Miodrag Bolic
Professor
School of Electrical Engineering and Computer Science (EECS)
Faculty of Engineering

Introduction to Uncertainty Evaluation in Engineering Measurements and Machine Learning Graduate Course

Outline

- Motivation
- Introduction
  - Uncertainty framework
  - Examples
- Confidence intervals
- Bayesian approach and Monte Carlo sampling
- Applications
- Conclusion

uOttawa

Motivation: Unresolved uncertainty questions

- How accurate are the resulting predictions?
- Are the mathematical and physical models correct?
- In general, how can we establish ”error bars” on the results?
- How can we use the knowledge of uncertainties during calibration for prediction?
- In systems with multiple processing steps, how do the uncertainties propagate from one step to another?

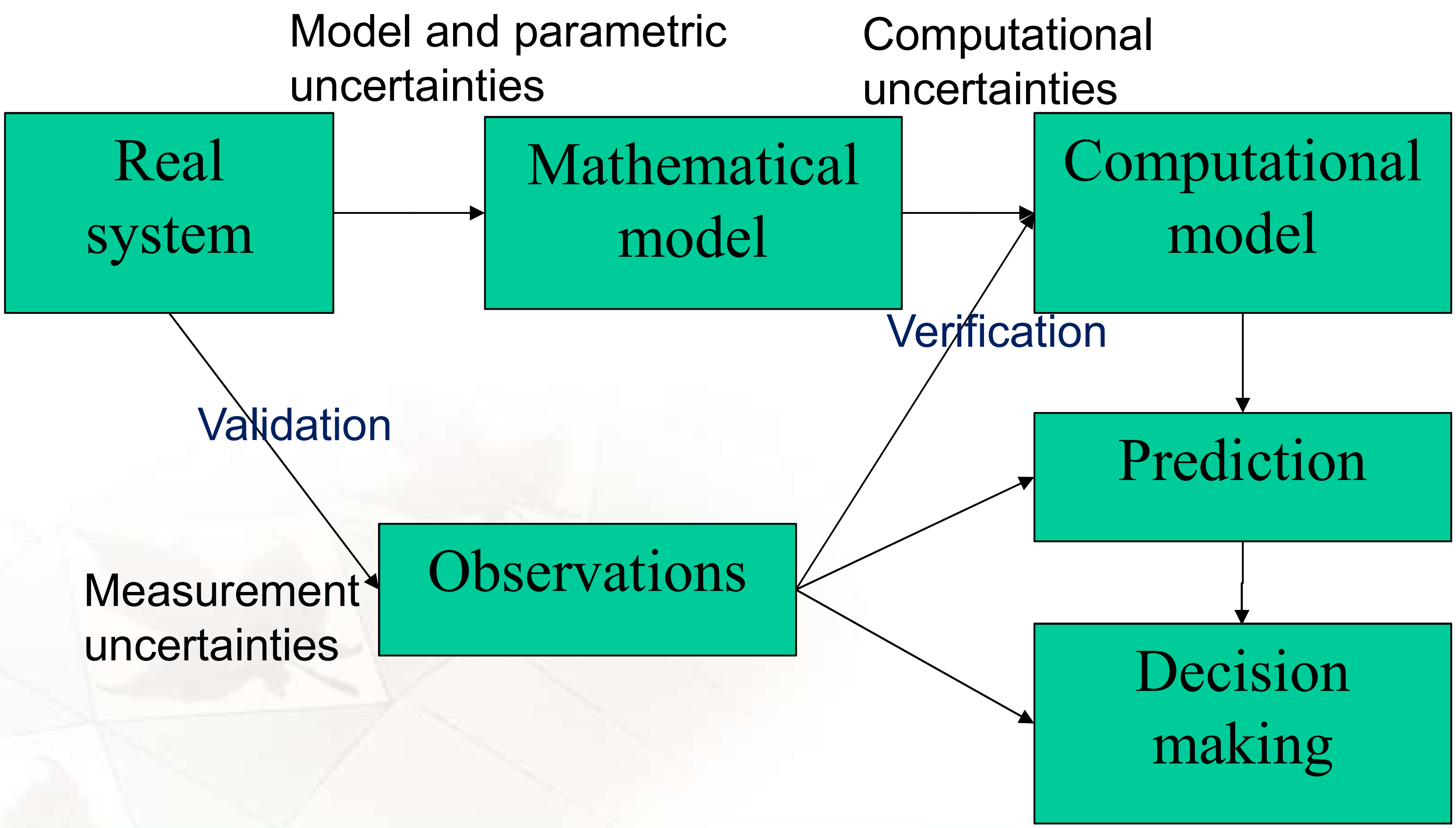
Uncertainty evaluation in instrumentation, processing and data analysis

- Current status
  - Not commonly performed
- Current approaches mainly based on metrology (GUM)
  - Deal mainly with propagation of uncertainty
- Opportunities
  - Advances in computing hardware and algorithms have dramatically improved the ability to simulate complex processes – sampling methods
  - Significant developments in mathematical and software tools for uncertainty quantifications in other areas
  - Focus is expanded to sensitivity analysis, calibration of models, uncertainties in predictions and decision making

Uncertainty quantification

- Uncertainty Quantification (UQ) aims at developing rigorous methods to characterize the impact of ”limited knowledge” on quantities of interest.
- Statistics of an outcome of interest, such as its expectation and the variance, commonly requires the evaluation of integrals
- Uncertainty is usually summarized through confidence intervals

Framework 1 - decision making under uncertainty



- Verification determines how well the computational model solves the math-model equations
- Validation determines how well the model represents the true physical system
  - Involves comparisons between QOIs computed by the model and corresponding true, physical QOIs inferred from physical observations or experiments.

Observing nature and predicting events

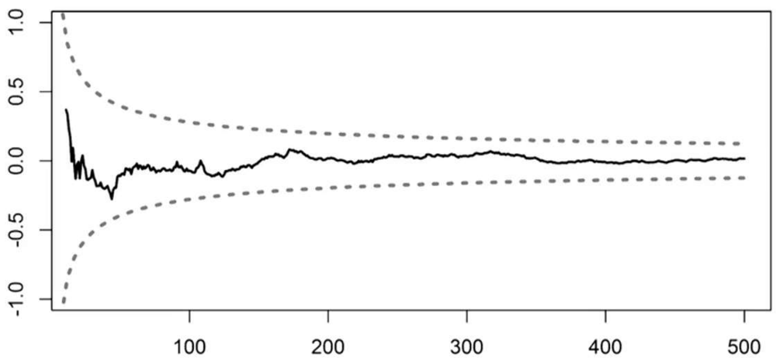
- Observations: we are unable to observe and/or predict nature accurately
  - the limited accuracy of measurement instruments,
  - the exceedingly high cost of performing accurate experiments and/or measurements,
  - the lack of accurate models or the computational need of using simplified ones.
- Predictions: the result of a combination of measurements, modeling and simulations
- Models are based on certain levels of approximation, introduced to make them manageable

Modeling Approach

- Advantages
  - Concise summary of present knowledge of operation of a particular system
  - Predict outcomes of modes of operation not easily studied experimentally
  - Clarify or simplify complex experimental data
  - Suggest new experiments to advance understanding of a system
- Limitations
  - Models often require many simplifying assumptions
    - beware of garbage in, garbage out
  - Validation of model predictions is essential

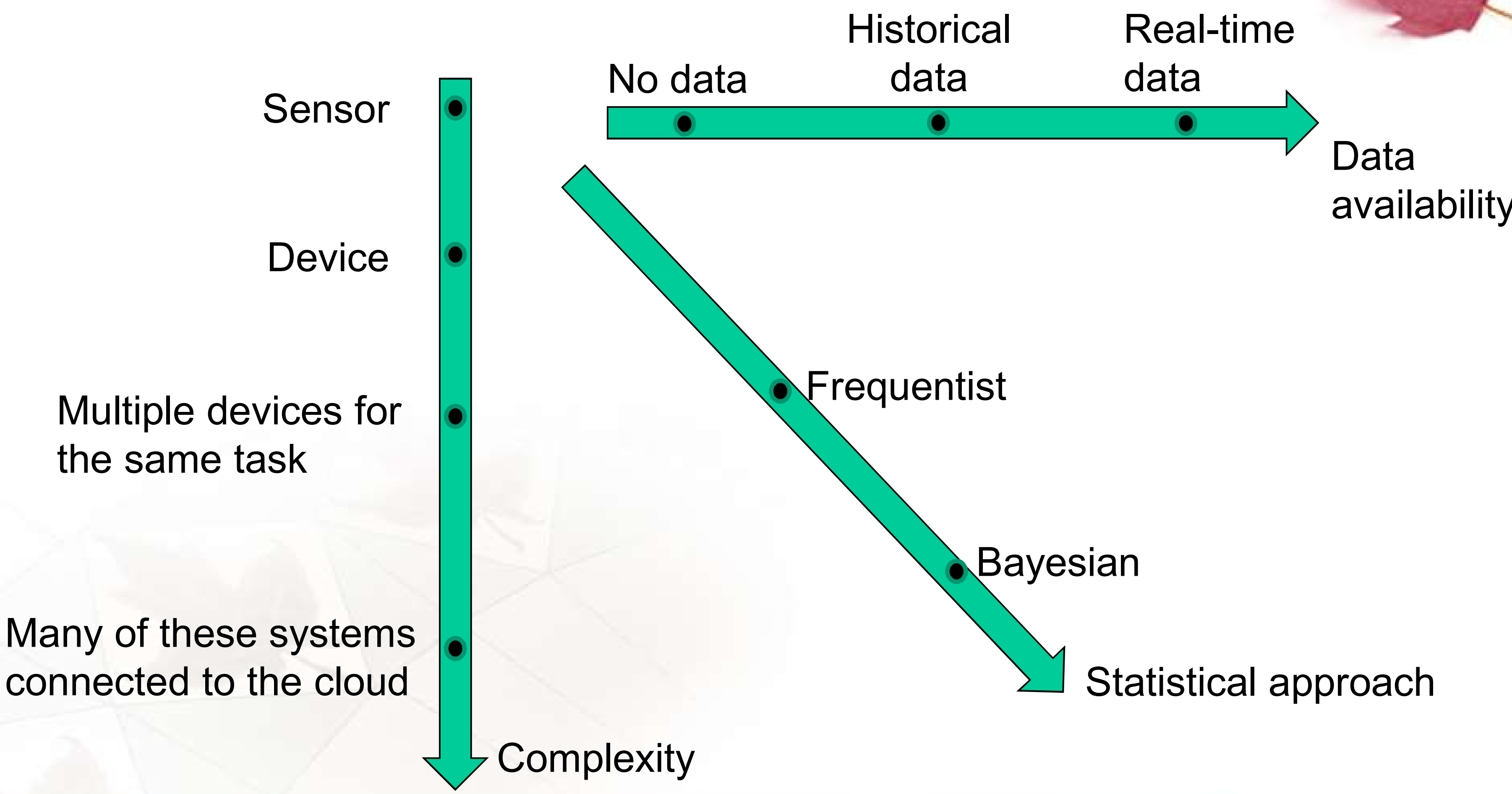
Examples of presenting uncertainty

- Standard error
  - Heart rate is (60 ± 4) beats/minute (mean ± standard error)
- Confidence levels
  - 95% confidence for the heart rate is [52,68] beats/minute
- Probability distributions
- Determining different moments or quantiles
- Prediction levels over time



uOttawa

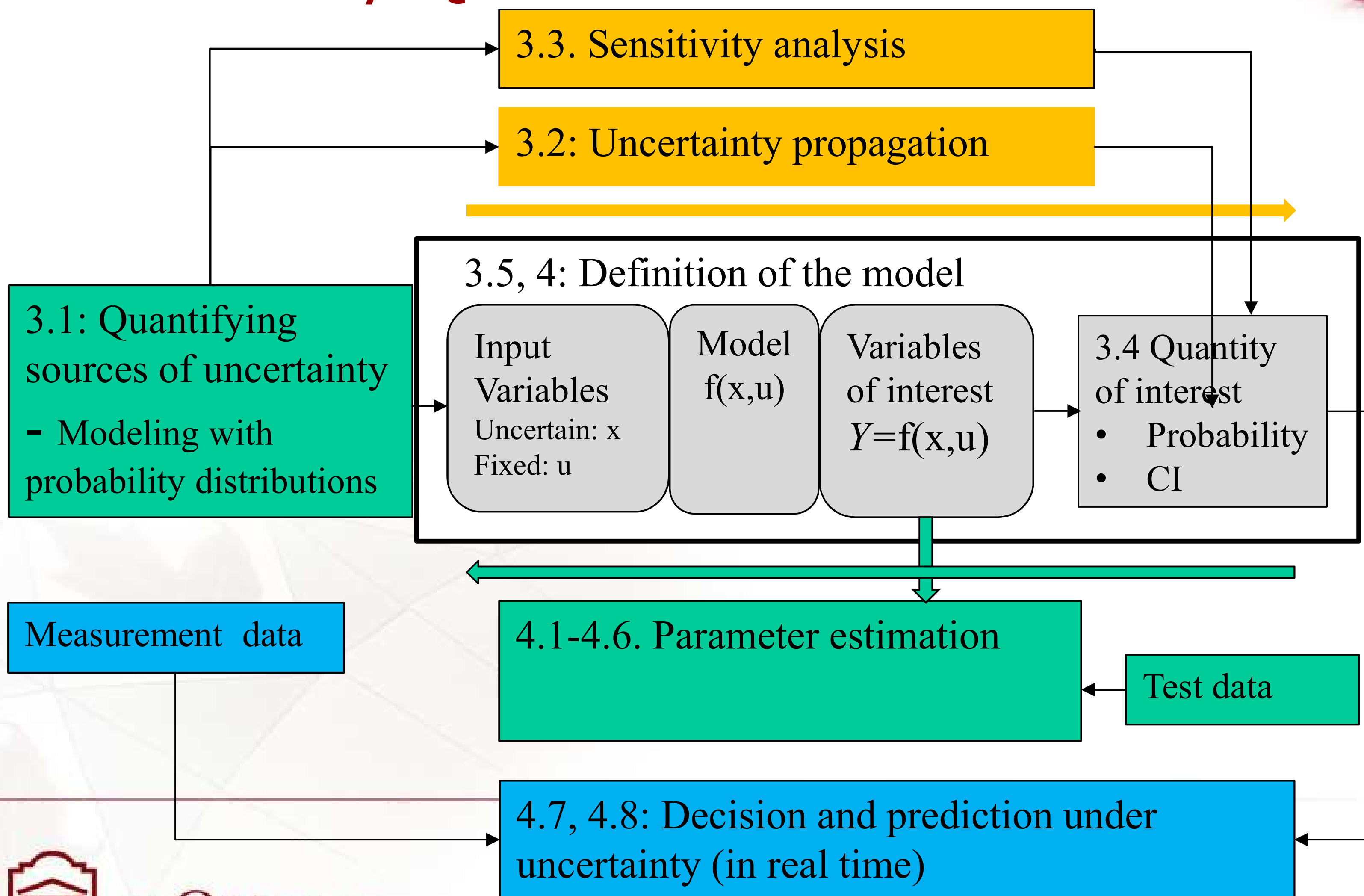
Uncertainty aspects



Uncertainty – classification based on data availability

- Uncertainty propagation when no data is available
  - Resampling methods
  - Sensitivity analysis
- Uncertainty evaluation when historical data is available
  - Model fitting and calibration
    - Bootstrap
- Uncertainty evaluation using real time data
  - Bootstrap for processing radar data
  - Monte Carlo methods

Framework 2: The workflow of Uncertainty Quantification



uOttawa

Based on OpenTURNS:
http://www.openturns.org/

Step B: Quantification of uncertainty sources

- A lot of data
  - Fitting of probability distributions
  - Statistical hypothesis test
- Few data ($n < 10$)
  - Hypothesis on parametric probability distribution
  - Expert judgement, then Bayesian inference
- No data
  - Expert judgment techniques

- Taking into account the dependency between inputs is a crucial issue in uncertainty analysis

uOttawa

Step B’: Model Calibration

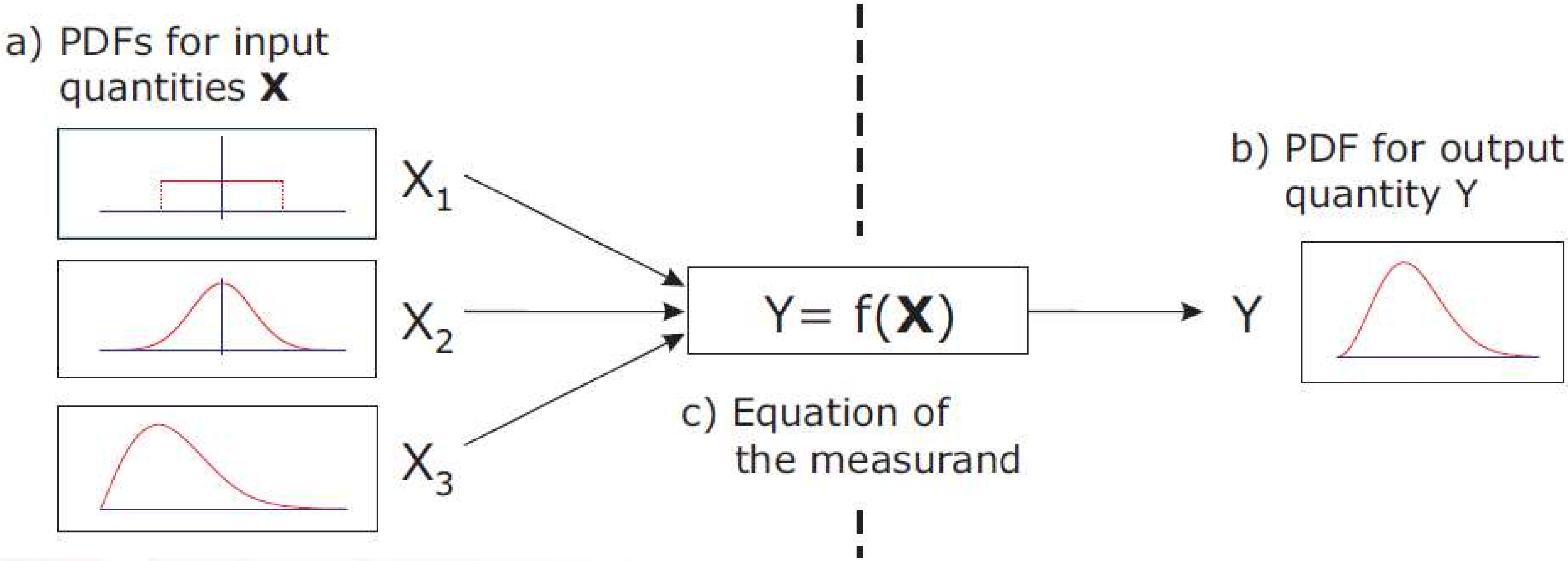
- Model calibration is the process of adjusting unknown model parameters in order to improve the agreement between model output and observed data
- Involves “tuning” values of the parameters of the model to best match the observed data
- Methods
  - Maximum likelihood methods
    - Model is used with fitted parameters to predict future behavior of the system
  - Bayesian methods for parameter estimation
    - the predictions allow for all sources of uncertainty, including the remaining uncertainty over the fitted parameters

Step C: Uncertainty propagation

- Aim is to quantify output uncertainties
- Allows us to place confidence on model predictions
  - a first step in providing trust in model predictions.
- Metrology: Uncertainty budget
  - Combine all the uncertainties and then see what components in your systems need to be replaced/improved
- Quality control:
  - Meeting design specification of your device

Step C: Propagation of uncertainty

- Perturbation methods
  - the solution is expressed using a suitable Taylor series expansion
- Sampling techniques
  - Monte Carlo based



Step C': Sensitivity analysis

- Local sensitivity: effect of x_i to the output while all other input factors x_j , $j \neq i$, are kept at the nominal values
  - Compute partial derivatives of the output functions with respect to the input parameters. $df(x_i)/dx_i$
  - Vary the input factors in a small interval around the nominal value.

  - When the model is nonlinear and various input parameters are affected by uncertainties of different order of magnitude, local sensitivity analysis should not be used.
- Global sensitivity: effect of x_i to the output while all other input factors x_j , $j \neq i$, are varied as well
  - Parameter space exploration with Monte Carlo simulations

Step C’: Sensitivity analysis

- Sensitivity analysis investigates the relationship between inputs and outputs of a model
  - it makes possible to relate the variability of the outputs to the variability of the inputs.
- Does not need input data and can be conducted on purely mathematical analysis
- Identifies the most important parameters in the model
- Helps reducing the dimension of the model by fixing unimportant parameters
- Focus: global variability of the model output, measured by its variance.

uOttawa

Step C′: Sensitivity analysis

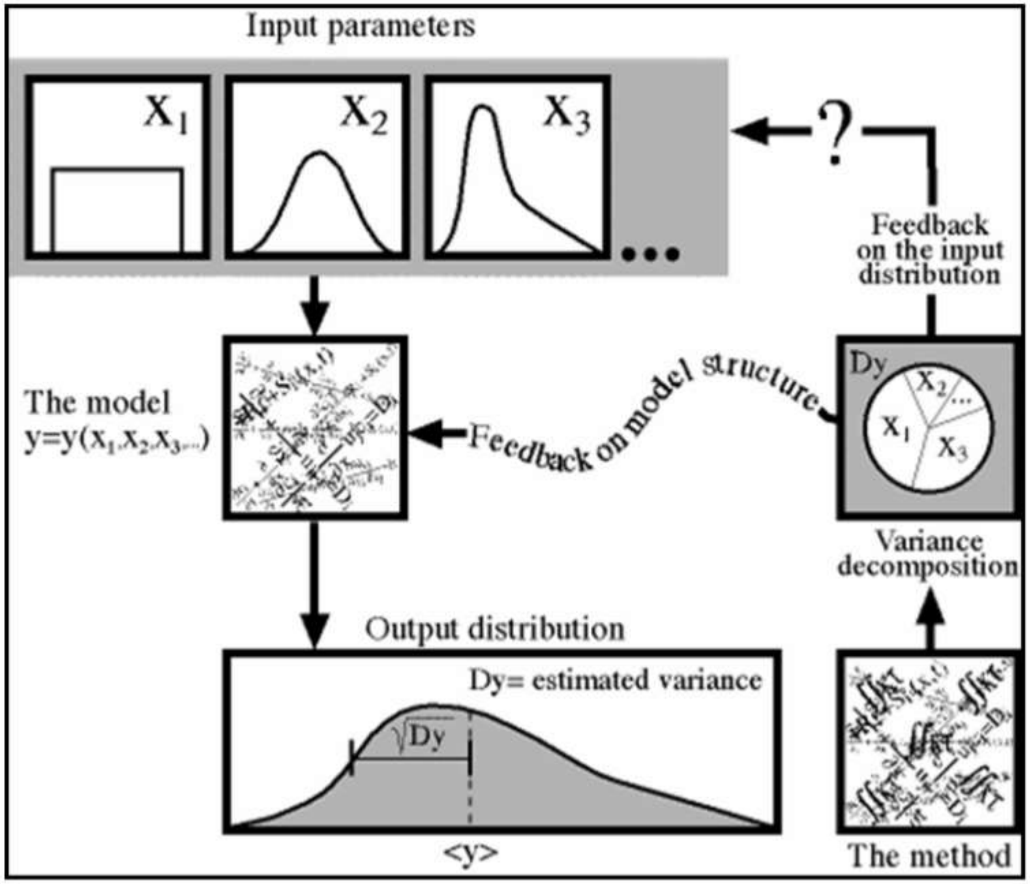
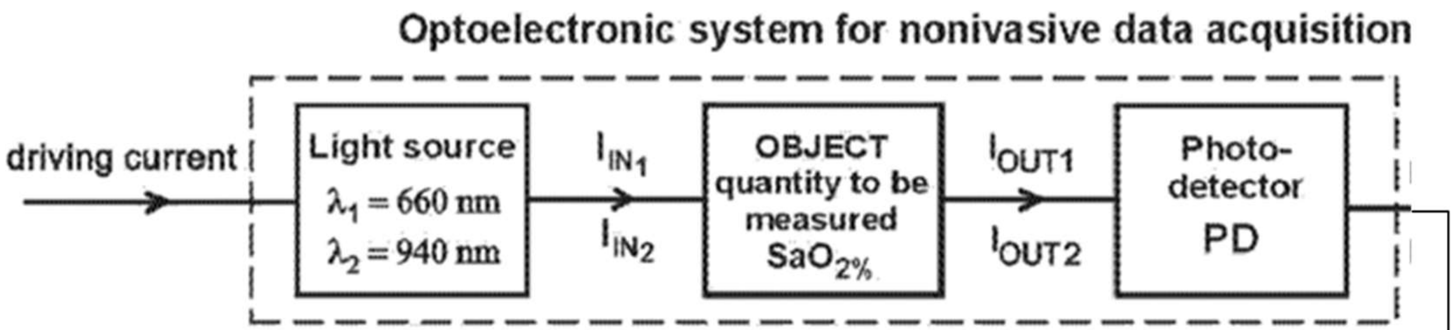


Figure 1: A schematic view of sampling-based sensitivity analysis, Saltelli [Sal00].

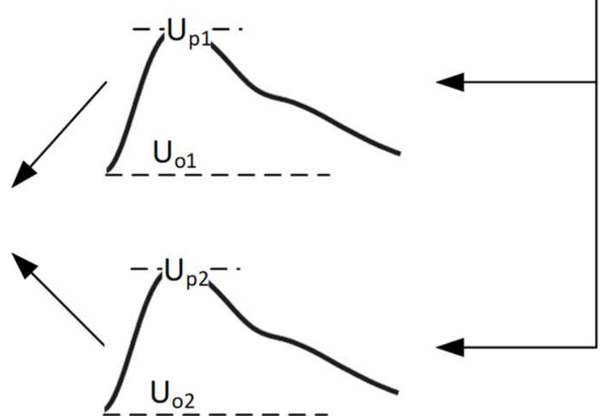
Step D: Confidence intervals for estimation for time series

- Non-parametric methods
  - Bootstrap for time series
- Parametric methods
  - Kalman filters for linear and Gaussian models
  - Particle filters
    - Ability to represent arbitrary densities
    - Adaptive focusing on probable regions of state-space
    - Dealing with non-Gaussian noise
    - The framework allows for including multiple models

Uncertainty propagation for pulse oximeter



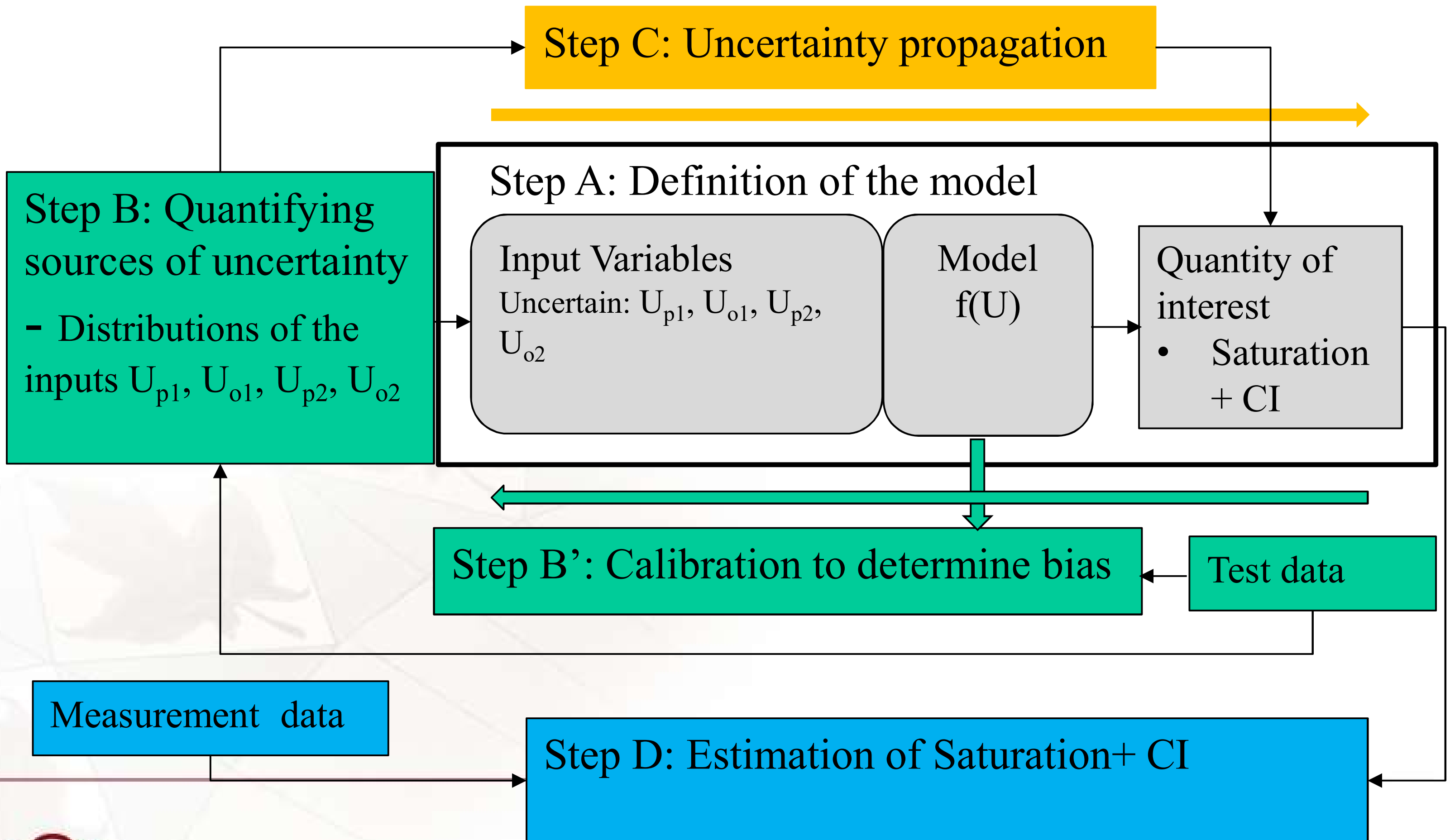
$$F = \mathrm{SyO_2} + b = \frac{1.11 - 0.22 \cdot \frac{U_{p1}}{U_{o1}} \cdot \frac{U_{o2}}{U_{p2}}}{1.00 - 0.05 \cdot \frac{U_{p1}}{U_{o1}} \cdot \frac{U_{o2}}{U_{p2}}} + b$$



A. Cysewska-Sobusiak, "Estimation of Uncertainty in Complex Biomeasurements," *IEEE Workshop on Advanced Methods for Uncertainty Estimation in Measurement*, 2007, pp. 24-29.

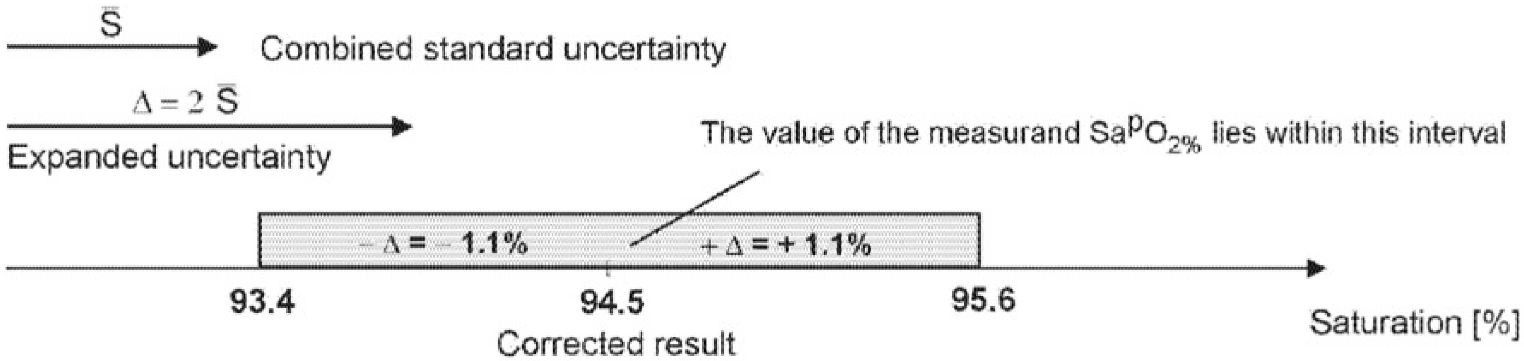
uOttawa

Framework 2: – Uncertainty propagation for pulse oximeter



uOttawa

Framework 2 – Uncertainty propagation for pulse oximeter



Applications

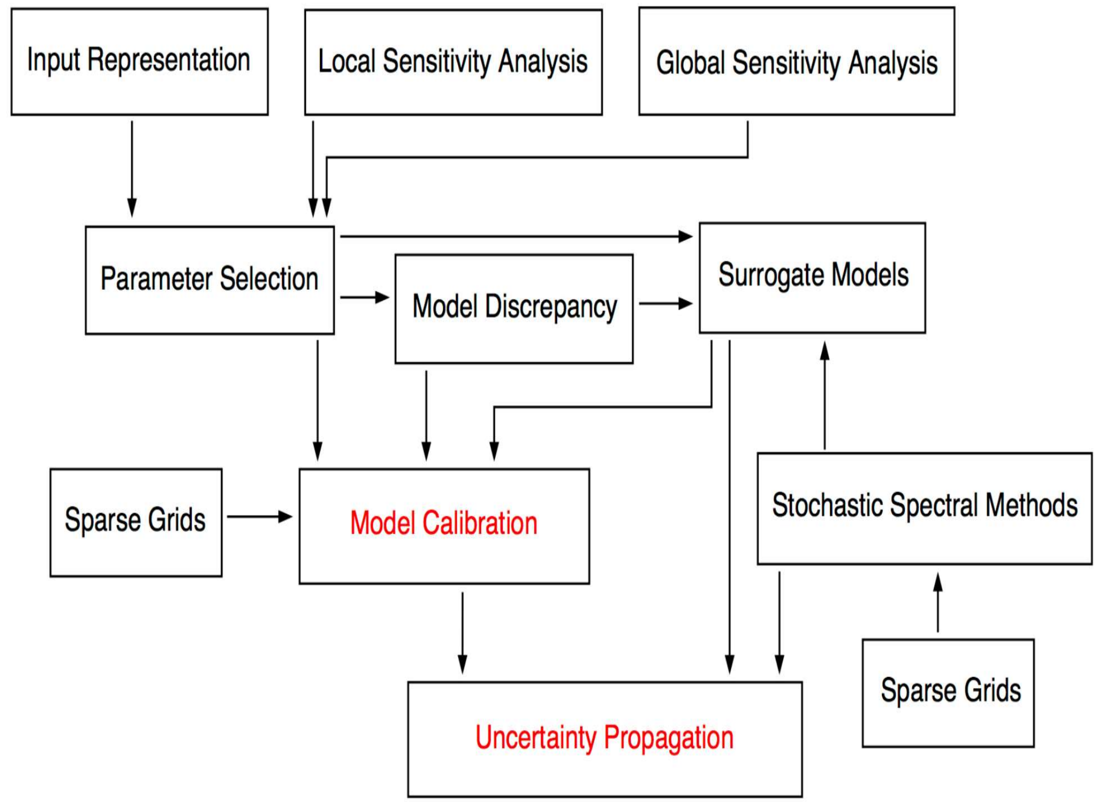
- Prognostics
- Metrology
- Uncertainty quantification in complex systems
- Probabilistic machine learning
- Reliability
- Decision making under uncertainty

Metrology

- The science of measurement, embracing both experimental and theoretical determinations at any level of uncertainty in any field of science and technology
- Uncertainty, as defined in the ISO Guide to the Expression of Uncertainty in Measurement (GUM) and the International Vocabulary of Basic and General Terms in Metrology (VIM), is a
- "parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand."

Uncertainty quantification in complex systems

- Weather models
- Hydrology
- Nuclear reactor design
- Biological models



uOttawa

Probabilistic machine learning

- Learning can be thought of as inferring plausible models to explain observed data.
- Main uses:
  - Make predictions about future data,
  - take decisions that are rational given these predictions.
- Uncertainty:
  - Observed data can be consistent with many models, and therefore which model is appropriate, given the data, is uncertain.
  - Predictions about future data and the future consequences of actions are uncertain.

uOttawa

Zoubin Ghahramani, Probabilistic machine learning and artificial intelligence, Nature, 2015

Prognostics

- Prognostic is predicting how long will take until a particular future event or state is reached.
- Classification
  - Reliability base prognostics
    - Predict mean life of the component
    - Failure rates
  - Early detection of anomalous state

Decision making under uncertainty

- Including various sources of uncertainty into decision making process
- Automated decision making systems
- Examples
  - Collision avoidance system
  - Surveillance systems

Tracking and sensor fusion

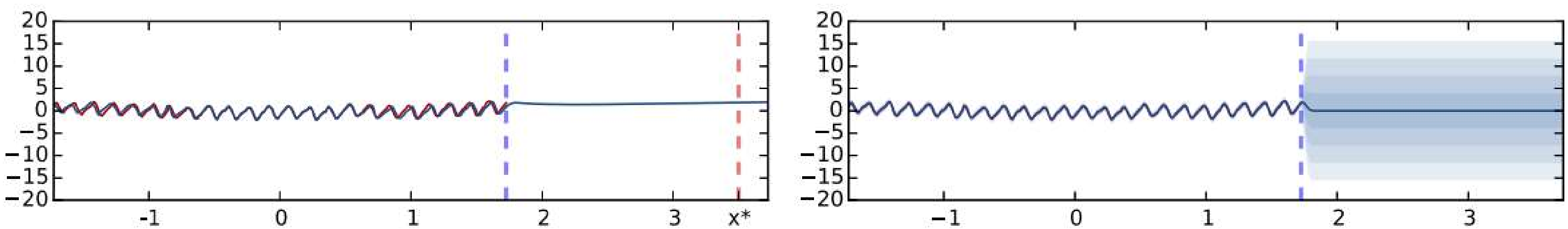
- How can one combine information from multiple imprecise sensors
- What is the accuracy of tracking of the objects
- Monte Carlo based filters – particle filters

Interesting applications

- Uncertainty in deep learning
- Digital twins
- Self-validating sensors
- Uncertainty in the cloud

Uncertainty in deep learning

- Bayesian machine learning deals with probabilistic models and uncertainty
- When using deep learning models, we generally only have point estimates of parameters and predictions.
- Combining Bayesian approach and neural networks*



(a) Standard deep learning model (b) Probabilistic model

Yarin Gal, What My Deep Model Doesn't Know..., 2015, http://mlg.eng.cam.ac.uk/yarin/blog_3d801aa532c1ce.html

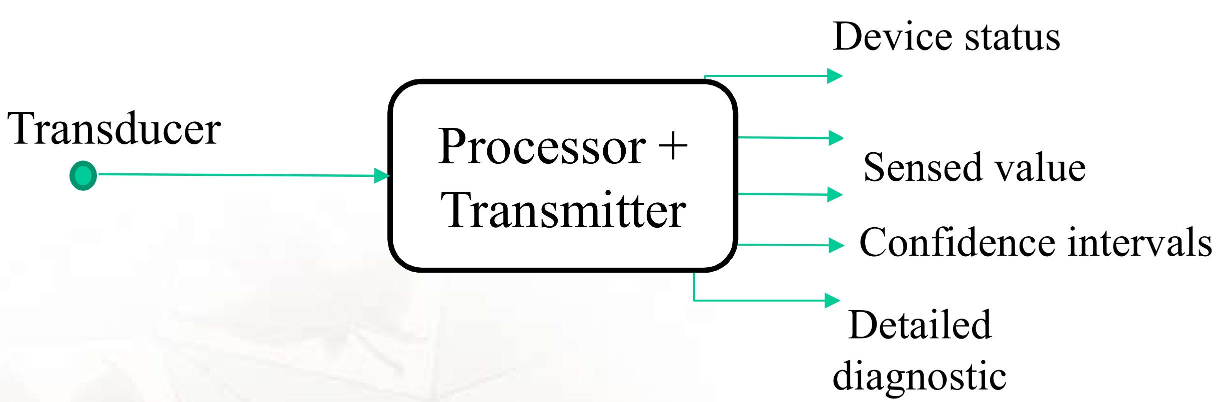
Digital twins

- Digital twins are dynamic digital or virtual software replications of physical assets, products and constructions
- Virtual replica is a digital twin that acts like the real thing
  - help us in detecting possible issues, test new settings, simulate all kinds of scenarios, analyze whatever needs to be analyzed, in fact, do pretty much everything we want in a virtual or digital environment *
- Future:
  - expand to more applications, use cases and industries
  - get combined with more technologies such as speech capabilities, augmented reality for an immersive experience, AI capabilities, more technologies enabling us to look inside the digital twin removing the need to go and check the ‘real’ thing

- Digital twins – rise of the digital twin in Industrial IoT and Industry 4.0
- https://www.i-scoop.eu/internet-of-things-guide/industrial-internet-things-iiot-saving-costs-innovation/digital-twins/

Self-validating (SEVA) sensors

- Sensors that provide uncertainty info with the data



Uncertainty in the cloud

- Goal:
  - Making sense in real-time of multiple, heterogenous, noisy and possibly incomplete data streams in order to support the decision process of very large number of concurrent users.
- Combination of stream or complex event processing and uncertainty
  - Using Bayesian networks for uncertainty quantification and propagation
- Current research is done on smart-homes but on very simple examples

Typical objectives in the applications

- Forward propagation (uncertainty propagation)
  - Suppose that the uncertainties about the inputs of the model can be summarized in a probability distribution. Given that, determine the induced probability distribution at the output
- Reliability
  - Given information about the input and forward process, determine the failure probability (probability that the output value is greater than some threshold)
- Prediction
- Inverse problem
  - State estimation (for quantity changing in time)
  - Parameter identification (usually for quantity non-changing)
  - Learning
- Model reduction – consider another function that approximates our model

Confidence Intervals

The value of the statistic in the data sample (eg., mean, median, etc.)

point estimate ± (measure of how confident we want to be) × (standard error)

From a Z table or a T table, depending on the sampling distribution of the statistic.

Standard error of the statistic.

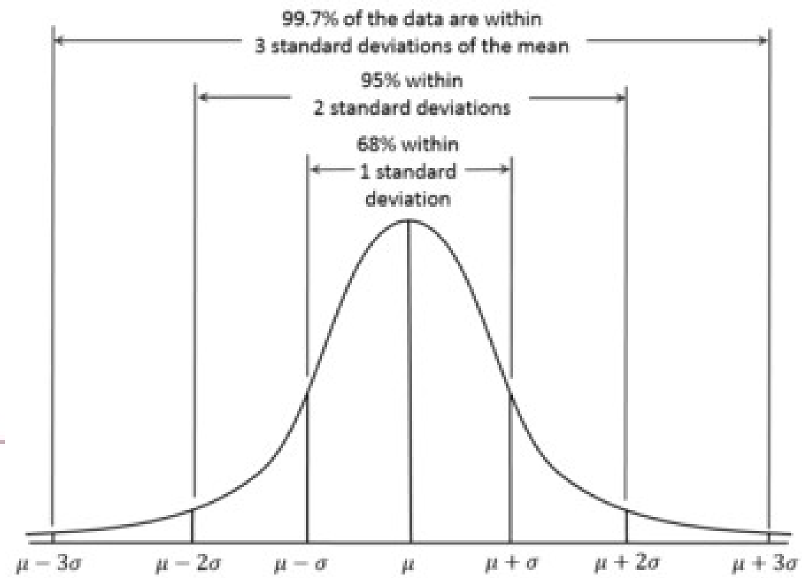
uOttawa

Confidence interval for the mean of Normal distribution with σ known

- Suppose that X=(x_1,…,x_n) are samples from Normal distribution $X_i \sim N(\mu, \sigma^2)$.
- Empirical mean $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$ and

To determine information about the unknown mean, we consider the sample mean $\bar{x}$. 95% of the area of a normal distribution lies within two standard deviations of the mean

$$P(\bar{x} - 2\frac{\sigma}{\sqrt{n}} < \mu < \bar{x} + 2\frac{\sigma}{\sqrt{n}}) \approx .95$$



uOttawa

Confidence interval

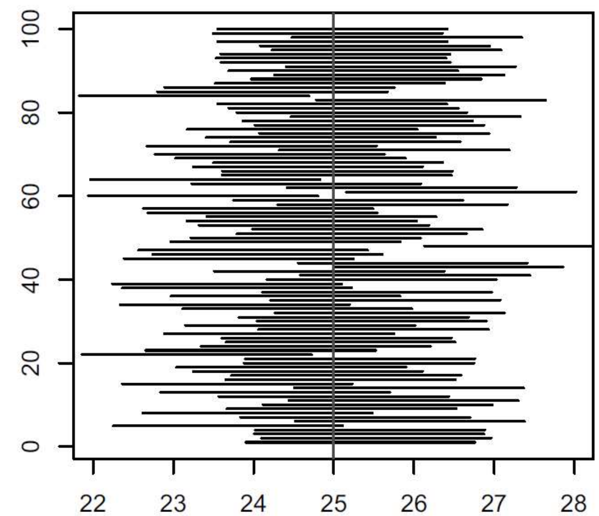
- The goal is to determine functions $q_L(x)$ and $q_U(x)$ that bound the location $q_L(x)$ < q < $q_U(x)$ of q based on realizations x=[x_1,…. x_n] of a random sample X=[X_1,…. X_n].
- The random interval [q_L(X), q_U(X)] is termed as interval estimator.
- The interval estimator in combination with a confidence coefficient is commonly called a confidence interval.
- The confidence coefficient (1- α)x100% can be interpreted as the frequency of times, in repeated sampling, that the interval will contain the target parameter q.

$$P[q_L(X) \leq q \leq q_U(X)] = 1 - \alpha$$

Confidence intervals interpretation

- 95% confidence interval means:

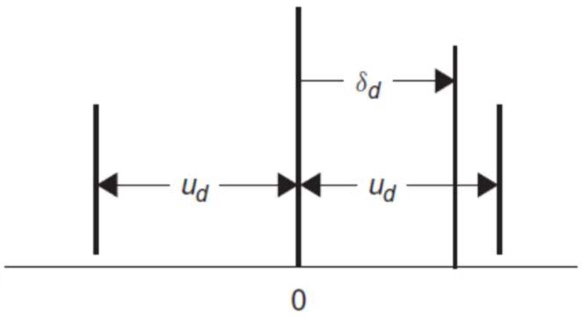
95% of similarly constructed confidence intervals will contain the true mean



~~The probability that the true mean lies between $q_L(x)$ and $q_U(x)$ is 95%~~

GUM-base approach
Types of uncertainty

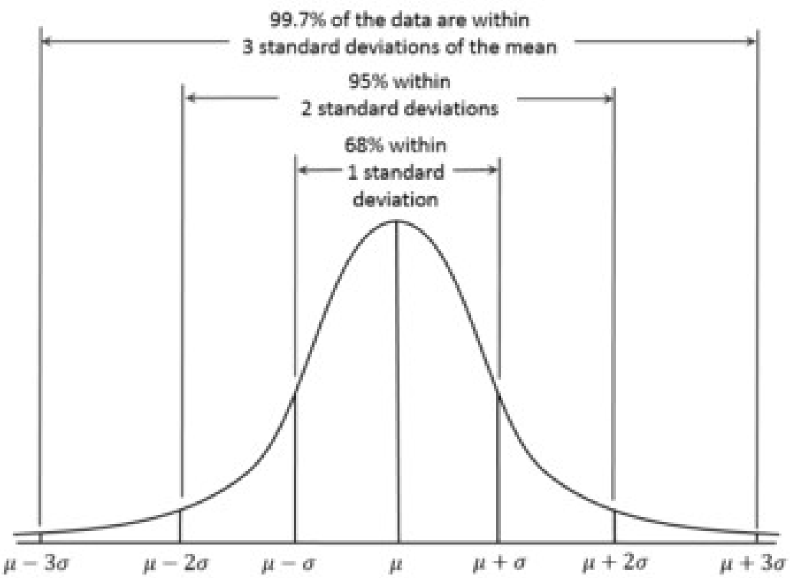
- An error δ = measured value– "true" value of density
- An uncertainty u is an estimate of an interval $\pm$u that should contain an error.
- GUM categorization :
  - Type A: "method of evaluation of uncertainty by the statistical analysis of series of observations"
  - Type B: "method of evaluation of uncertainty by means other than the statistical analysis of series of observations"



uOttawa

Expended Uncertainty

- Uncertainty
  - Systematic (bias) b_x
  - Random (standard deviation): s_x
- Uncertainty can be defined as
  - $u_x^2 = b_x^2 + s_x^2$



- Expended uncertainty is defined as
  - $U = k_{\%} u_x$

Definitions

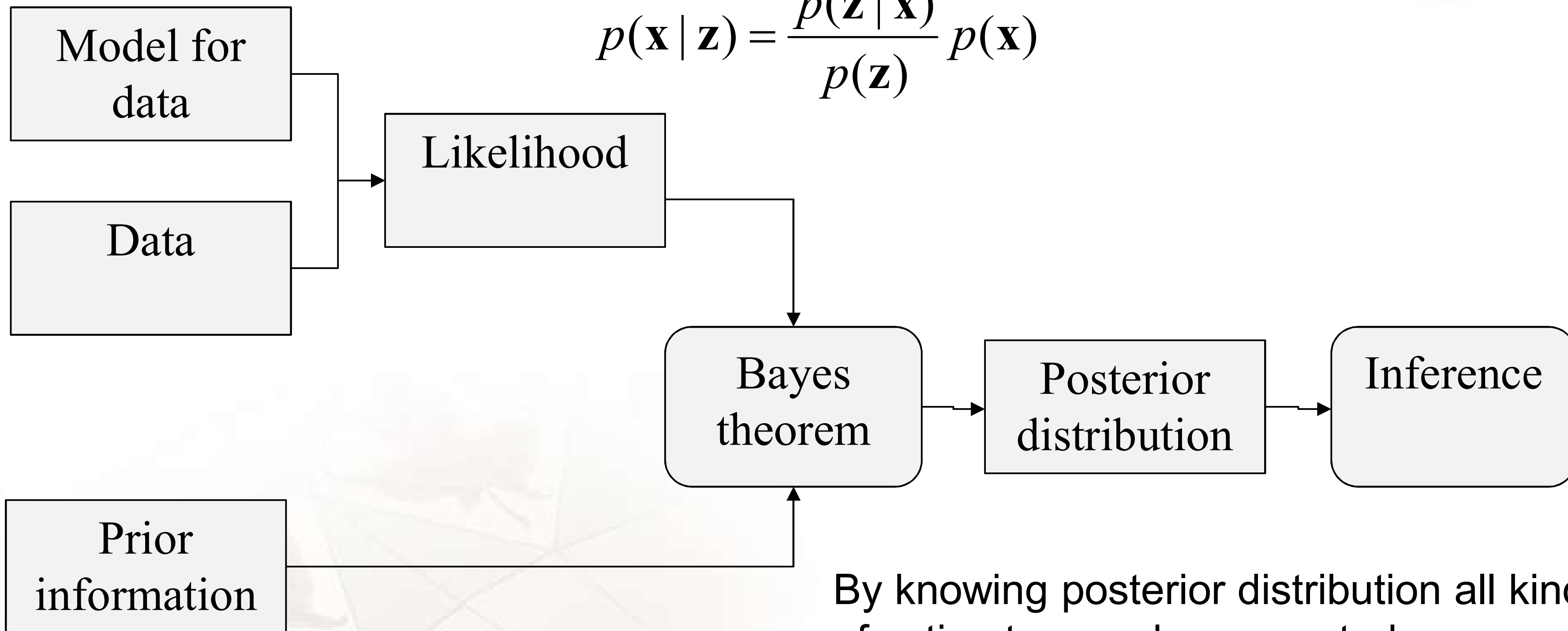
- Standard uncertainty
  - uncertainty of the result of a single type of measurement includes Type A and/or Type B uncertainties
- Expanded uncertainty
  - the standard uncertainty multiplied by a coverage factor
- Standard error SE
  - Standard deviation of the sample statistics

Other statistical intervals

- Prediction intervals
  - An intervals that would contain a future randomly selected observation from the distribution, with a specific degree of confidence.
  - Example: predict sample mean of *m* future samples
- Statistical tolerance limits create an interval that bounds a specified percentage of the population at a given level of confidence.
  - (such as 99% of the population with 95% confidence)
  - These intervals are often used to demonstrate compliance with a set of requirements or specification limits.

Bayesian inference method

$$p(\mathbf{x}\,|\,\mathbf{z}) = \frac{p(\mathbf{z}\,|\,\mathbf{x})}{p(\mathbf{z})}\,p(\mathbf{x})$$



By knowing posterior distribution all kinds of estimates can be computed:

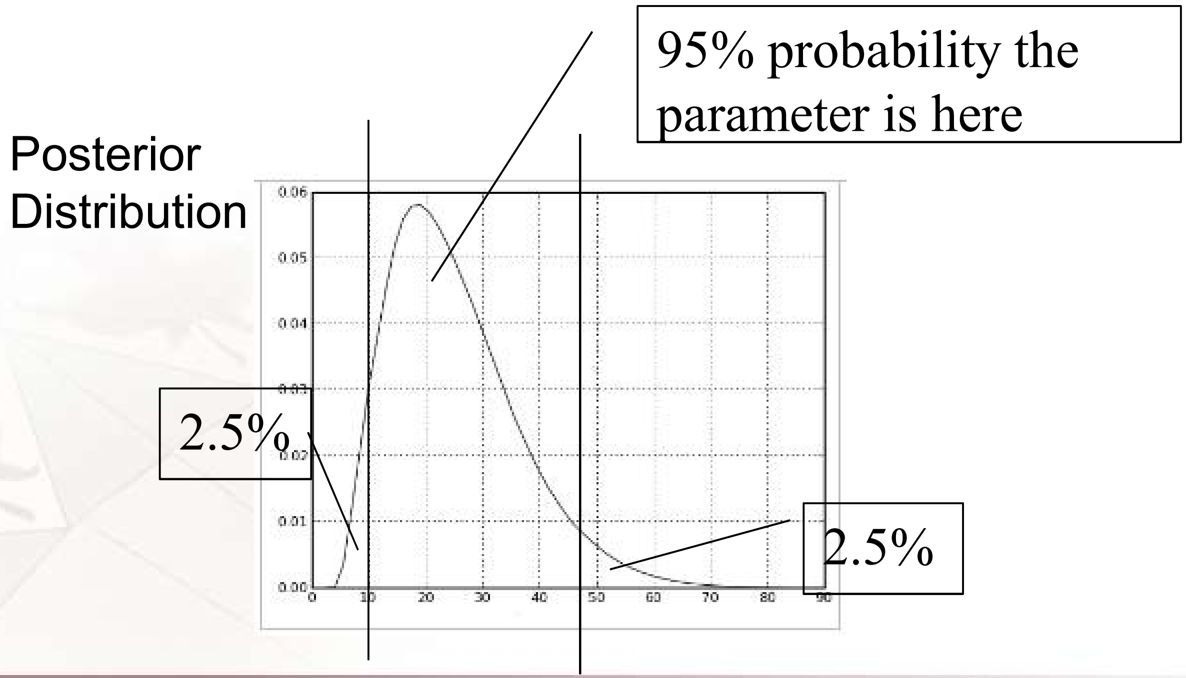
$$E(f(x)) = \int f(x)\,p(\mathbf{x}\,|\,\mathbf{z})\,d\mathbf{x}$$

uOttawa

W. Q. Meeker, et. al., “Statistical intervals, A Guide for Practitioners and Researchers,” Second Edition, Wiley, 2017

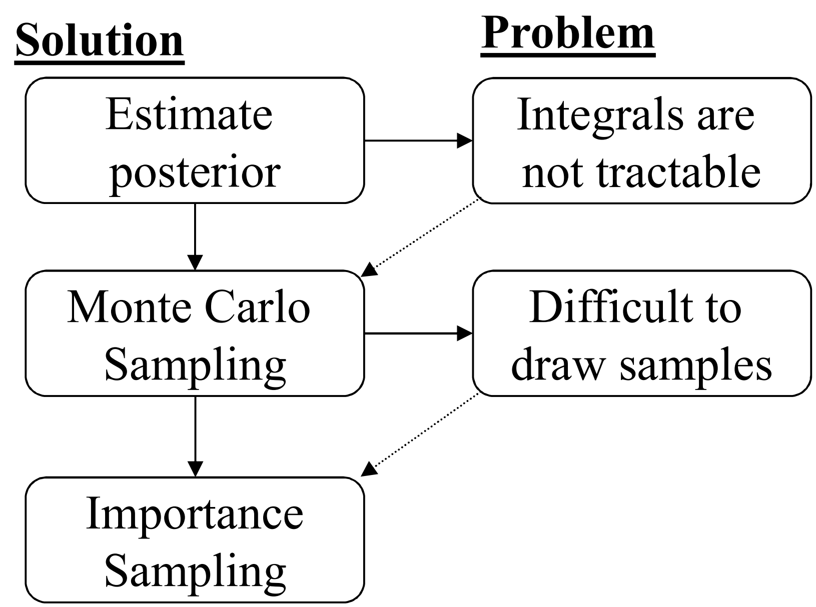
Credible intervals

- Interpretation: the probability that the true mean is contained within the given interval is 95%.



Monte Carlo methods

- Use
  - Solving integrals
  - Propagating uncertainties
  - Sequential Monte Carlo methods for parameter estimation



Evaluating integrals using Monte Carlo methods

- Example: Estimate the variance of a zero mean Gaussian process

$$v = \int_{-\infty}^{+\infty} x^2 p(x) dx$$

- Monte Carlo approach:

1. Simulate M random variables from a Gaussian distribution

$$x^{(m)} \sim N(0, \sigma^2)$$

2. Compute the average

$$v = \frac{1}{M} \sum_{m=1}^{M} (x^{(m)})^2$$

Importance sampling

- Classical Monte Carlo integration – Difficult to draw samples from the desired distribution
- Importance sampling solution:
  1. Draw samples from another (proposal) distribution
  2. Weight them according to how they fit the original distribution

- Free to choose the proposal density
- Important:
  - It should be easy to sample from the proposal density
  - Proposal density should resemble the original density as closely as possible

uOttawa

Importance sampling

- Evaluation of integrals

$$E(f(X)) = \int_X f(x)p(x)dx = \int_X f(x)\frac{p(x)}{\pi(x)}\pi(x)dx$$

- Monte Carlo approach:

1. Simulate M random variables from proposal density $\pi(x)$

$$x^{(m)} \sim \pi(x)$$

2. Compute the average

$$E(f(x)) \approx \frac{1}{M}\sum_{m=1}^{M} f(x^{(m)})\underbrace{\frac{p(x^{(m)})}{\pi(x^{(m)})}}_{w^{(m)}}$$

Bayesian Uncertainty Quantification

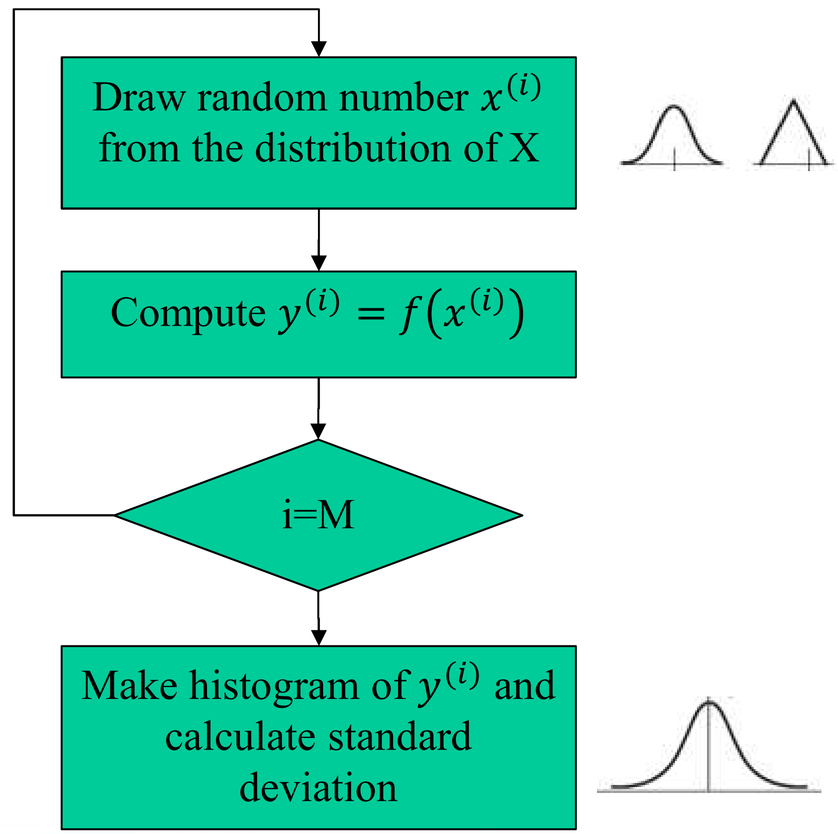
- Issues to be considered
  - Selection of prior PDFs
  - Ranking the alternative models in order to select the best model
  - Incorporating measurement and calibration uncertainties
  - Real-time processing

Step C': Propagation of uncertainties based on Monte Carlo

- Propagate of uncertainties "through" function *f*

  $y = f(x)$

- Distribution of measurement errors and input uncertainties has been determined
- Works for non-linear models
- Disadvantages
  - Slow convergence



uOttawa

Monte Carlo based propagation of uncertainty

I. To get $P(a < y < b)$ let N be the number of $y^{(i)}$ such that $a < y^{(i)} < b$ and compute

$$P(a < y < b) \approx \frac{N}{M}.$$

II. To get σ_Y, compute the sample mean $\bar{y} = \frac{1}{M}\sum_{i=1}^{M} y^{(i)}$

$$\sigma_Y \approx \sqrt{\frac{1}{M-1}\sum_{i=1}^{M}\left(y^{(i)} - \bar{y}\right)^2}$$

III. Get the q^{th} quantile of the empirical distribution of Y

Uncertainty related resources - Tools

- **SimLab**
  - https://ec.europa.eu/jrc/en/samo/simlab
- **OpenTurns**
  - http://www.openturns.org/
  - C++ with Python wrappers
- UQLab
  - http://www.uqlab.com/
  - Matlab
- MIT Uncertainty Quantification Library (MUQ)
  - C++
- …

Uncertainty related resources - Courses

- With Videos
  - Uncertainty Quantification in Engineering Science
    - http://eclass.uth.gr/eclass/courses/MHXB124/
  - Introduction to Uncertainty Quantification
    - https://www.ima.umn.edu/2014-2015/ND6.15-26.15/#
- Without videos
  - MA 540 Uncertainty Quantification for Physical and Biological Models
    - http://www4.ncsu.edu/~rsmith/MA540_s17.html

Uncertainty related resources - Books

- F. Pavese, A. B. Forbes, Data Modeling for Metrology and Testing in Measurement Science, Springer, 2009.
- S. V. Gupta, Measurement Uncertainties, Physical Parameters and Calibration of Instruments, Springer-Verlag Berlin Heidelberg 2012.
- I. Lira, Evaluating the Measurement Uncertainty: Fundamentals and Practical Guidance, IoP 2002.
- H. W. Coleman, W. G. Steele, Experimentation, validation and uncertainty analysis for Engineers, Wiley, 2009.

- A. Zoubir, D. R. Iskander, Bootstrap techniques for signal processing, Cambridge University Press, 2004.
- W. Q. Meeker, G. J. Hahn, L. A. Escobar, Statistical Intervals: A Guide for Practitioners and Researchers, 2nd Edition, Wiley, 2017.
- R. C. Smith, Uncertainty Classification: Theory, Implementation and Applications, SIAM, 2014.

- K. Beven, Environmental Modelling: An Uncertain Future?, Taylor & Francis e-Library, 2010.

References

- Sankaran Mahadevan, “Modeling and Data Uncertainties,” presentation, NASA/NAI Summer Design Institute on Uncertainty, Hampton, VA, July 20, 2011
- William F. Guthrie,1 Hung-kung Liu,2 Andrew L. Rukhin,3 Blaza Toman, Jack C. M. Wang,5 Nien fan Zhang, **Three Statistical Paradigms for the Assessment and Interpretation of Measurement Uncertainty, from Data Modeling for Metrology and Testing in Measurement Science by Franco Pavese and Alistair B. Forbes**
- BIPM, IEC, IFCC, ISO, IUPAC, IUPAP, and OIML. Guide to the expression of uncertainty in measurement, International Organization for Standardization. GUM 1995 with minor corrections. Corrected version 2010. JCGM 100:2008.
- BIPM, IEC, IFCC, ISO, IUPAC, IUPAP, and OIML. Evaluation of measurement data — Supplement 1 to the Guide to the expression of uncertainty in measurement — Propagation of distributions using a Monte Carlo method. JCGM 101:2008.