spatial.
[d]PE, parameter estimation; 1, local; 2, global; 3, hybrid; 4, importance sampling; 5, MCMC sampling.
[e]UAua, uncertainty analysis; 1, Monte Carlo; 2, stratified sampling; 3, importance sampling; 4, approximate.
[f]SA, sensitivity analysis; 1, screening; 2, local; 3, correlation based; 4, regression based; 5, variance based.
[g]MMA, multimodel analysis; 1, qualitative; 2, quantitative.
[h]BN, Bayesian networks; 1, hierarchical Bayesian network; 2, Bayesian decision network.
[i]CIT, number of citations determined by a search of SCOPUS database.
[j]AV, available materials; 1, method description only; 2, source code; 3, manual; 4, executable.
[k]DIS, form of software distribution; 1, Web download; 2, on request; 3, software not available.

Snapshot of tools - S to W

SARS-RT (Sensitivity Analysis based on Regional Splits and Regression Trees)					3-4			11	1	3
SCE (Shuffled Complex Evolution)			2					533	2-4	1
SCEM (Shuffled Complex Evolution Metropolis)			5	3	1			74	2-4	1
SIMLAB (Simulation Laboratory for UA/SA)				1-2	1,3-5			101	2-4	1
SODA (Simultaneous Optimization and Data Assimilation method)		1	5	3	1			26	1	3
SOLO (Self-Organizing Linear Output map)		2						29	2	2
SRSM (Stochastic Response Surface Method)	n/a - tool for surrogate-based modeling							32	2	1
SUFI,SUFI-2 (Sequential Uncertainty-FItting algorithm)			4					16	1	3
SUNGLASSES (Sources of UNcertainty GLobal Assessment using Split SamplES)				3				3	2-4	1
UCODE (Universal CODE for Inverse Modeling)			1	4	2			148	2-4	1
UNCERT (UNCERTainty analysis, geostatistics and visualization toolkit)	1-3							20	2-4	1
UNCSIM (UNCertainty SIMulator)		1	2,4-5	1-3	2			8	2-4	1
WebGUAC (Website Guidance for Uncertainty Assessment and Communication)						1		17	n/a	