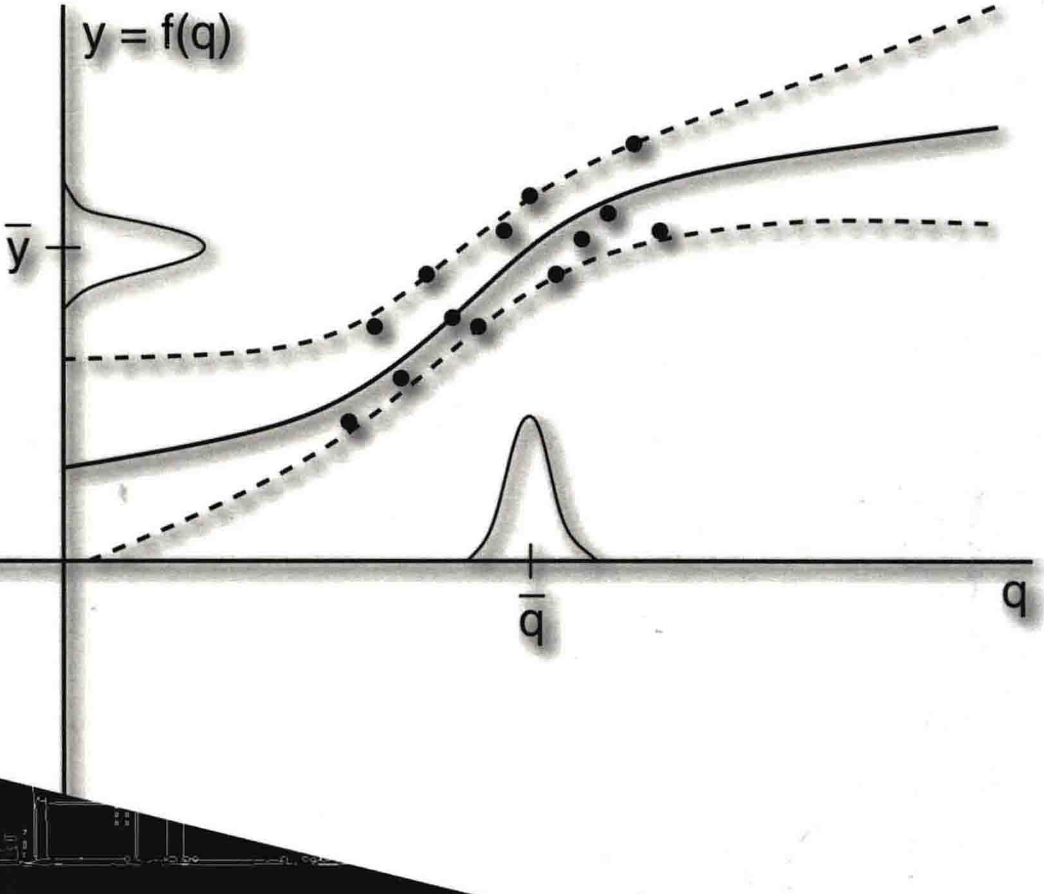
RALPH C. SMITH

Uncertainty Quantification

Theory, Implementation, and Applications



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Computational Science & Engineering

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Uncertainty Quantification

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Preface

Uncertainty quantification is both a new field and one that is as old as the disciplines of probability and statistics. The present novelty lies in the synthesis of probability, statistics, model development, mathematical and numerical analysis, large-scale simulations, experiments, and disciplinary sciences to provide a computational framework for quantifying input and response uncertainties in a manner that facilitates predictions with quantified and reduced uncertainty. This is the topic of this book.

Uncertainty quantification for physical models can be motivated in the context of weather modeling. Models for complex phenomena, such as dust-induced cloud formation, are approximate and uncertain, as are the parameters in these models. Additional errors and uncertainties are introduced by the numerical algorithms and experimental data used to approximate and calibrate the models. In the first step of the prediction process, data assimilation or model calibration techniques are used to determine input parameters and initial conditions so that quantities of interest, such as temperature or relative humidity, match current conditions. The second step entails the prediction of future weather conditions with uncertainties quantified by probabilistic statements—e.g., 95% change of rain—or uncertainty cones of the type reported for hurricanes or tropical storms.

Whereas model calibration and uncertainty propagation comprise the primary aspects of the prediction process, their implementation for large-scale applications requires a wide range of supporting topics. These include aspects of probability, statistics, analysis, and numerical analysis as well as the following topics: parameter selection, surrogate model construction, local and global sensitivity analysis, and quantification of model discrepancies. The interdisciplinary nature of the field is augmented by the fact that all of these components must be investigated and implemented in the context of the underlying applications.

The explosive growth of uncertainty quantification as an interdisciplinary field is due to a number of factors: increasing emphasis on models having quantified uncertainties for large-scale applications, novel algorithm development, and new computational architectures that facilitate implementation of these algorithms.

In Chapter 2, we detail five applications where model predictions with quantified uncertainties are critical for understanding and predicting scientific phenomena and making informed decisions and designs based on these predictions. These applications are weather models, climate models, subsurface hydrology and geology models, nuclear reactor models, and models for biological phenomena. Whereas the presence and role of uncertainties in these applications has long been recognized, the development of computational models that quantify and incorporate uncertainties is receiving increased attention. The reliance of scientists and policy makers on such models is expected to grow rapidly as the field of uncertainty quantification for predictive sciences matures and computational resources evolve.

The relatively recent development of supporting mathematical and statistical theory and algorithms is a second factor supporting the growth of the field. For example, the adaptive DRAM and DREAM algorithms discussed in Chapter 8 for Bayesian model calibration were developed within the last ten years. These algorithms are presently being investigated in the context of climate and groundwater models. Similarly, much of the sparse grid theory discussed in Chapter 11 was developed in the last twenty years, although the original concept is much older.

The availability of massively parallel computer architectures and hardware has further bolstered uncertainty quantification for complex and large-scale applications. The DREAM algorithms are inherently parallel, and recent versions of DRAM are being implemented on parallel architectures. It is anticipated that field programmable gate arrays (FPGAs) will be increasingly utilized for uncertainty quantification as high-level tools are developed to reduce programming overhead. The fact that we operate in increasingly data-rich environments will also benefit uncertainty quantification, and we anticipate increased interaction between data mining, high-dimensional visualization, and uncertainty quantification.

The growth in the field has spawned the introduction of interdisciplinary courses on uncertainty quantification, and this text owes its genesis to the author's development of such a course at North Carolina State University in 2008. This text was written with the goal of introducing advanced undergraduates, graduate students, postdocs, and researchers in mathematics, statistics, engineering, and natural and biological sciences to the various topics comprising uncertainty quantification for predictive models. To achieve this, we motivate a number of the topics using very basic examples that should be familiar to most readers. We have included numerous definitions and significant detail to provide a common footing for a wide range of readers. Because this is a new and evolving field, we indicate open research questions at various points in the text and provide research references in the Notes and References at the end of each chapter.

Various resources will be maintained at the website http://www.siam.org/books/cs12 to augment the text and provide a mechanism to update the material. This includes data employed in exercises as well as a future erratum.

This text has benefited significantly from graduate students, postdocs, and colleagues whose comments have improved the exposition and reduced the number of typos by orders of magnitude. Specifically, sincere thanks are extended to Nate Burch, Amanda Coons, John Crews, John Harlim, Zhengzheng Hu, Zack Kenz, Christine Latten, Jerry McMahan Jr., Keri Rehm, Mami Wentworth, and Lucus Van Blaircum for their attention to detail and candid feedback regarding parts of the manuscript. The author is also extremely grateful to Brian Adams and Karen Willcox for their feedback during the review process; the book is significantly improved due to their detailed comments.

The support provided by several funding agencies has been instrumental both for related research and the writing of this text. These agencies include the Air Force Office of Scientific Research (Dynamics and Control Program), the Department of Energy Consortium for Advanced Simulation of Light Water Reactors (CASL), and the National Science Foundation (Research Training Groups in the Mathematical Sciences). Part of this text was written while the author was a Faculty Fellow in the 2011–12 Statistical and Applied Mathematical Sciences Institute (SAMSI) *Program on Uncertainty Quantification.* Collaboration and interactions during this year significantly influenced aspects of the book, and the author very gratefully acknowledges the scientific and financial contributions from this program. Finally, I would like to thank Elizabeth Greenspan from SIAM for her assistance and encouragement throughout the process of writing this book.

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July 1, 2013

Notation

This compilation does not include all of the symbols used throughout the text, and we neglect those that appear one time in a specific context such as those in the models of Chapter 2. Instead, it is meant to clarify the role of symbols that appear multiple times throughout the discussion.

Symbol	Meaning	Page
$\partial\mathcal{D}, \partial\Omega$	Boundaries of regions $\mathcal{D}$ and Ω	62, 63
$\alpha(q^*\|q^{k-1})$	Probability of accepting candidate q^*	159
γ_i	Normalization factor for $\langle\cdot,\cdot\rangle_\rho$	209
Γ_i, Γ	Range of i^{th} random parameter, random vector	108
$\delta, \delta(x_i), \delta(t_i)$	Model discrepancy or error	133, 257
ε, ϵ	Random and realized measurement errors	82, 132
Λ_{M_1}	Lebesgue constant	252
μ	Mean	70
μ_i, μ_i^*	Morris sensitivity measures	332
ν	Dimension of model response $y(t,q)$	61
$\pi_0(q), \pi(q\|y)$	Bayesian prior and posterior density	100
$\pi(y\|q)$	Bayesian likelihood function	100
$\rho_{Q_i}(q_i), \rho_Q(q)$	Density for i^{th} random parameter, random vector	108
σ_0^2	Unknown measurement error variance	135
$\hat{\sigma}^2, \sigma^2$	Estimator and estimate for σ_0^2	135
σ_j	Singular values of the matrix A	117
Σ	Matrix of singular values of matrix A	117
υ	Realized measurements of Υ	132, 156
Υ	Random variable for measurements	82
$\phi_i(x)$	Spatial basis functions	219
χ	Independent variables $\chi = [x,t] \in \mathcal{D} \times \mathcal{T} \equiv \Omega$	63
$\psi_k(Q), \Psi_k(Q)$	Univariate, multivariate orthogonal polynomials	209, 213
$\mathcal{A}(q,p)$	Sparse grid quadrature operator	247
$B(u,q), B(q)u$	Boundary operators	62, 63

Symbol	Meaning	Page
$\mathcal{C}$	Observation matrix or vector	61
$d_i(q), d_i^\sigma(q)$	Morris elementary effects for i^{th} input	331
D, D_i, D_{ij}	Total and partial variances of response Y	324
$\mathcal{D}$	Spatial domain in $\mathbb{R}^1, \mathbb{R}^2$, or $\mathbb{R}^3$	62
$f(q), f(t,x,q)$	Model response	132
$\widetilde{f}(q), \widetilde{f}(t,x,q)$	Surrogate model	274
$F(q)$	Source terms	62
H_u, H_q, H_F	Hilbert spaces for state, parameters, and source	63
$H_i(Q)$	Hermite polynomials	210
$\mathcal{H}(q,p)$	Sparse quadrature grid	248
$\mathbf{i}', \mathbf{j}', \mathbf{k}'$	Multi-indices	212
$I^{(p)}f$	Integral operator in $\mathbb{R}^p$	240
$\mathbb{I}(\ell)$	Multi-index sets	246
$\mathcal{I}_\ell^{(p)}u$	Interpolation operator in $\mathbb{R}^p$	254
$I(q)$	Identifiable subspace	113
$\mathcal{I}(q)$	Space of influential parameters	114
$\mathcal{J}(q)$	Least squares functional	135
$J(q^*\|q^{k-1})$	Proposal or jumping distribution	159
$\ell(q\|\upsilon)$	Log-likelihood function	83
$L(q\|\upsilon)$	Likelihood function	83
$L(q)u$	Linear operator	63
$L_m(q)$	Lagrange interpolating polynomial	251
$L^2_{\rho_i}(\Gamma_i), L^2_\rho(\Gamma)$	Square integrable functions on Γ_i, Γ	215
M, M_ℓ	Number of collocation points or samples	253
n	Number of measurements or model evaluations	61
N	Dimension of state u	61
$NI(q)$	Unidentifiable subspace	113
$\mathcal{NI}(q)$	Space of noninfluential parameters	114
$\mathcal{N}(A)$	Null space of the matrix A	116
$\mathcal{N}(u,q)$	Linear or nonlinear differential operator	62
p	Number of parameters	100
$P_i(Q)$	Legendre polynomials	211
$\mathbb{P}_k$	Space of polynomials with argument less than or equal to k	208
$\widehat{\mathbb{P}}_k$	Polynomials in $\mathbb{P}_k$ that are orthogonal to $\mathbb{P}_{k-1}$	208

Symbol	Meaning	Page
q_0	True but unknown parameter	82
$q = [q_1, \ldots, q_p]$	Realizations of Q	100
q^*	Proposed Markov chain parameter	159
q^{k-1}	Parameter at $k-1$ step in Markov chain	159
q^r, q^m	Quadrature, collocation, and sample points	211, 217
$\hat{q}_{OLS}, q_{OLS}$	Least squares estimator, estimate for q_0	82
q_{MAP}	Maximum a posteriori estimate	157
q_{MLE}	Maximum likelihood estimate	84
$Q = [Q_1, \ldots, Q_p]$	Random vector of parameters	100
Q	Orthogonal matrix in QR factorization	118
$\mathbb{Q}$	Admissible parameter space	82
$\mathcal{Q}$	Sample space	82
$\mathcal{Q}^{(p)}$	Quadrature operator in $\mathbb{R}^p$	240
r	Rank of matrix A	117
R, R_ℓ	Number of quadrature points	243
R	Upper triangular matrix in QR factorization	118
$\widehat{R}, R$	Residual estimator and estimate	136
$\mathcal{R}$	Number of sparse grid quadrature points	248
$\mathcal{R}(u, q)$	General observation or response	63
$\mathcal{R}(A)$	Range of the matrix A	116
s_i	Local sensitivity indices	192, 322
S_i^σ	Sigma-normalized sensitivity indices	322
S_i, S_{ij}, S_{T_i}	Sobol sensitivity indices	324
SS_q	Sum of squares error	156
$\mathcal{T}$	Temporal domain	63
$u(q), u(t, x, q)$	State variable	61
$\widetilde{u}(q), \widetilde{u}(t, x, q)$	Surrogate state representation	279
V, V^J	Spaces of spatial test functions	219
V_k	Chain covariance matrix	172
w^r	Quadrature weights	211
X	Deterministic $n \times p$ design matrix	131
$\mathcal{X}(q)$	Sensitivity matrix	144
y	Realizations of Y	132
Y	Random variable for model response	321
Z, Z^K	Spaces of parameter test functions	219

Acronyms and Initialisms

Term	Meaning	Page
ANOVA	Analysis of variance	291
AR	Autoregressive (model)	89
ASAP	Adjoint sensitivity analysis procedure	306
BWR	Boiling water reactor	36
càdlàg	Continue à droite, limite à gauche	69
CASL	Consortium for Advanced Simulation of Light Water Reactors	37
cdf	Cumulative distribution function	68
CESM	Community Earth System Model	30
CFCs	chlorofluorocarbons	25
CRUD	Chalk River unidentified deposit	43
CVTs	Centroidal Voronoi tesselations	285
DAKOTA	Design Analysis Kit for Optimization and Terascale Applications	236
DOE	Department of Energy	37
DRAM	Delayed rejection adaptive Metropolis	172
DREAM	DiffeRential Evolution Adaptive Metropolis	181
ECMWF	European Centre for Medium-Range Weather Forecasts	16
FPGAs	Field programmable gate arrays	x
FSAP	Forward sensitivity analysis procedure	306
gcd	Greatest common divisor	94
GCR	Gas-cooled reactor	36
GP	Gaussian process	89
gPC	Generalized polynomial chaos	207
HDMR	High-dimensional model representation	289
HIV	Human immunodeficiency virus	45
iid	Independent and identically distributed	79

Term	Meaning	Page
IPCC	Intergovernmental Panel on Climate Change	32
kde	Kernel density estimation	75
LANL	Los Alamos National Laboratory	41
LQR	Linear quadratic regulator	50
MAP	Maximum a posteriori (estimate)	157
MCMC	Markov chain Monte Carlo	159
MLE	Maximum likelihood estimate	84
NISP	Nonintrusive spectral projection	225
NWP	Numerical weather prediction	16
ODE	Ordinary differential equation	51
OLS	Ordinary least squares	82
ORNL	Oak Ridge National Laboratory	41
PC	Polynomial chaos	207
PCA	Principal component analysis	109
PDE	Partial differential equation	51
pdf	Probability density function	69
POD	Proper orthogonal decomposition	285
PRA	Probabilistic risk assessment	44
PWR	Pressurized water reactor	36
Q-Q	Quantile-quantile	74
QoI	Quantity of interest	4
SAMSI	Statistical and Applied Mathematical Sciences Institute	xi
SDE	Stochastic differential equation	97
SIR	Susceptible, infected, recovered (model)	55
SVD	Singular value decomposition	117
WMO	World Meteorological Organization	17

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