

# Illustration of three different approaches to estimate measurement uncertainties

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<https://github.com/dhueser/MDA-Vorlesung-iprom-tu-bs>

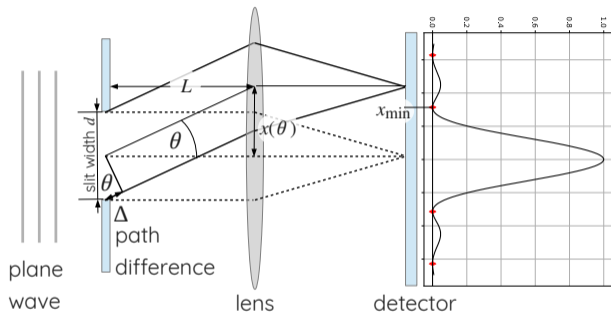
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# Content

1. JCGM 100 – GUM: Uncertainty propagation of explicit, univariate and linearizable models
2. JCGM 101 – GUM-S1: Monte Carlo method - simulation of very large samples of direct measurands histogramming the indirect measurand  $Y_\nu$  using the model  $f(Y_\nu, (x_{1,\nu_1}, \dots, x_{N,\nu_N})) = 0$
3. JCGM 102 – GUM-S2: Bayesian statistics

# 1 JCGM 100 – GUM: explicite, univariate and linearizable models

Example: Fraunhofer diffraction of single slit



direct measurands:

- ▶ distance slit – lens:  $L$
- ▶ wavelength of light:  $\lambda$
- ▶ position of  $x_{\min}$  estimated from
  1. pixel positions:  $x$
  2. gray values:  $g(x)$

slit width  $d$  – coarse model:

$$d \approx \frac{\lambda L}{x_{\min}}$$

uncertainties are assumed to be bell like (Gaussian or t-distributions):

- ▶ uncertainty of  $L$  from set up:  $u(L)$
- ▶ uncertainty of  $\lambda$  due to finite coherence:  $u(\lambda)$
- ▶ uncertainty of  $x_{\min}$  due to pixel noise and pixel sizes:  $u(x_{\min})$

# 1 JCGM 100 – GUM: explicite, univariate and linearizable models

Example: Fraunhofer diffraction of single slit

slit width  $d$  – model equation

$$d \approx \frac{\lambda L}{x_{\min}}$$

combined uncertainty

$$u(d) = \sqrt{(c_L u(L))^2 + (c_\lambda u(\lambda))^2 + (c_{x_{\min}} u(x_{\min}))^2}$$

measurand	estimate	standard uncertainty	sensitivity	$ c u $ in $\mu\text{m}$
$L$ :	$\bar{L} = 4000 \mu\text{m}$	$u(L) = 20 \mu\text{m}$	$c_L = \left. \frac{\partial}{\partial L} d \right _{\bar{L}, \bar{\lambda}, \bar{x}_{\min}} = \frac{\bar{\lambda}}{\bar{x}_{\min}} = 0.0014238$	0.02858
$\lambda$ :	$\bar{\lambda} = 0.550 \mu\text{m}$	$u(\lambda) = 0.002 \mu\text{m}$	$c_\lambda = \left. \frac{\partial}{\partial \lambda} d \right _{\bar{L}, \bar{\lambda}, \bar{x}_{\min}} = \frac{\bar{L}}{\bar{x}_{\min}} = 10.35465$	0.02071
$x_{\min}$ :	$\bar{x}_{\min} = 386.3 \mu\text{m}$	$u(x_{\min}) = 5.9 \mu\text{m}$	$c_{x_{\min}} = \left. \frac{\partial}{\partial x_{\min}} d \right _{\bar{L}, \bar{\lambda}, \bar{x}_{\min}} = -\frac{\bar{\lambda} \bar{L}}{\bar{x}_{\min}^2} = -0.01474257$	0.08698

$$\hookrightarrow \bar{d} \approx \frac{\bar{\lambda} \bar{L}}{\bar{x}_{\min}} = 5.695 \mu\text{m}$$

$$u(d) = 0.094 \mu\text{m}$$

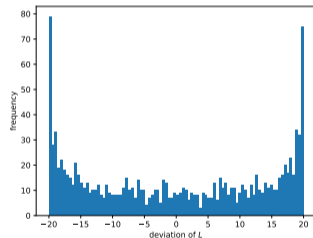
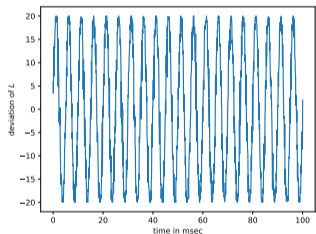
$$d = (5.695 \pm 0.187) \mu\text{m for } k = 2$$

## 2 JCGM 101 – GUM-S1: Monte Carlo method

Example: Fraunhofer diffraction of single slit

may be life of an experimentalist is not so easy ...

- ▶ how to proceed if the distribution of distance  $L$  between slit and lens is not bell shaped, but U-shaped due to vibrations?



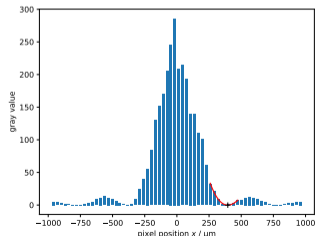
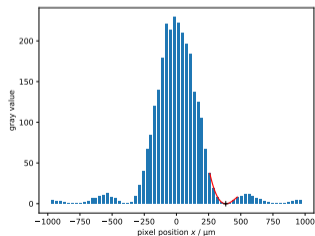
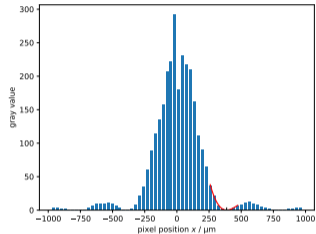
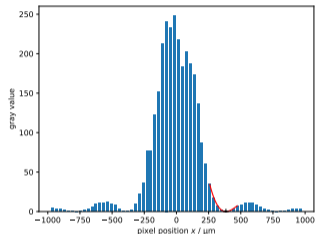
this distribution is not at all Gaussian

- ▶ which are the influences on the uncertainty of  $x_{\min}$ ?

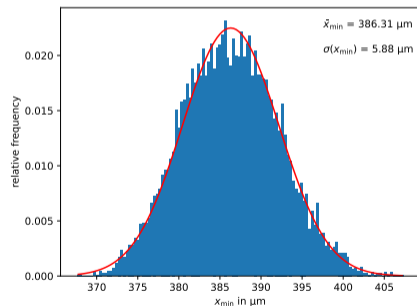
## 2 JCGM 101 – GUM-S1: Monte Carlo method

Example: Fraunhofer diffraction of single slit

may be life of an experimentalist is not so easy ... influences on the uncertainty of  $x_{\min}$ ?



- ▶ pixel noise
- ▶ pixel size precision



this distribution is not quite Gaussian

## 2 JCGM 101 – GUM-S1: Monte Carlo method

Example: Fraunhofer diffraction of single slit

may be life of an experimentalist is not so easy ... influences on the uncertainty of  $\lambda$ ?

this distribution is very much a Gaussian - lucky

Gaussian spectrum of a not ideally monochromatic light source

$$S(k) = \frac{1}{2\sqrt{\pi} \Delta k} e^{-\left(\frac{k-k_0}{2\Delta k}\right)^2}$$

where  $k$  is the wave number  $k = \frac{2\pi}{\lambda}$ ;  $k_0 = \frac{2\pi}{\lambda_0}$

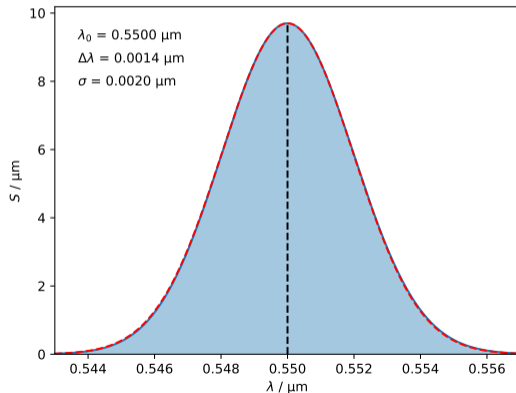
$$\Delta k = \frac{2\pi}{\lambda_0} \Delta \lambda$$

$$S(\lambda) = \frac{\lambda_0^2}{4\sqrt{\pi}^3 \Delta \lambda} e^{-\left(\frac{(\lambda_0-\lambda)\lambda_0}{2\lambda \Delta \lambda}\right)^2}$$

$\lambda_0 = 0.5500 \mu\text{m}$  und  $\Delta \lambda = 0.0014 \mu\text{m}$

$$S(\lambda) \approx a e^{-\frac{1}{2} \left(\frac{\lambda_0-\lambda}{\sigma}\right)^2}$$

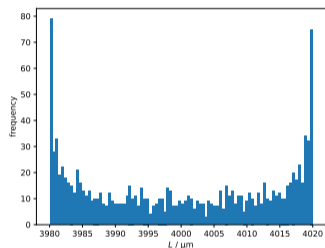
$\sigma = 0.0020 \mu\text{m}$



## 2 JCGM 101 – GUM-S1: Monte Carlo method

Example: Fraunhofer diffraction of single slit

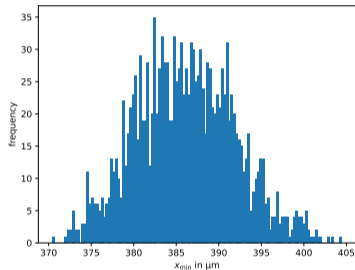
use random number generator and probability densities  $p$  to generate synthetic data samples



$p_L : L \mapsto p_L(L|\bar{L}, a_L)$  with  
 $\bar{L} = 4000 \mu\text{m}$  and  $a_L = 20 \mu\text{m}$

$$\{L_1, \dots, L_{i_L}, \dots, L_{N_L}\}$$

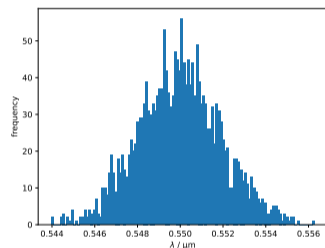
here  $N_L = 1200$



$p_{x_{\min}} : x_{\min} \mapsto p_{x_{\min}}(x_{\min}|g_{i_{x_{\min}}}(x_j), x_j)$   
 $j$ : pixel index,  $g_{i_{x_{\min}}}(x_j)$ : gray values

$$\{x_{\min,1}, \dots, x_{\min,i_x}, \dots, x_{\min,N_x}\}$$

here  $N_x = 1500$



$p_\lambda : \lambda \mapsto p_\lambda(\lambda|\lambda_0, \Delta\lambda)$  with  
 $\lambda_0 = 0.5500 \mu\text{m}$ ;  $\Delta\lambda = 0.0014 \mu\text{m}$

$$\{\lambda_1, \dots, \lambda_{i_\lambda}, \dots, \lambda_{N_\lambda}\}$$

here  $N_\lambda = 2000$



## 2 JCGM 101 – GUM-S1: Monte Carlo method

Example: Fraunhofer diffraction of single slit

- ▶ generate synthetic data samples

$$\{L_1, \dots, L_{i_L}, \dots, L_{N_L}\} \quad \text{and} \quad \{x_{\min,1}, \dots, x_{\min,i_x}, \dots, x_{\min,N_x}\} \quad \text{and} \quad \{\lambda_1, \dots, \lambda_{i_\lambda}, \dots, \lambda_{N_\lambda}\}$$

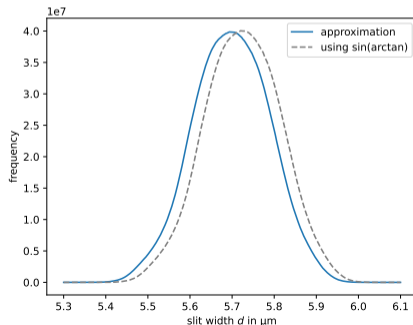
- ▶ calculate  $N_L \times N_x \times N_\lambda$  slit width values using the model

$$d_{i_L, i_x, i_\lambda} = \frac{\lambda_{i_\lambda} L_{i_L}}{x_{\min, i_x}} \quad \text{resp.} \quad d_{i_L, i_x, i_\lambda} = \frac{\lambda_{i_\lambda}}{\sin\left(\arctan\left(\frac{x_{\min, i_x}}{L_{i_L}}\right)\right)}$$

histogramm  $h : d_k \mapsto h(d_k)$  where  $d_k$  are the bins  $k = 1, \dots, N_{\text{bin}}$   
here  $N_{\text{bin}} = 300$

$$\bar{d} = \frac{1}{N_{\text{tot}}} \sum_{k=1}^{N_{\text{bin}}} d_k h(d_k) \quad \text{for} \quad N_{\text{tot}} = \sum_{k=1}^{N_{\text{bin}}} h(d_k)$$

$$\text{and} \quad \sigma(d) = \sqrt{\frac{1}{N_{\text{tot}} - 1} \sum_{k=1}^{N_{\text{bin}}} (d_k - \bar{d})^2 h(d_k)}$$



## 2 JCGM 101 – GUM-S1: Monte Carlo method

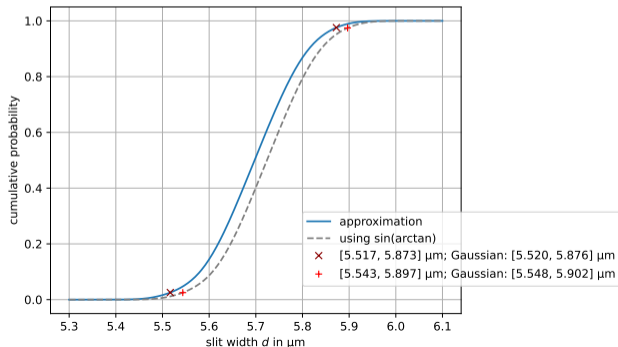
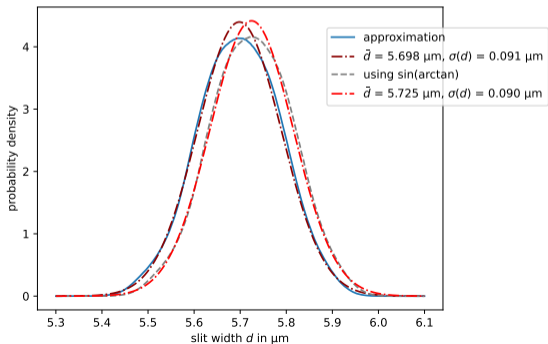
Example: Fraunhofer diffraction of single slit

probability density of indirect measurand slit width  $d$ :  $p_d: d \mapsto p_d(d)$

$$p_d(d) \propto \int dL \int d\lambda \int dx_{\min} \delta(d - f(L, \lambda, x_{\min})) p_L(L|\bar{L}, a_L) p_{x_{\min}}(x_{\min}|g_{i_{x_{\min}}}(x_j), x_j) p_\lambda(\lambda|\lambda_0, \Delta\lambda)$$

measurement result:

- ▶ estimate of the measurand  $d$ :  $\bar{d} = \int d p(d) dd$
- ▶ and its uncertainty interval for 95% confidence level



### 3 JCGM 102 – GUM-S2: Bayesian statistics

- ▶ probability density of indirect measurand slit width  $d$ :  $p_d: d \mapsto p_d(d)$

$$p_d(d) \propto \int dL \int d\lambda \int dx_{\min} \delta(d - f(L, \lambda, x_{\min})) p_L(L|\bar{L}, a_L) p_{x_{\min}}(x_{\min}|g_{i_{x_{\min}}}(x_j), x_j) p_\lambda(\lambda|\lambda_0, \Delta\lambda)$$

- ▶ the Dirac distribution  $\delta(d - f(L, \lambda, x_{\min}))$  means that for each tuple  $(L_{i_L}, \lambda_{i_\lambda}, x_{\min, i_x})$  the model function  $f(L, \lambda, x_{\min})$ 
  - ▶ is directly used
  - ▶ no uncertainty is assigned to the model itself
  - ▶ all uncertainty has its origin in the uncertainties of the direct measurands  $L$ ,  $\lambda$ , and  $x_{\min}$
- ▶ using a model means incorporating à priori knowledge, therefore the peak shaped (infinitely thin) distribution  $\delta(d - f(L, \lambda, x_{\min}))$  is a prior probability density distribution
- ▶ in Bayesian statistics, the model prior is a probability density distribution of finite width:  
 $p_f: (d, L, \lambda, x_{\min}) \mapsto p_f(d, L, \lambda, x_{\min})$
- ▶ furthermore Bayesian statistics allows for incorporating à priori knowledge of the indirect measurand:  
 $p_d: d \mapsto p_d(d|\bar{d}_0, \sigma_{d,0})$  respectively  $p_d(d|\bar{d}_0)p_\sigma(\sigma(d)|\sigma_{d,0})$

### 3 JCGM 102 – GUM-S2: Bayesian statistics

- ▶ probability density of indirect measurand slit width  $d$ :  $p_d: d \mapsto p_d(d)$  for sharp model prior

$$p_d(d) \propto \int dL \int d\lambda \int dx_{\min} \delta(d - f(L, \lambda, x_{\min})) p_L(L|\bar{L}, a_L) p_{x_{\min}}(x_{\min}|g_{i_{x_{\min}}}(x_j), x_j) p_\lambda(\lambda|\lambda_0, \Delta\lambda)$$

- ▶ using a model means incorporating à priori knowledge, therefore the peak shaped (infinitely thin) distribution  $\delta(d - f(L, \lambda, x_{\min}))$  is a prior probability density distribution
- ▶ in Bayesian statistics, the model prior is a probability density distribution of finite width:  
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- ▶ furthermore Bayesian statistics allows for incorporating à priori knowledge of the indirect measurand:  
 $p_d: d \mapsto p_d(d|\bar{d}_0, \sigma_{d,0})$  respectively  $p_d(d|\bar{d}_0) p_\sigma(\sigma(d)|\sigma_{d,0})$
- ▶ probability density of indirect measurand slit width  $d$ :  $p_d: d \mapsto p_d(d)$  for model prior  $p_f(d, L, \lambda, x_{\min})$  and prior  $p_d(d|\bar{d}_0) p_\sigma(\sigma(d)|\sigma_{d,0})$

$$p_d(d) \propto \int dL \int d\lambda \int dx_{\min}$$

$$p_f(d, L, \lambda, x_{\min}) p_d(d|\bar{d}_0) p_\sigma(\sigma(d)|\sigma_{d,0}) p_\lambda(\lambda|\lambda_0, \Delta\lambda) p_L(L|\{\dots, L_k, \dots\}) p_{x_{\min}}(x_{\min}|\{\dots, g_i(\{\dots, x_j, \dots\}), \dots\})$$

$L_k$  and  $g_i$ : currently measured;  $\lambda_0, \Delta\lambda$ : obtained previously when initially setting up the experiment

### 3 JCGM 102 – GUM-S2: Bayesian statistics

- ▶ since  $\lambda_0, \Delta\lambda$  were obtained previously when initially setting up the instrument, they are also priors
- ▶  $L_k$  and  $g_i$  are currently measured observations
- ▶ their probability density distributions are referred to as likelihoods

$$p_d(d|\dots) \propto \int dL \int d\lambda \int dx_{\min}$$

$$\underbrace{p_f(d, L, \lambda, x_{\min}) p_d(d|\bar{d}_0) p_\sigma(\sigma(d)|\sigma_{d,0}) p_\lambda(\lambda|\lambda_0, \Delta\lambda)}_{\text{prior distributions}} \underbrace{p_L(L|\{\dots, L_k, \dots\}) p_{x_{\min}}(x_{\min}|\{\dots, g_i(\{\dots, x_j, \dots\}), \dots\})}_{\text{likelihoods}}$$

- ▶ the resultant probability density distribution  $p_d(d|\dots)$  is called posterior
- ▶ now, consider a less complex example with two direct measurands, one currently measured, the other as à priori knowledge

### 3 JCGM 102 – GUM-S2: Bayesian statistics

Example: measurand with calibration factor

- ▶ indirect measurand: some physical quantity  $Y$  with some physical unit, denote it with the German word for unit: “Einheit” E
- ▶ direct measurand  $X_M$ : raw signal as voltage  $U$ , physical unit Volt V
- ▶ direct measurand  $X_K$ : the calibration factor  $K$  with unit  $\frac{E}{V}$
- ▶ model

$$Y = f(X_K, X_M) = X_K X_M$$

### 3 JCGM 102 – GUM-S2: Bayesian statistics

Example: measurand with calibration factor

- ▶ Sample of observations of raw voltage signal with sample size  $J_M = 9$ :

$X_M/V$	479.58	526.47	516.77	522.01	506.61	497.99	481.71	484.90	491.41
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- ▶ calibration factor  $X_K$

$$X_K = (K_0 \pm U_K) \frac{E}{V} = (0.0925 \pm 0.0180) \frac{E}{V} \quad \text{mit} \quad k = 2 \quad \text{und} \quad \nu_K = 45$$

$k = 2$  rounded value of  $t$  quantile ( $k = 2.0141$ ) for 95 % confidence level  
with  $\nu_K = 45$  degrees of freedom

### 3 JCGM 102 – GUM-S2: Bayesian statistics

Example: measurand with calibration factor

mean and empirical standard deviation from sample of direct measurand  $X_M$ :

$$\bar{x}_M = \frac{1}{9} \sum_{j=1}^9 X_{M,j} = 500.83 \text{ V}$$

$$s_M = \sqrt{\frac{1}{\nu_M} \sum_{j=1}^9 (X_{M,j} - \bar{x}_M)^2} = 17.8927 \text{ V} \approx 17.89 \text{ V}$$

with  $\nu_M = 8$  degrees of freedom



### 3 JCGM 102 – GUM-S2: Bayesian statistics

Example: measurand with calibration factor

▶  $s_{KM} = K_0 s_M = 0.0925 \frac{\text{E}}{\text{V}} \cdot 17.8927 \text{ V} = 1.655 \text{ E}$

▶  $s_K = \frac{U_K}{2} = 0.0090$

▶  $\sigma_f = 0.003 \cdot s_{KM} = 0.00497$

▶ coverage interval for 95% confidence level:

▶ t-quantile for 52 d.o.f.:  $k = 2.306$

▶ then coverage interval: [36.691 E, 55.962 E]

task: use Bayesian method to determine

▶ the expectation value (estimate of measurand) and

▶ the coverage interval 95% credibility from posterior

$$\underbrace{p(Y, X_K, X_M | (X_{M,1}, \dots, X_{M,J}), K_0, s_K)}_{\text{posterior}} \propto \underbrace{e^{-\frac{1}{2} \left( \frac{Y - X_K X_M}{\sigma_f} \right)^2}}_{\text{model prior}} \underbrace{e^{-\frac{1}{2} \left( \frac{X_K - K_0}{s_K} \right)^2}}_{\text{prior calib.}} \underbrace{\prod_{j=1}^J e^{-\frac{1}{2} \left( \frac{X_M - X_{M,j}}{s_M} \right)^2}}_{\text{likelihood}}$$

marginal distribution:

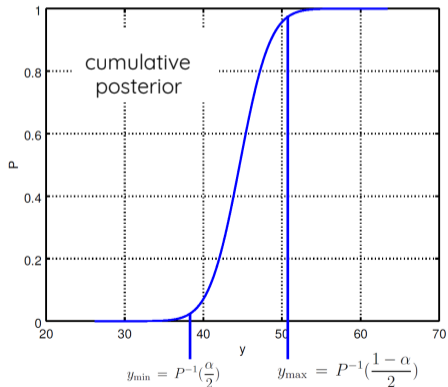
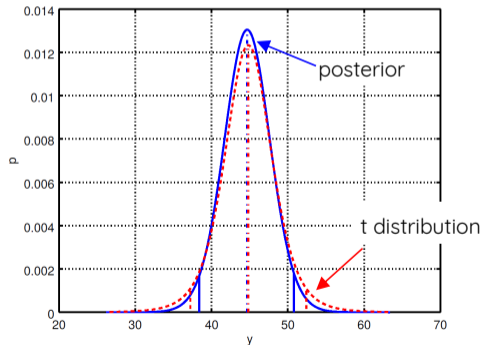
$$\underbrace{p(Y | (X_{M,1}, \dots, X_{M,J}), K_0, s_K)}_{\text{posterior}} \propto \int dX_M \int dX_K \underbrace{e^{-\frac{1}{2} \left( \frac{Y - X_K X_M}{\sigma_f} \right)^2}}_{\text{model prior}} \underbrace{e^{-\frac{1}{2} \left( \frac{X_K - K_0}{s_K} \right)^2}}_{\text{prior calib.}} \underbrace{\prod_{j=1}^J e^{-\frac{1}{2} \left( \frac{X_M - X_{M,j}}{s_M} \right)^2}}_{\text{likelihood}}$$

### 3 JCGM 102 – GUM-S2: Bayesian statistics

Example: measurand with calibration factor

task: from posterior distribution determine

- ▶ expectation value (estimate of measurand) and
- ▶ the coverage interval 95% credibility



### 3 JCGM 102 – GUM-S2: Bayesian statistics

Example: measurand with calibration factor

- ▶ normalize posterior
- ▶ marginal distribution

$$p(Y|(X_{M,1}, \dots, X_{M,J}), K_0, s_K) = \frac{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\frac{1}{2} \left( \frac{Y - X_K X_M}{\sigma_f} \right)^2} e^{-\frac{1}{2} \left( \frac{X_K - K_0}{s_K} \right)^2} \prod_{j=1}^J e^{-\frac{1}{2} \left( \frac{X_M - X_{M,j}}{s_M} \right)^2} dX_M dX_K}{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\frac{1}{2} \left( \frac{Y - X_K X_M}{\sigma_f} \right)^2} e^{-\frac{1}{2} \left( \frac{X_K - K_0}{s_K} \right)^2} \prod_{j=1}^J e^{-\frac{1}{2} \left( \frac{X_M - X_{M,j}}{s_M} \right)^2} dX_M dX_K dY}$$

### 3 JCGM 102 – GUM-S2: Bayesian statistics

Example: measurand with calibration factor

estimate  $\bar{y}$  – expectation value of the posterior

$$\bar{y} = \int_{-\infty}^{\infty} Y p(Y|(X_{M,1}, \dots, X_{M,J}), K_0, s_K) dY = 46.278 \text{ E}$$

cumulative posterior to obtain coverage interval  $[y_1, y_2]$

$$P(Y) = \int_{-\infty}^Y p(Y'| (X_{M,1}, \dots, X_{M,J}), K_0, s_K) dY'$$

for a probability of 95% (credibility)

$$P(y_1) = 0.025 \Leftrightarrow y_1 = P^{-1}(0.025) = 36.855 \text{ E}$$

$$P(y_2) = 0.975 \Leftrightarrow y_2 = P^{-1}(0.975) = 56.185 \text{ E thus } [\bar{y} - 9.423, \bar{y} + 9.907] \text{ E}$$

### 3 JCGM 102 – GUM-S2: Bayesian statistics vs. JCGM 100 – GUM

Example: measurand with calibration factor

- ▶ expectation value from classical method:  
product of  $\bar{x}_M = 500.83 \text{ V}$  and  $K_0 = 0.0925 \frac{\text{E}}{\text{V}}$

$$\bar{y} = K_0 \bar{x}_M = 46.327 \text{ E}$$

- ▶ Bayesian result  $\bar{y} = 46.278 \text{ E}$
- ▶ difference  $0.049 \text{ E}$  – it is one promille

### 3 JCGM 102 – GUM-S2: Bayesian statistics vs. JCGM 100 – GUM

Example: measurand with calibration factor

- uncertainty due to propagation according to GUM JCGM 100 (no correlation  $\rho_{M,K} = 0$ )

$$u^2(Y) = \left( \frac{\partial}{\partial X_M} X_M X_K \right)_{\bar{x}_{M,K_0}}^2 s_M^2 + \left( \frac{\partial}{\partial X_K} X_M X_K \right)_{\bar{x}_{M,K_0}}^2 s_K^2$$

$$u(Y) = \sqrt{K_0^2 s_M^2 + \bar{x}_M^2 s_K^2} = 4.802 \text{ E}$$

### 3 JCGM 102 – GUM-S2: Bayesian statistics vs. JCGM 100 – GUM

Example: measurand with calibration factor

- ▶ number of degrees of freedom from Satterthwaite's equation

$$\frac{u(Y)^4}{\nu_y} = \frac{K_0^4 s_M^4}{\nu_M} + \frac{\bar{x}_M^4 s_K^4}{\nu_K}$$

mit  $\nu_K = 45$ ,  $\nu_M = 8$ ,  $K_0 = 0.0925 \frac{\text{E}}{\text{V}}$ ,  $s_K = 0.009 \frac{\text{E}}{\text{V}}$ ,  $\bar{x}_M = 500.83 \text{ V}$ ,  $s_M = 17.89 \text{ V}$

$$\nu_y = u(Y)^4 \left( \frac{K_0^4 s_M^4}{\nu_M} + \frac{\bar{x}_M^4 s_K^4}{\nu_K} \right)^{-1} = 52.58 \approx 52$$

$$\nu_y = \left\lfloor u(Y)^4 \left( \sum_{i=1}^N \frac{(c_i s_i)^4}{\nu_i} \right)^{-1} \right\rfloor$$

### 3 JCGM 102 – GUM-S2: Bayesian statistics vs. JCGM 100 – GUM

Example: measurand with calibration factor compared with JCGM 100 – GUM

Confidence interval

[36.691 E, 55.962 E]

Credible interval

[36.855 E, 56.185 E]

Measurement result

$$Y = (46.327 \pm 9.635) E \quad Y = (46.278 - 9.423 + 9.907) E$$



### 3 JCGM 102 – GUM-S2: Bayesian statistics vs. JCGM 100 – GUM

The different concepts

