A BRIEF VIEW OF VERIFICATION, VALIDATION, AND UNCERTAINTY QUANTIFICATION

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Foundations of Verification, Validation, and
Uncertainty Quantification

Albuquerque, New Mexico

June 10, 2010

OUTLINE

1. Definitions and Philosophical Issues
2. Model Calibration, Validation, and Uncertainty Quantification
3. Mathematical Challenges

SCIENCE: (From the Latin, scientia “knowledge” or scire “to know”)
The (enterprise dedicated to the) systematic acquisition of knowledge.

Knowledge can be obtained in two (or three) ways:

(1) Observation
(2) Theory
} ➽ The classical Pillars of Science

(3) Computer Modeling and Simulation,
Data Processing (CS) ➽ The third Pillar

THEORY:

One or more hypotheses or analytical constructions that make assertions about the “underlying reality” that brings about a phenomenon.

OBSERVATION:

An act or instance of observing or recognizing physical events through the use of senses - or the use of instruments.

MATHEMATICAL MODEL:

A collection of mathematical constructions that describe a system: a mathematical representation of the essential aspects of a system **that presents the knowledge of the system in a usable form, thus a mathematical representation of theory and of observations**.

COMPUTATIONAL MODEL:

A discretization (or corruption) of a mathematical model designed to render it to a form that can be processed by computing devices.

CALIBRATION:

The assignment or adjustment of values of parameters of a model designed to bring model output (“predictions”) into agreement with experimental measurements.

PREDICTION:

The forecast of an event (a predicted event cannot be measured or observed, for then it ceases to be a prediction).

QUANTITIES OF INTEREST:

Specific objectives that can be expressed as the target outputs of a model (mathematically, they are often defined by functionals of the solutions and provide focus on the goal of scientific computation).

UNCERTAINTY:

The lack of certainty – a state of having limited knowledge where it is impossible to describe existing state or future outcomes. The lack of sureness about something.

Aleatory Uncertainty – Uncertainty due to variation in the physical system - it is stochastic and irreducible.

Epistemic Uncertainty – Uncertainty due to lack of knowledge of the quantities are processes identified with a system.

Some Quotable Philosophers and Mathematicians

Thomas Bayes	1702–1761	Essay towards Solving a Problem in the Doctrine of Chances, 1764
David Hume	1711–1776	A Treatise on Human Nature, 1739
Hans Reichenbach	1891–1953	The Rise of Scientific Philosophy, 1951
Sir Karl Popper	1902–1994	The Logic of Scientific Discovery, 1954
Colin Howson and Peter Urbach	1945 –, 1941–	Scientific Reasoning – The Bayesian Approach, 1989, 2006

(and others: Kant, Eddington, Laplace, Poincare, $\cdots$)

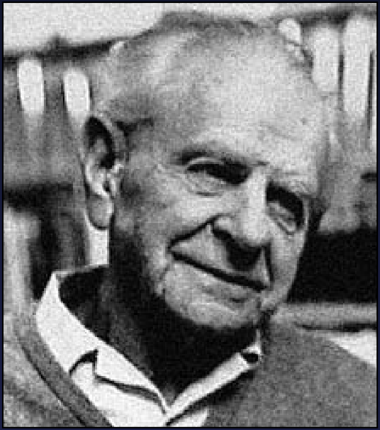
David Hume (1711 - 1776): Skepticism

The Problem of Induction

The philosophical question
of whether
inductive reasoning
leads to knowledge

Induction presupposes that
a sequence of events
will occur in the future
as it always has in the past

Sir Karl Popper (1902 - 1994)



The Principle of Falsification

A hypothesis can be accepted as
a legitimate scientific theory
if it can possibly be refuted by
observational evidence

- A theory can never be validated; it can only be invalidated by (contradictory) experimental evidence.
- Corroboration of a theory (survival of many attempts to falsify) does not mean a theory is likely to be true.

Scientific Reasoning – The Bayesian Approach (Howson and Urbach, 1989, 2006)

- "Most of the twentieth century was dominated by the classical approach, and in that period, Bayesianism was scarcely taught in universities and Bayesians were widely dismissed as thoroughly misguided."
- "…during the 1980's, a regular trickle of around 200 articles published annually with the words or prefix 'Bayes' in their titles. Suddenly, in 1991, this number shot up to 600 and by 1994 exceeded 800; by 2000 it reached almost 1,400."
- "…classical objections and the need for priori have been shown to be baseless." (H&U)

Thomas Bayes (1702 - 1761)

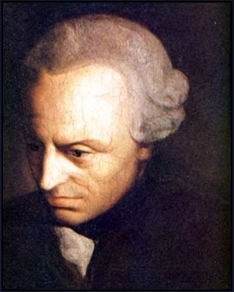
"Theories have to be judged in terms of their probabilities in light of the evidence."

Henri Poincaré (1854 – 1912)

"The physicist is often in the same position ad the gambler who reckons up his chances. Every time he reasons by induction, he more or less requires the calculus of probabilities."

"It is often stated that one should experiment preconceived ideas. This is simply impossible: not only would this make every experiment sterile, but even if we were ready to do so, we could not implement this principle. Everyone stands by his own conception of the world, which he cannot get rid of so easily."

A Few Other Quotes:



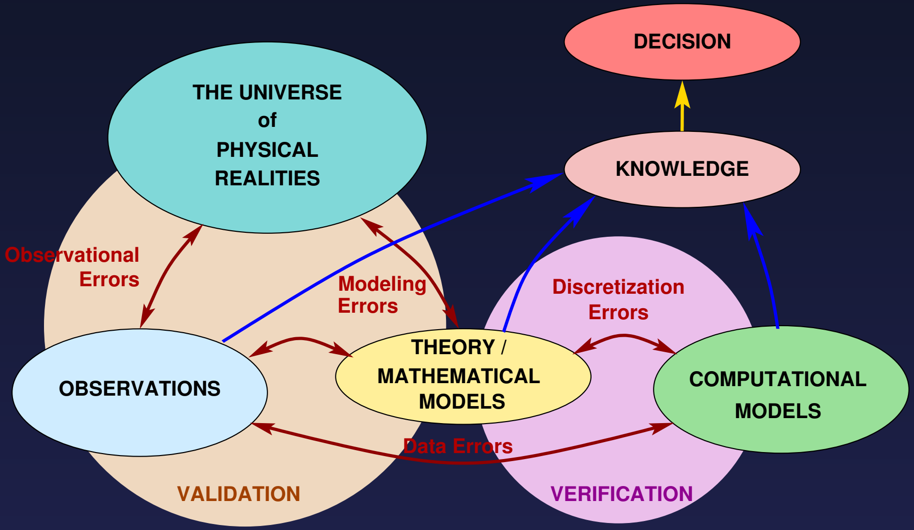
Immanuel Kant (1724 – 1804)

“Philosophy needs a science to determine the possibility, the principle, and the scope of our whole prior knowledge.”

Sir Arthur Eddington (1882 – 1944)

“Experimentalists will be surprised to learn that we will not accept any experimental evidence that is not confirmed by theory.”

The Imperfect Paths to Knowledge



The Path to Truth . . .

"If error is corrected
whenever it is recognized as such,
the path to error
is the path of truth."

Hans Reichenbach (1891- 1953)
The Rise of Scientific Philosophy, 1951.

VALIDATION:

The **process** of determining the accuracy with which a model can predict observed physical events (or the important features of a physical reality).

P. Roache (2009): “The process of determining the degree to which a model (and its associated data) is an accurate representation of the real world from the perspective of the intended uses of the model”.

”Do we solve the right equations?” (Boehm, 1981)

VERIFICATION:

The **process** of determining the accuracy with which a computational model can produce results deliverable by the mathematical model on which it is based:

- CODE VERIFICATION
- SOLUTION VERIFICATION

"Do we solve the equations right?" (Boehm, 1981)

Solution verification is an activity that pertains to **a posteriori error estimation**, i.e. that aims at quantifying the discretization error $\mathbf{u}-\mathbf{u}_h$:

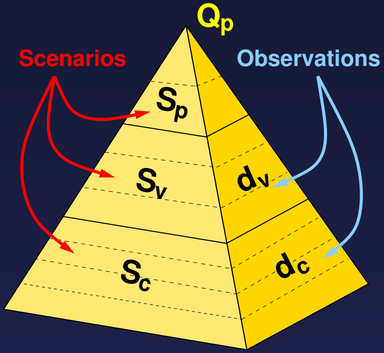
- With respect to a norm: $\|\mathbf{u} - \mathbf{u}_h\|$
- Most importantly, with respect to a quantity of interest:

  $|Q(\mathbf{u}) - Q(\mathbf{u}_h)|$

THE PREDICTION PYRAMD: Hierarchy of Models

Subjective probability

RANDOMNESS $\Leftrightarrow$ LACK OF KNOWLEDGE



$$\mathcal{A}\big(\mathbf{m}, \mathcal{S}, \mathbf{u}(\mathbf{m}, \mathcal{S})\big) = 0$$

$$\Downarrow$$

$$\mathcal{A}\big(\sigma_M(\mathbf{m}), \mathcal{S}, \mathbf{u}(\sigma_M(\mathbf{m}), \mathcal{S})\big) = 0$$

$$\Downarrow$$

$$Q\big(u(\sigma_M(\mathbf{m}, \mathcal{S})\big) = q_c(\mathbf{m})$$

A Bayesian Approach

$\mathbf{m} \in \mathcal{M}$
(model manifold)
$\rho_M(\mathbf{m})=$ prior pdf

$\underbrace{\theta(\mathbf{d}|\mathbf{m})}_{\text{theory pdf}}$

$\mathbf{d} \in \mathcal{D}$
(data manifold)
$\rho_D(\mathbf{d})=$ prior pdf

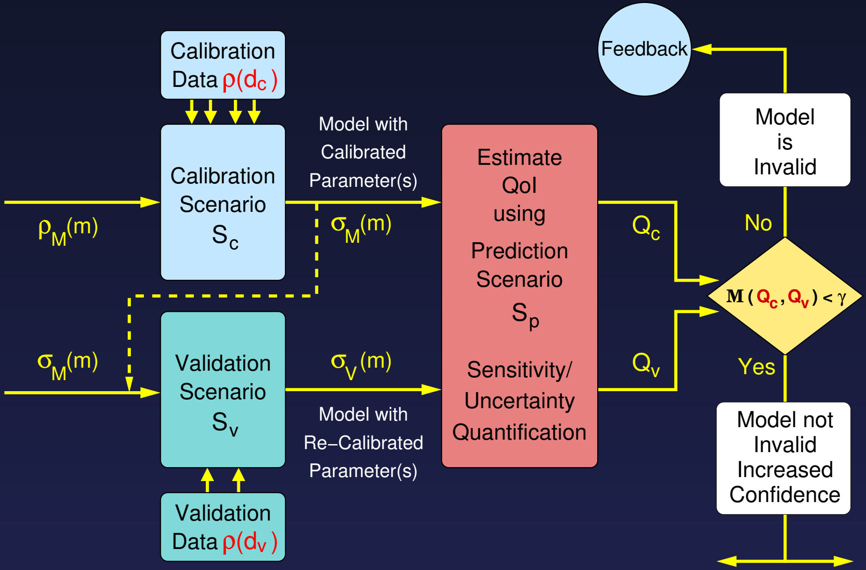
$\Downarrow \quad \Downarrow \quad \Downarrow$

$$\sigma(\mathbf{m}|\mathbf{d}) \propto \theta(\mathbf{d}|\mathbf{m})\rho_M(\mathbf{m})/\rho_D(\mathbf{d})$$

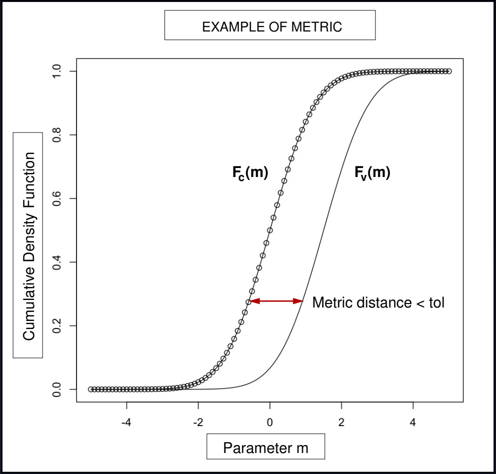
$\Downarrow$

$$\sigma_M(\mathbf{m}) = \text{posterior pdf} = \int_{\mathcal{D}} \sigma(\mathbf{m}|\mathbf{d})d\mathbf{d} \;\propto\; \rho_M(\mathbf{m})\; L(\mathbf{m})$$

One Possible Validation Process



Uncertainty Quantification and Acceptance Metric



Probability density functions:

$$Q_P\big(\mathbf{u}(\sigma_M(\mathbf{m}), \mathcal{S}_p)\big) = Q_C(\mathbf{m})$$
$$Q_P\big(\mathbf{u}(\sigma_V(\mathbf{m}), \mathcal{S}_p)\big) = Q_V(\mathbf{m})$$

Cumulative density functions:

$$F_C(\mathbf{m}) = \int_{-\infty}^{\mathbf{m}} q_C(\mathbf{m}')\, dm'$$
$$F_V(\mathbf{m}) = \int_{-\infty}^{\mathbf{m}} q_V(\mathbf{m}')\, dm'$$

Generalizations: Model Selection and Predications with Limited Data

- Dempster-Shafer Evidence Theory – plausibility and belief measures of uncertainty
- Evidence and Plausibility of Model Classes
- Possibility Theory
- Fuzzy Sets – parametric worst case scenarios
- Rough Sets
- Decision Theory
- Imprecise Probability, Monotone Non-Additive Measures
- Sets of Desirable Gambles
- Choquet Capacities
- Generalized Bayes Rules

$\vdots$

Model Choice Theories

Intra-Class

$$\underbrace{\rho(\mathbf{m}_j|\mathbf{d}|\mathbf{M}_j)}_{\text{posterior pdf}} = \frac{\overbrace{\theta(\mathbf{d}|\mathbf{m}_j,\mathbf{M}_j)}^{\text{likelihood}}\ \overbrace{\rho_M(\mathbf{m}_j|\mathbf{M}_j)}^{\text{prior}}}{\underbrace{\rho(\mathbf{d}|\mathbf{M}_j)}_{\text{evidence}}}, \quad \mathbf{M}_j \in \mathcal{M}, j = 1, 2, \cdots, N$$

Inter-Class

$$\underbrace{\rho(\mathbf{M}_j|\mathbf{d}|\mathcal{M})}_{\text{posterior plausibility}} = \frac{\overbrace{\rho(\mathbf{d}|\mathbf{M}_j)}^{\text{evidence}}\ \overbrace{\rho_M(\mathbf{M}_j|\mathcal{M})}^{\text{prior plausibility}}}{\rho(\mathbf{d}|\mathcal{M})}, \quad \mathbf{M}_j \in \mathcal{M}, j = 1, 2, \cdots, N$$

Open and Challenging Mathematical and Computational Problems

- Statistical Inverse Analysis:
  - Development of fast sampling methods for calibration, uncertainty propagation, and sensitivity analysis in the case of large parameter spaces (curse of dimensionality).
  - Methodology for selecting adequate observational data.
  - etc.
- Assessment and control of validation processes:
  - Selection and analysis of acceptance metrics/criteria and of tolerances for decision-making.
  - Development of adaptive approaches for the Bayesian method (selection of prior probability density function, misfit, likelihood, etc.)
  - Adaptive algorithms for feedback control.
  - Techniques for estimating modeling error.
  - etc.

Open and Challenging Mathematical and Computational Problems

- Solution of Very Large Stochastic Systems:
  - Stochastic PDE's (Polynomial Chaos, Stochastic Galerkin, $\cdots$)
  - Stochastic molecular models.
  - Stochastic multiphysics and multiscale coupling methods (e.g. molecular/continuum modeling).
  - Stochastic optimal control.
- Systematic Methodologies for Code and Solution Verification.

Thank you – and good luck!