Review on methods to estimate measurement uncertainties

The various concepts of the “GUM” and its supplements

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Content

1. Definitions of measurand and measurement uncertainty
2. Modelling indirect measurands
3. Propagation of measurement uncertainties
   3.1 Linear and linearizable explicit dependence of an indirect measurand on direct measurands
   3.2 Combination of probability density distributions ...
      - ... without à priori information
      - ... with à priori information, updating estimates by increase of knowledge
4. Guides of the *Joint Committee for Guides in Metrology*

1 Definitions of measurand and measurement uncertainty

VIM International vocabulary of metrology – Basic and general concepts and associated terms
3rd edition (2012 - JCGM 200:2008 with minor corrections)
https://www.bipm.org/utils/common/documents/jcgm/JCGM_200_2012.pdf
currently under revision:

https://www.bipm.org/documents/20126/54295284/VIM4_CD_210111c.pdf

Measurand

quantity intended to be measured

Measurement

process of experimentally obtaining one or more quantity values that can reasonably be attributed to a quantity

Quantity

property of a phenomenon, body, or substance, where the property has a magnitude that can be expressed as a number and a reference

1 Definitions of measurand and measurement uncertainty

observe

acquire

acquire

observe

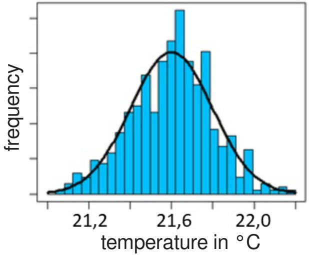
observing repetitively

set of observations: sample

values are scattering

frequency: how often

probability



1 Definitions of measurand and measurement uncertainty

VIM:

Measurement result/ result of measurement

set of quantity values being attributed to a measurand together with any other available relevant information

Note 1:

A measurement result generally contains "relevant information" about the set of quantity values, such that some may be more representative of the measurand than others.
This may be expressed in the form of a probability density function (PDF).

Note 2:

A measurement result is generally expressed as a single measured quantity value and a measurement uncertainty. ...

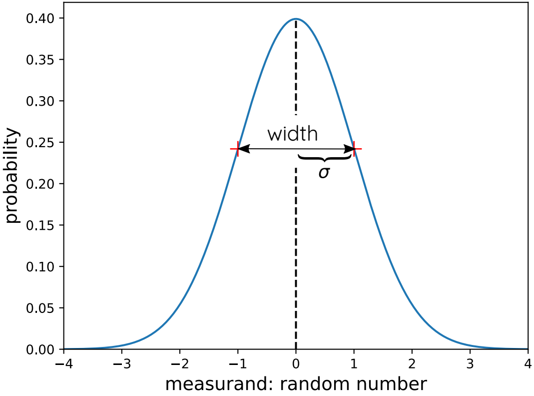
1 Definitions of measurand and measurement uncertainty

- "relevant information" belonging to the estimator of a measurand is given to express its uncertainty
- measure for the "scattering" characteristics of observations
- the "scattering" is expressed by the probability density distribution of the measurand's observations
- a single parameter to quantify the "scattering" is the width of the probability distribution
- which is the variance, resp. the square root of the variance

1 Definitions of measurand and measurement uncertainty

probability density distribution

$$p\colon X \mapsto p(X)$$



Variance $\propto$ second statistical moment

$$\int_{-\infty}^{\infty} X^2\, p(X)\, \mathrm{d}X$$

in case of a normal distribution (Gaussian)

$$p(X) \;=\; \frac{1}{\sqrt{2\pi}\sigma}\, e^{-\frac{1}{2}\left(\frac{X}{\sigma}\right)^2}$$

the variance is

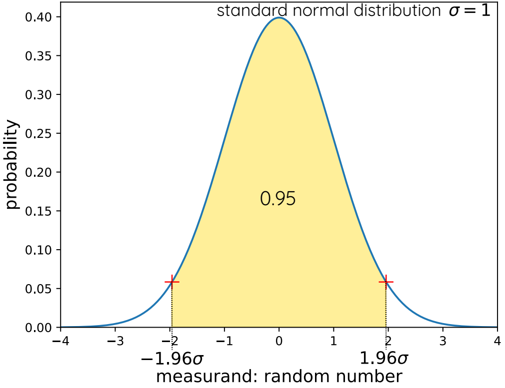
$$\int\limits_{-\infty}^{\infty} X^2\, \frac{1}{\sqrt{2\pi}\sigma}\, e^{-\frac{1}{2}\left(\frac{X}{\sigma}\right)^2}\, \mathrm{d}X \;=\; \sigma^2$$

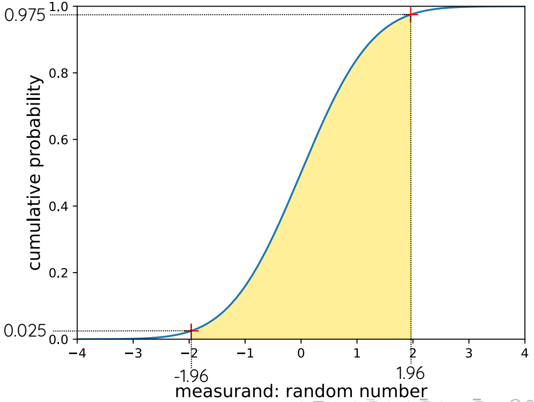
1 Definitions of measurand and measurement uncertainty

- coverage interval $[\mu - k\sigma, \mu + k\sigma]$
- in case of a normal distribution:
- 95% confidence level: $k = 1.96$

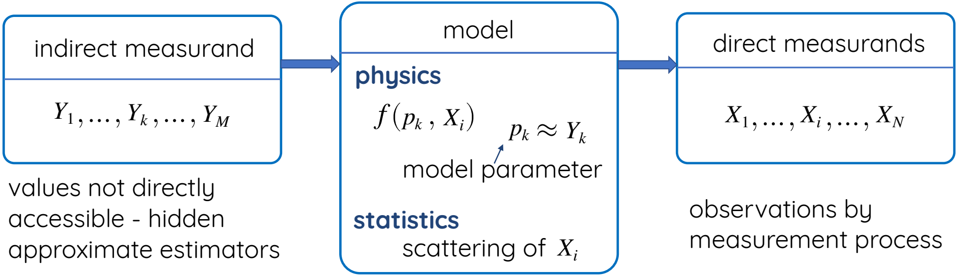
cumulative probability distribution of a random number X:

$$P(X) = \int_{-\infty}^{X} p(X')\,\mathrm{d}X'$$





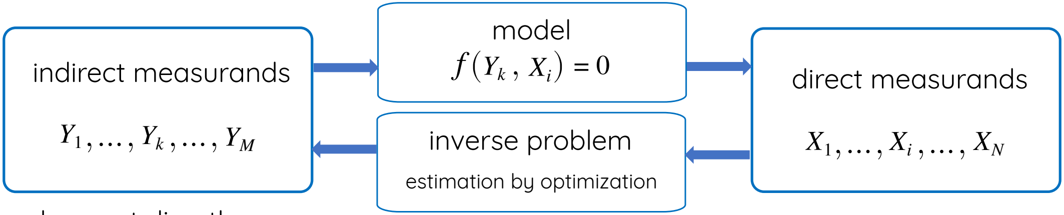
2 Modelling indirect measurands



Causes of deviations:

- scattering of values of direct measurands
- approximations when setting up a model ...
  - ... simplification of the description of physical processes (neglecting smaller effects)
  - ... neglection of external influences

2 Modelling indirect measurands



values not directly accessible - hidden approximate estimators

observations by measurement process

2 Modelling indirect measurands

Direct measurand $\mathbf{X} = (X_1, \ldots, X_N)^\mathsf{T}$

Indirect measurand (model parameter) to be estimated $\mathbf{Y} = (Y_1, \ldots, Y_M)^\mathsf{T}$

	univariate: 1 indirect quantity	multivariate: $M > 1$ indirect quantities
explicite	$Y = f(\mathbf{X})$	$\mathbf{Y} = \vec{f}(\mathbf{X})$
implicite	$f(Y, \mathbf{X}) = 0$	$f(\mathbf{Y}, \mathbf{X}) = 0$ or $\vec{f}(\mathbf{Y}, \mathbf{X}) = 0$

2 Modelling indirect measurands

Example: Fraunhofer diffraction of single slit

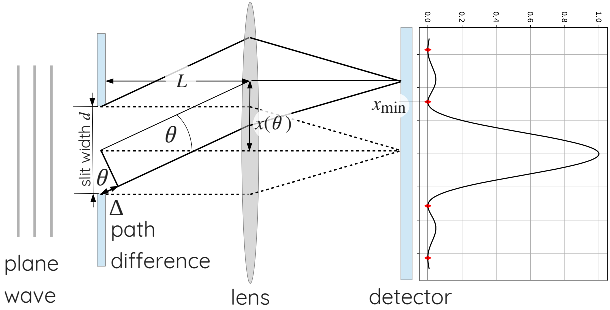
- path difference:

$$\Delta = \frac{d}{2} \sin(\theta)$$

- phase difference:

$$\varphi = \frac{2\pi}{\lambda} \Delta$$

where λ is the wavelength of the light



- model of single slit diffraction in Fraunhofer approximation:

$$I = I_0 \frac{\sin(\varphi)^2}{\varphi^2} \quad \text{and} \quad x = L\tan(\theta) \hookrightarrow \theta = \arctan\left(\frac{x}{L}\right)$$

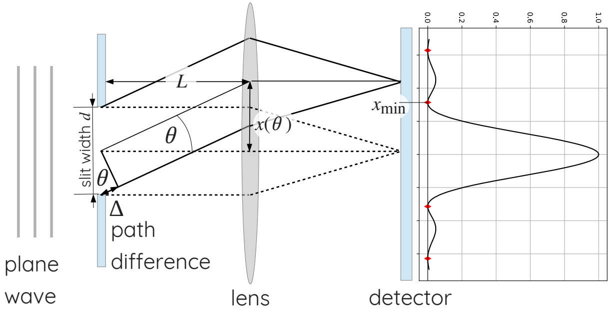
2 Modelling indirect measurands

Example: Fraunhofer diffraction of single slit

- detector signal: $g(x)$ where g denotes the gray values of the discrete detector elements
- minima at destructive interference

$$\Delta_{\min} = n\frac{\lambda}{2} \quad n \in \mathbb{N}_{>0}$$

- first order minimum

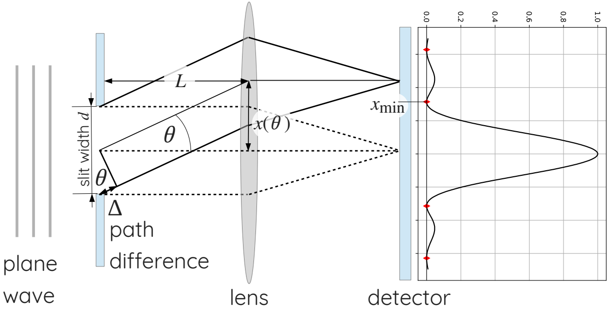


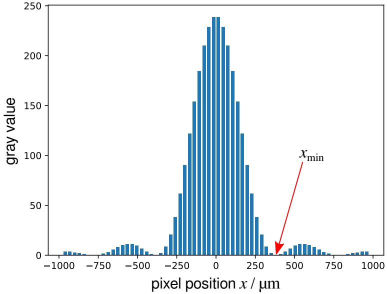
$$\frac{d}{2}\sin(\theta_{\min}) = \frac{\lambda}{2} \hookrightarrow \frac{d}{2}\sin\left(\arctan\left(\frac{x_{\min}}{L}\right)\right) = \frac{\lambda}{2}$$

indirect measurand slit width: $d = \dfrac{\lambda}{\sin\left(\arctan\left(\frac{x_{\min}}{L}\right)\right)} \approx \dfrac{\lambda L}{x_{\min}}$

2 Modelling indirect measurands

Example: Fraunhofer diffraction of single slit





direct measurands:

- distance slit – lens: L
- wavelength of light: λ
- positions of detector elements (pixel): x
- gray values of detector elements: $g(x)$

- indirect measurand $x_{\min}$ estimated from discrete $g\colon i\Delta x \mapsto g(i\Delta x)$
- where Δx is pixel distance, i is pixel number

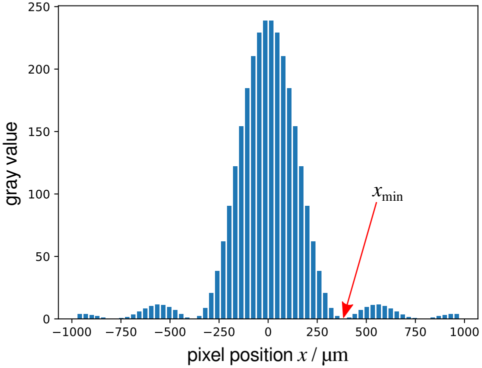
2 Modelling indirect measurands

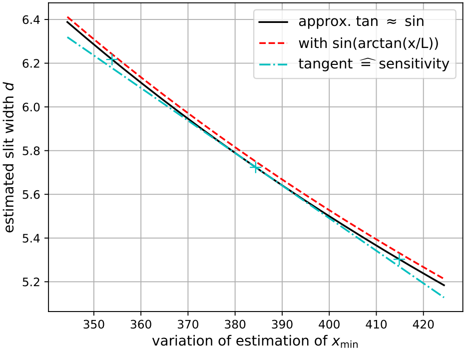
Example: Fraunhofer diffraction of single slit

measurand		uncertainty u
distance slit – lens: L	$\hookrightarrow$	à priori knowledge of exp. setup: $u(L)$
wavelength of light: λ	$\hookrightarrow$	à priori knowledge of light source: $u(\lambda)$
positions of detector elements (pixel): x	$\hookrightarrow$	à priori knowledge of detector: $u(x)$
gray values of detector elements: $g(x)$	$\hookrightarrow$	à priori knowledge of detector: $u(g)$
first order minimum x_{min}:	$\hookrightarrow$	propagation of $u(x)$ and $u(g)$ and
implicite dependence on x, g		optimization process $\min\{g(x)\}$: $u(x_{\mathrm{min}})$
slit width d	$\hookrightarrow$	propagation of $u(x_{\mathrm{min}})$, $u(L)$, and $u(\lambda)$: $u(d)$
explicite dependence on x_{min}, L, and λ		

One indirect measurand d explicitely dependent on three direct measurands $x_{\min}$, L, and λ

$$d(x_{\min}, L, \lambda) = \frac{\lambda}{\sin\left(\arctan\left(\frac{x_{\min}}{L}\right)\right)} \approx \frac{\lambda L}{x_{\min}}$$





Examine sensitivity of indirect measurand with respect to variations of direct measurands

- Gradient (slope; tangential hyperplane) at estimated values of $\hat{x}_{\min}$, $\hat{L}$, and $\hat{\lambda}$

$$\left(\frac{\partial}{\partial x_{\min}} d(x_{\min}, L, \lambda) \bigg|_{\hat{x}_{\min}}, \; \frac{\partial}{\partial L} d(x_{\min}, L, \lambda) \bigg|_{\hat{L}}, \; \frac{\partial}{\partial \lambda} d(x_{\min}, L, \lambda) \bigg|_{\hat{\lambda}} \right)^{\mathsf{T}}$$

  how much does d change if $x_{\min}$, L, and λ change

- d is linearly dependent on λ, so $\frac{\partial}{\partial \lambda} d(x_{\min}, L, \lambda) = const.$ independent of $\hat{\lambda}$

- d is linearly dependent on L in case of the approximation $d \approx \frac{\lambda L}{x_{\min}}$

- $d(x_{\min}, L, \lambda)$ is linearizable if $u(x_{\min}) \lesssim \Delta x$ (where Δx is the pixel size)

- how much does d change if $x_{\min}$, L, and λ change
- change/ variation/ scattering of $x_{\min}$, L, and λ:
  $u(x_{\min})$, $u(L)$, and $u(\lambda)$
- $u_{x_{\min}}(d) = \frac{\partial}{\partial x_{\min}} d(x_{\min}, L, \lambda)\Big|_{\hat{x}_{\min}} u(x_{\min})$,
- $u_L(d) = \frac{\partial}{\partial L} d(x_{\min}, L, \lambda)\Big|_{\hat{L}} u(L)$,
- $u_\lambda(d) = \frac{\partial}{\partial \lambda} d(x_{\min}, L, \lambda) u(\lambda)$
- independent variations of $x_{\min}$, L, and λ $\hookrightarrow$ Pythagorean sum

$$u^2(d) = u^2_{x_{\min}}(d) + u^2_L(d) + u^2_\lambda(d)$$

3 Propagation of measurement uncertainties

3.1 Linear and linearizable explicit dependence

JCGM 100:2008 (GUM 1995 with minor corrections)
Evaluation of measurement data - Guide to the expression of uncertainty in measurement

- uncertainties of x_{min}, L, and λ are not correlated $\hookrightarrow$ propagation:

$$u^2(d) = \left(\frac{\partial d}{\partial x_{\mathrm{min}}}\right)^2\Bigg|_{\hat{x}_{\mathrm{min}}} + \left(\frac{\partial d}{\partial L}\right)^2\Bigg|_{\hat{L}} u^2(L) + \left(\frac{\partial d}{\partial \lambda}\right)^2 u^2(\lambda)$$

- propagation law for models of linearizable sensitivity to variation of direct measurands

$$u^2\left(Y\right) = \sum_{i=1}^{N} c_i^2 u^2(X_i) + 2\sum_{i=1}^{N-1}\sum_{k=i+1}^{N} c_i c_k \rho(X_i, X_k) u(X_i) u(X_k)$$

- where Y is the indirect measurand and where $c_i = \frac{\partial Y}{\partial X_i}\Big|_{\hat{X}_i}$ are the sensitivities
- where $\rho(X_i, X_k)$ are possible correlations of pairs of direct measurands (X_i, X_k)

3 Propagation of measurement uncertainties

3.2 Combination of probability density distributions – Probability calculus

- Probability theory
- terms:
  - finite countable set = sample space Ω
  - an event E is a finte subset of Ω: $E = \{x_1, x_2, \ldots\}$
- foundation of the probability theory: Kolmogorov axioms (in 1930th)
  1. For any $x \in \Omega$ and also for any event E the probability p is a real number between 0 and 1.
  2. The probability of an event that will certainly occur is 1:

$$\sum_{x \in \Omega} p(x) = 1$$

  3. Any countable sequence of disjoint sets (synonymous with mutually exclusive events) $E_1, E_2, \ldots$ satisfies

$$p\left(\bigcup_{i=1}^{\infty} E_i\right) = \sum_{i=1}^{\infty} p(E_i).$$

- **Joint Probability (event intersection):**
  - A statistical measure that calculates the likelihood of two events E_i and E_j occurring together resp. occur in identically performed experiments; i.e. they intersect
  - Both events must be independent of each other
  - if $p(E_i)$ is the probability that E_i happens and $p(E_j)$ is the probability that E_j occurs, then the probability $p(E_i \cap E_j)$ that both occur simultaneously is the product of the probabilities $p(E_i \cap E_j) = p(E_i)p(E_j)$
- Example: deck with 52 cards having 12 figures: 4 Jacks, 4 Kings, 4 Queens, two of them are red (diamonds and hearts) and two black (spades and clubs)
  - event $E_1 = J$ pick a Jack; event $E_2 = r$ pick a red card
  - probability $p(J) = \frac{4}{52}$ 4 Jacks are in the deck; probability $p(r) = \frac{26}{52} = \frac{1}{2}$ half of the cards are red
  - $p(J \cap r) = p(J)\,p(r) = \frac{4}{52}\frac{1}{2} = \frac{1}{26}$

- **Conditional Probability:**
  - the probability that one event E_j will occur given that another event E_i occurs
  - denotion: $p(E_j|E_i)$
- **Chain rule:**

  The conditional probability can be used to calculate the joint probability,

$$p(E_i \cap E_j) = p(E_i, E_j) = p(E_j|E_i)\, p(E_i)$$

- Example: deck with 52 cards having 12 figures: 4 Jacks, 4 Kings, 4 Queens
  - probability to pick a figure from the deck $p(F) = \frac{12}{52}$
  - probability to pick a Jack from the set of figures $p(J|F) = \frac{4}{12}$
  - $p(J|F)\, p(F) = \frac{4}{12} \cdot \frac{12}{52} = \frac{4}{52} = p(J)$
  - probability to pick a Jack from the deck $p(J) = \frac{4}{52}$

- Sample of observations $\{x_1, \ldots, x_n\}$ obtained by identical and independent measurements:
  - measurand X with expectation value μ and variance σ^2
  - stochastic process: Gaussian distribution
  - probability to measure the value x_i

$$p(x_i) = \frac{1}{\sqrt{2\pi}\,\sigma} e^{-\frac{1}{2}\left(\frac{x_i-\mu}{\sigma}\right)^2}$$

  - Joint probability that the values $x_1, \ldots, x_n$ are observed

$$p(x_1, \ldots, x_n) = \prod_{i=1}^{n} p(x_i)$$

for Gaussian probability density distributions

$$p(x_1, \ldots, x_n) = \frac{1}{\left(\sqrt{2\pi}\,\sigma\right)^n} \prod_{i=1}^{n} e^{-\frac{1}{2}\left(\frac{x_i-\mu}{\sigma}\right)^2} = \frac{1}{\left(\sqrt{2\pi}\,\sigma\right)^n} e^{-\frac{1}{2}\sum_{i=1}^{n}\left(\frac{x_i-\mu}{\sigma}\right)^2}$$

- One measurement: set of observations $\{x_{1,i_1}, \ldots, x_{N,i_N}\}$:
  - direct measurands $\mathbf{X} = (X_1, \ldots, X_N)$ with expectation values $\mu_1, \ldots, \mu_N$ and variances $\sigma_1^2, \ldots, \sigma_N^2$ (in case of correlations with covariances $\sigma_{i,j}$)
  - Joint probability that for measurand X_1 the value x_{1,i_1} is observed, ... for measurand X_N the value x_{N,i_N} is observed

$$p(x_{1,i_1}, \ldots, x_{N,i_N}) = \prod_{\nu=1}^{N} p(x_{\nu,i_\nu})$$

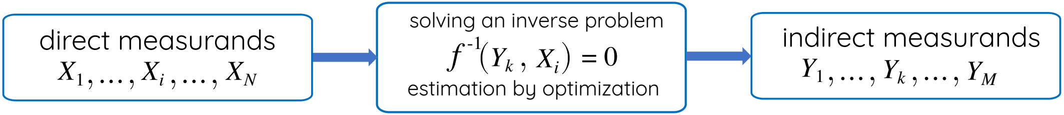
- Model $f(\mathbf{Y}, \mathbf{X}) = 0$: relation indirect measurands $\mathbf{Y}$ – direct measurements $\mathbf{X}$
  - Conditional probability

$$p(\mathbf{Y}|\{x_{1,i_1}, \ldots, x_{N,i_N}\}) = \int_{\mathbf{X}} \delta(f(\mathbf{Y}, \mathbf{X}', \{x_{1,i_1}, \ldots, x_{N,i_N}\})) \prod_{\nu=1}^{N} p_\nu(X'_\nu | x_{\nu,i_\nu})\, \mathrm{d}^N \mathbf{X}'$$

where $\delta(f(Y, \mathbf{X}))$ denotes the Dirac peak, here meaning that the assumption is made that the model itself does not scatter

3 Propagation of measurement uncertainties

3.2 Combination of probability density distributions – Bayes; à priori knowledge; revisions



estimator (= estimated value) y_1 of indirect measurand Y_1, ...
estimator y_M of indirect measurands Y_M
Update estimators of indirect measurands by new measurement campaign κ

$$\left.\begin{array}{c} \underbrace{(x_{1,\kappa}, \ldots, x_{N,\kappa})}_{\text{new observations}} \\[2ex] \underbrace{(y_{1,\kappa-1}, \ldots, y_{M,\kappa-1})}_{\text{previous estimators}} \end{array}\right\} \xrightarrow{\text{solve inverse problem}} \underbrace{(y_{1,\kappa}, \ldots, y_{M,\kappa})}_{\text{revised estimators}}$$

3 Propagation of measurement uncertainties

3.2 Combination of probability density distributions – Bayes; à priori knowledge; revisions

- Conditional probability

$$p(\mathbf{Y}|(x_{1,\kappa},\ldots,x_{N,\kappa}),(y_{1,\kappa-1},\ldots,y_{M,\kappa-1})) = \int_{\mathbf{X}} p_f(f(\mathbf{Y},\mathbf{X}')) \prod_{\nu=1}^{N} p_\nu(\mathbf{X}'|x_{\nu,\kappa}) \prod_{\mu=1}^{M} p_\mu(\mathbf{Y}|y_{\mu,\kappa-1})\, \mathrm{d}^N\mathbf{X}'$$

- $p_f(f(Y,\mathbf{X}))$ is the probability density distribution of the model itself; the model is à priori knowledge, so it is called *model prior*

- $p_\mu(\mathbf{Y}|y_{\mu,\kappa-1})$ for $\mu = 1,\ldots,M$ are the *priors of the indirect measurands*, the probability density distributions of the indirect measurands due to previous knowledge (campaigns)

- $\prod_{\nu=1}^{N} p_\nu(\mathbf{X}|x_{\nu,\kappa})$ is the *likelihood*

- $p(\mathbf{Y}|(x_{1,\kappa},\ldots,x_{N,\kappa}),(y_{1,\kappa-1},\ldots,y_{M,\kappa-1}))$ is denoted *posterior*

3 Propagation of measurement uncertainties

3.2 Combination of probability density distributions – Bayes; à priori knowledge; revisions

- General idea: estimate measurands $\mathbf{X} = (X_1, \ldots, X_N)$ given observations $(x_{1,1}, \ldots, x_{1,J_1}), \ldots, (x_{N,1}, \ldots, x_{N,J_N})$

$$p(\mathbf{X}|(x_{1,1}, \ldots, x_{1,J_1}), \ldots, (x_{N,1}, \ldots, x_{N,J_N}))$$

- without à priori data:
  - Either: estimate measurands $\mathbf{X}$ by maximizing likelihood within one optimization process delivering a covariance matrix, i.e. the uncertainties of the measurands

$$\max_{(X_1,\ldots,X_N)} \{p(\mathbf{X}|(x_{1,1}, \ldots, x_{1,J}), \ldots, (x_{N,1}, \ldots, x_{N,J}))\}$$

  - Or: Determine the conditional probability distribution given the knowledge on the uncertainty of direct measurands by simulation of observations of the direct measurands

1. use experimental observations $(x_{i,1}, \ldots, x_{i,J_i})$ to get an idea of the uncertainty of a direct measurand
2. generate large samples of simulated observations $(x_{i,1}, \ldots, x_{i,K_i})$ with $K_i \gg J_i$
3. calculate the joint probability density distribution by histogramming all values Y_ν for all $\nu = 1, \ldots, K_1 \times K_2 \times \ldots K_N$

$$f(Y_\nu, (x_{1,\nu_1}, \ldots, x_{N,\nu_N})) = 0$$

- together with all information available, also à priori

$$\max_{\mathbf{Y}, u(Y_1),\ldots,u(Y_M)} \{p(\mathbf{Y}, (u(Y_1), \ldots, u(Y_M))|(x_{1,\kappa}, \ldots, x_{N,\kappa}), (y_{1,\kappa-1}, \ldots, y_{M,\kappa-1}), (u(y_{1,\kappa-1}), \ldots, u(y_{M,\kappa-1})))\}$$

4. Guides of the *Joint Committee for Guides in Metrology*

`https://www.bipm.org/en/committees/jc/jcgm/publications`

explizite and univariate: $Y = f(\mathbf{X})$ with **univariate =** one indirect measurand Y

- JCGM 100:2008 (revision of GUM 1995) *Evaluation of measurement data - Guide to the expression of uncertainty in measurement*
  - linear

    $$Y = f(\mathbf{X}) = \sum_{i=1}^{N} c_i X_i$$

    linearizable

    $$Y = f(\mathbf{X}) = f(\mathbf{X})|_{\bar{\mathbf{x}}} + \sum_{i=1}^{N} \underbrace{\left.\frac{\partial f}{\partial X_i}\right|_{\bar{\mathbf{x}}}}_{c_i} \Delta X_i$$

  - random numbers: normal or t-distribution

4. Guides of the *Joint Committee for Guides in Metrology*

- JCGM 101:2008 "GUM-S1" ... *Propagation of distributions using a Monte Carlo method*;
  explicite and implicite, univariate models
  - not easily linearizable
  - no closed analytic representation existent

  simulate $(x_{1,\nu}, \ldots, x_{N,\nu})$ and calculate the joint probability density distribution
  by histogramming values Y_ν for all for all $\nu = 1, \ldots, K_1 \times K_2 \times \ldots K_N$ using the model for the indirect measurand $f(Y_\nu, (x_{1,\nu_i}, \ldots, x_{N,\nu_N})) = 0$
- JCGM 102:2011 "GUM-S2" ... *Extension to any number of output quantities*
  - univariate ($M = 1$, indirect measurand Y) or
    multivariate (several $M > 1$ indirect measurands $\mathbf{Y}$)
  - explicite or implicite
  - analytically or via Monte-Carlo methods
  - incorporation of à priori information (Bayesian methods)
- JCGM GUM 6:2020 ... *Developing and using measurement models*
- JCGM 104:2009 ... *An introduction to the GUM and related documents*
- JCGM 106:2012 ... *The role of measurement uncertainty in conformity assessment*