Physikalisch-Technische Bundesanstalt
Braunschweig und Berlin
Nationales Metrologieinstitut

Rejection sampling for Bayesian uncertainty evaluation using the Monte Carlo techniques of GUM-S1

M. Marschall, G. Wübbeler and C. Elster

The underlying question

Can we perform informative Bayesian uncertainty evaluation within the framework of GUM-Supplement 1?

First message

The Type-A uncertainty evaluation in GUM-S1 is equivalent to a Bayesian procedure with a specific non-informative prior.

C. Elster and B. Toman, “Bayesian uncertainty analysis under prior ignorance of the measurand versus analysis using the supplement 1 to the guide: a comparison,” ***Metrologia*** *2009.*

I. Lira and D. Grientschnig, “Equivalence of alternative Bayesian procedures for evaluating measurement uncertainty,” ***Metrologia****, 2010.*

O. Bodnar, G. Wübbeler, and C. Elster, “On the application of Supplement 1 to the GUM to non-linear problems,” ***Metrologia****, 2011.*

A. Forbes and J. Sousa, “The GUM, Bayesian inference and the observation and measurement equations,” ***Measurement****, 2011.*

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Replacement of the non-informative prior with an informative prior within the Type-A procedure does not preserve this equivalence.

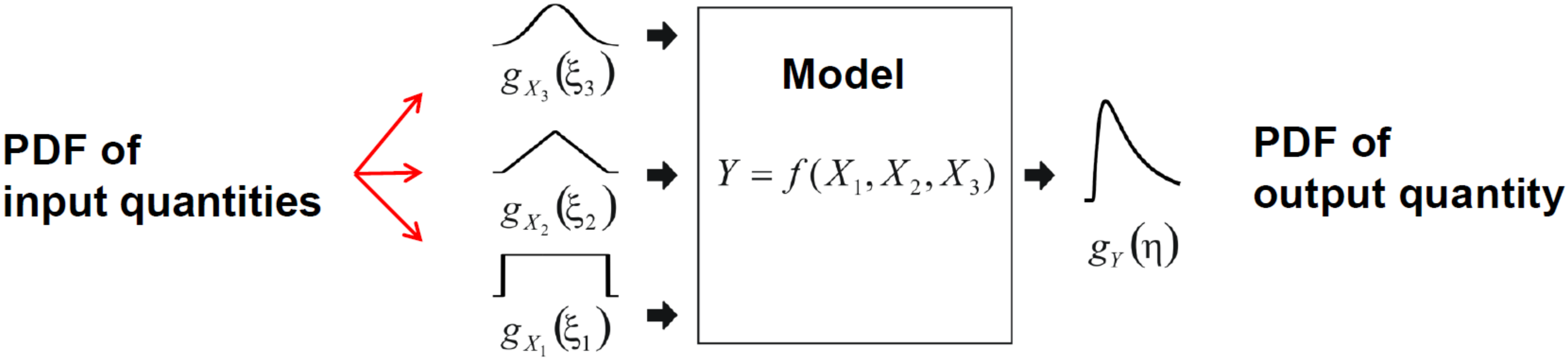
Marschall, M., Wübbeler, G., and Elster, C, “Rejection sampling for Bayesian uncertainty evaluation using the Monte Carlo techniques of GUM-S1,” ***Metrologia****, 2021*

Second message

The tools provided by GUM-S1 enable a fully informative Bayesian uncertainty evaluation.

Marschall, M., Wübbeler, G., and Elster, C, “Rejection sampling for Bayesian uncertainty evaluation using the Monte Carlo techniques of GUM-S1,” ***Metrologia***, *2021*

Link to software repository: https://gitlab1.ptb.de/marsch02/gums1-rejection-sampler



Degree-of-belief distributions assigned to input quantities

+

Monte Carlo sampling to obtain output PDF

First message

Replacement of the non-informative prior with an informative prior within the Type-A procedure does not preserve the equivalence to an informative Bayesian procedure.

Naive informative GUM-S1

Replacing the non-informative prior for X with the informative prior induced by the knowledge about Y.

$$\left(1 + \frac{u(z_0)^2}{u(y_0)^2}\right) < \frac{u_{naive}(y)^2}{u_{Bayes}(y)^2} < \left(1 + 2\frac{u(z_0)^2}{u(y_0)^2}\right)$$

Uncertainty ratio can become arbitrary large!

- Linear measurement model $Y = X + Z$
- X indication quantity with single recording x_1 drawn from $N(X, \sigma^2)$
- Z type-B with assigned PDF of $N(z_0, u(z_0)^2)$
- Y measurand with prior knowledge PDF of $N(y_0, u(y_0)^2)$

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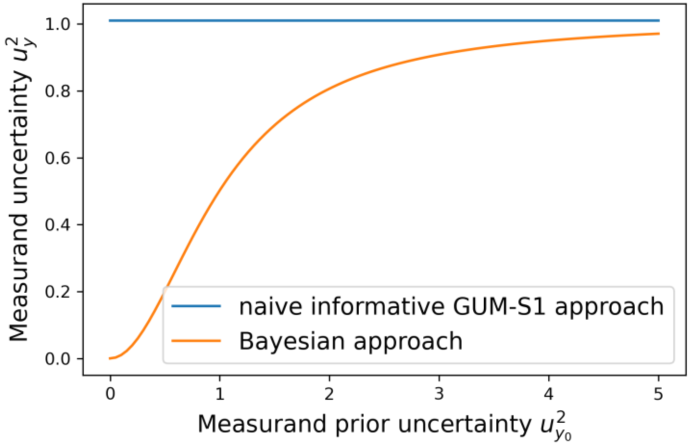

- Linear measurement model $Y = X + Z$
- X indication quantity with single recording x_1 drawn from $N(X, \sigma^2)$ $\sigma = 0.1$
- Z type-B with assigned PDF of $N(z_0, u(z_0)^2)$ $z_0 = 1, u(z_0)^2 = 1$
- Y measurand with prior knowledge PDF of $N(y_0, u(y_0)^2)$ $y_0 = 1$

Naive informative GUM-S1

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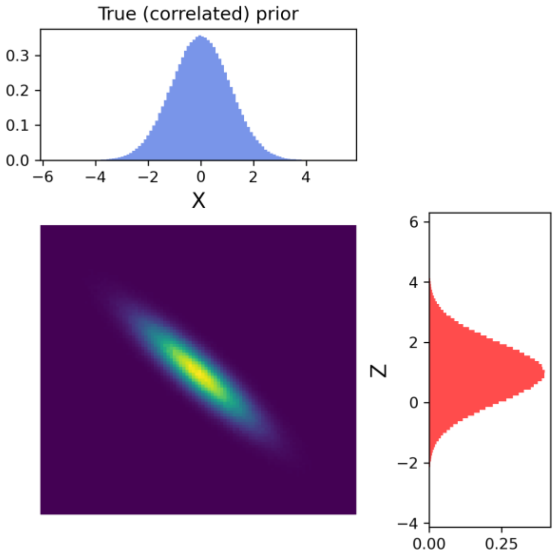
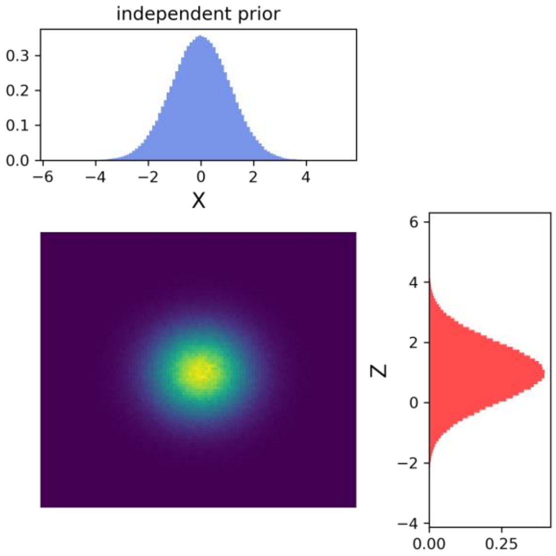


True joint prior PDF induced by prior knowledge of Y



Joint prior PDF assigned by naive informative GUM-S1

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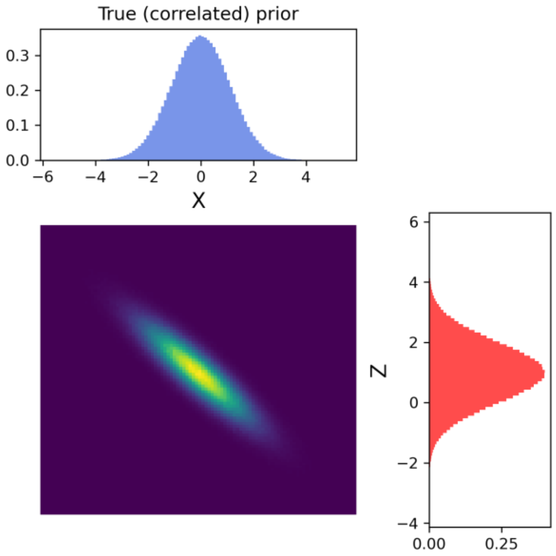
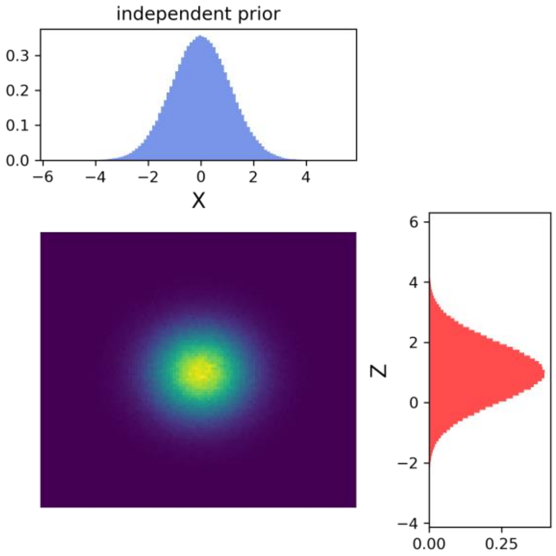


True joint prior PDF induced by prior knowledge of Y

X and Z are *a priori* dependent.

Taking an independent PDF for X is not appropriate.



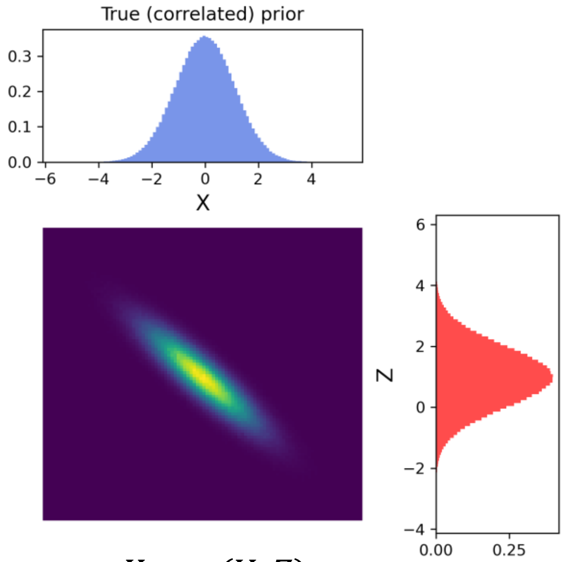
Joint prior PDF assigned by naive informative GUM-S1

Second message

The tools provided by GUM-S1 enable a fully informative Bayesian uncertainty evaluation.

Can we do better and fully Bayesian?

1. Generate samples from joint prior (GUM-S1 for observation equation)



$$X = g(Y, Z)$$

Can we do better and fully Bayesian?

1. Generate samples from joint prior (GUM-S1 for observation equation)
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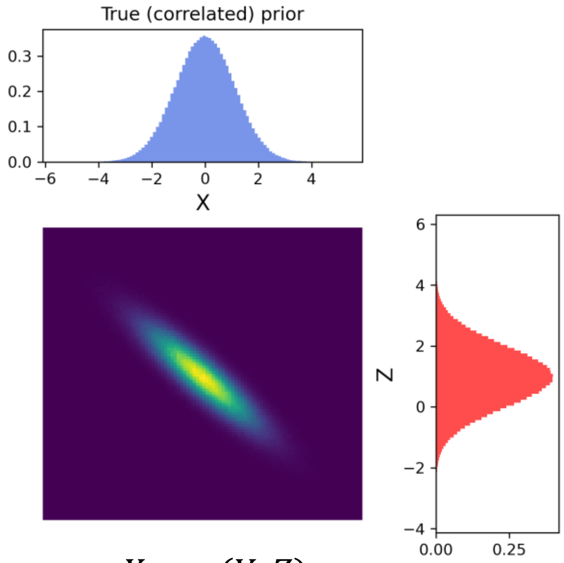

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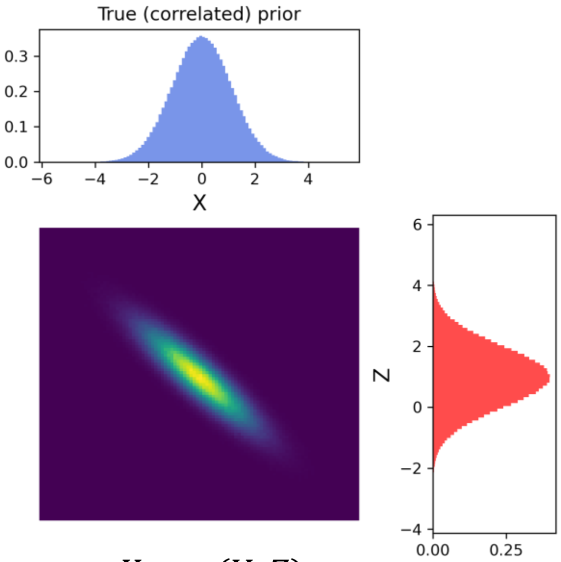

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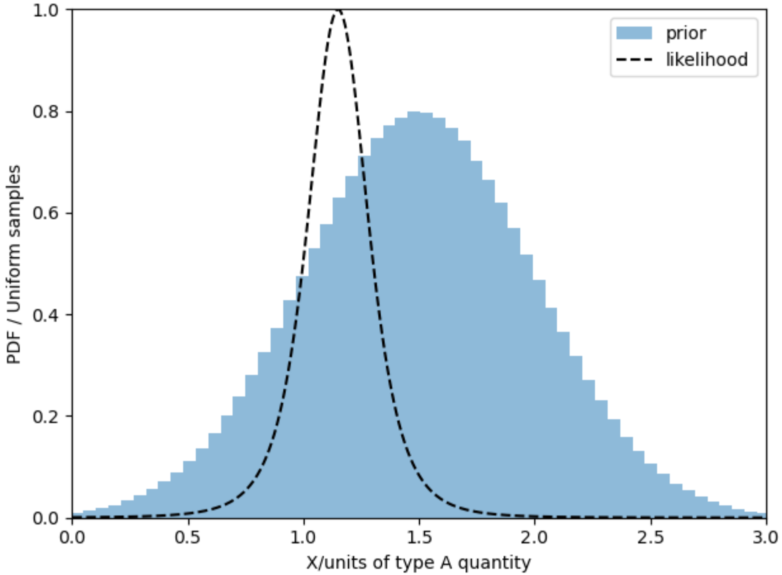

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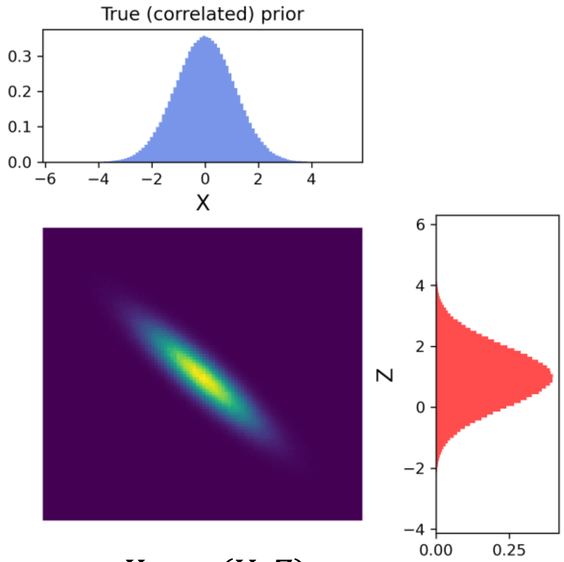

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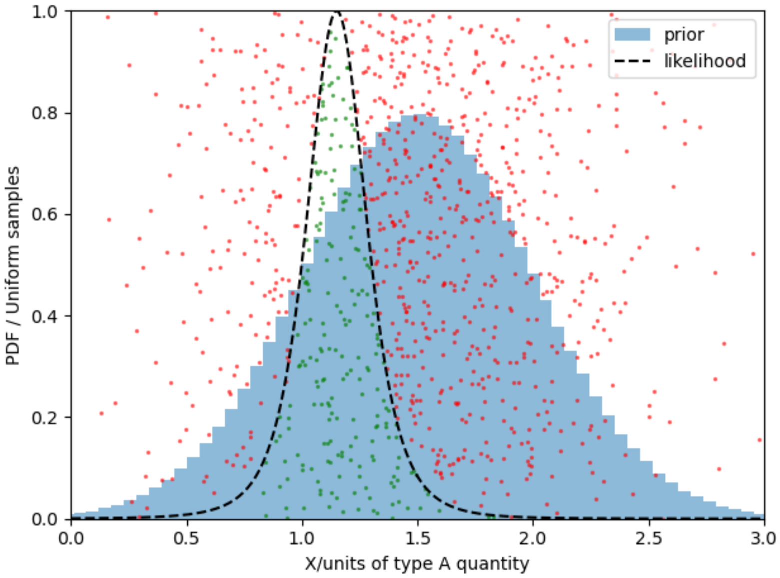

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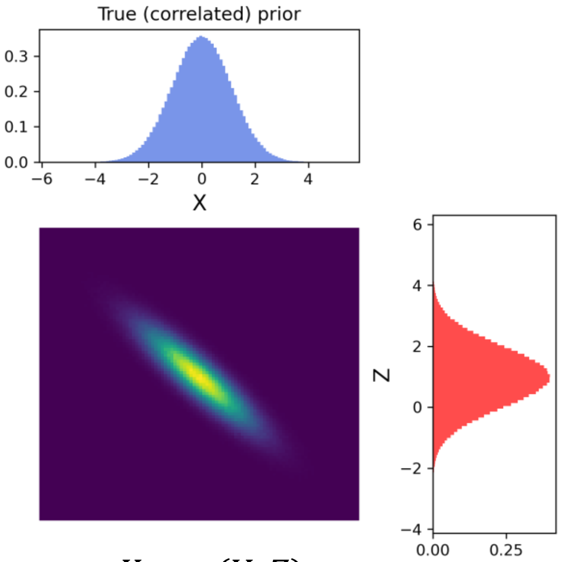

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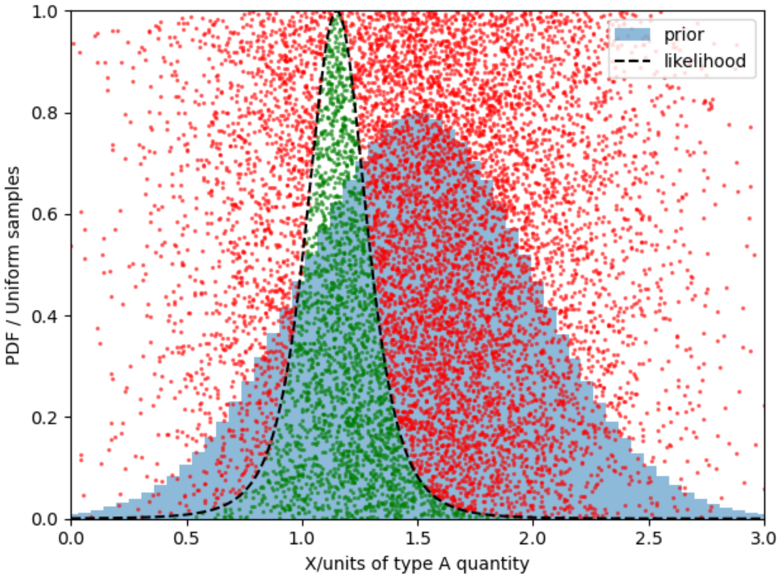

Rejection sampling for metrological relevant applications

- Fast and easy to implement
- Provably convergent sampling scheme
- Generates i.i.d. samples from posterior (without MCMC sampling)

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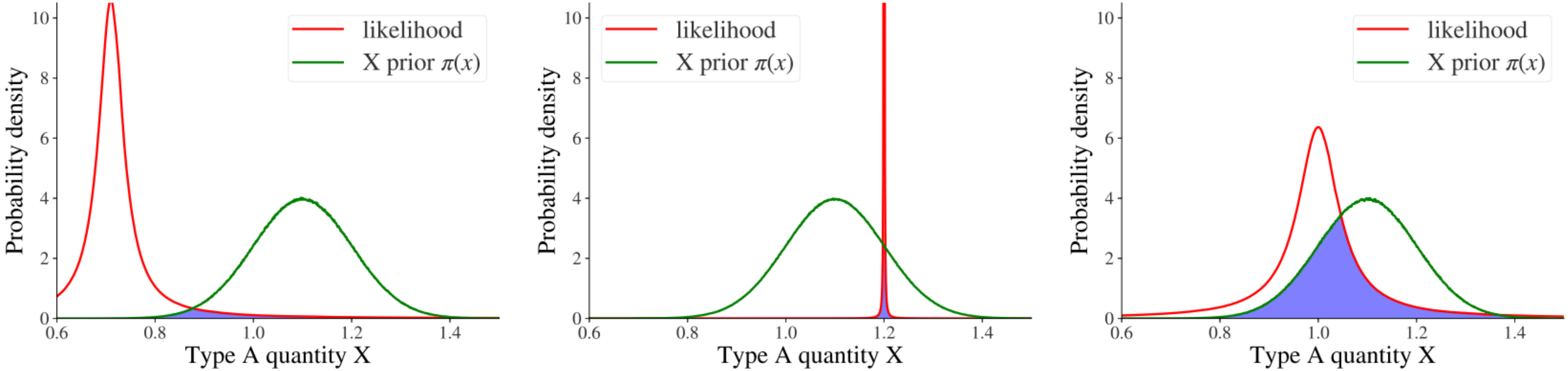

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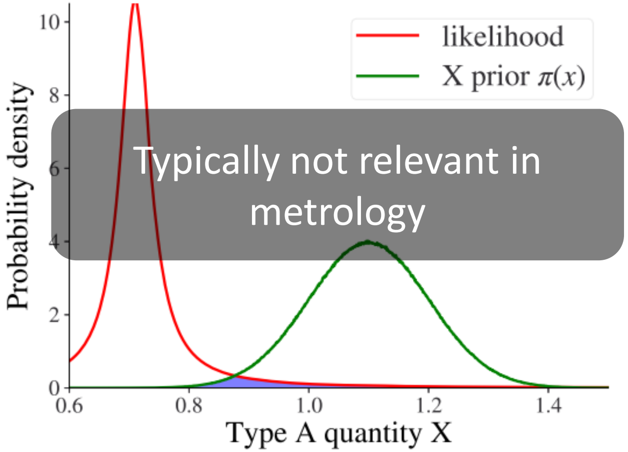
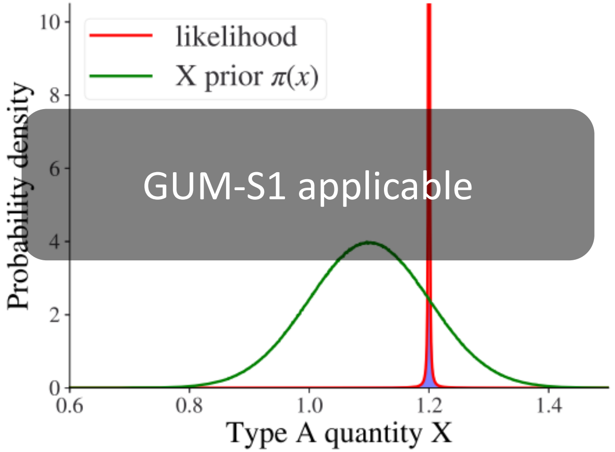
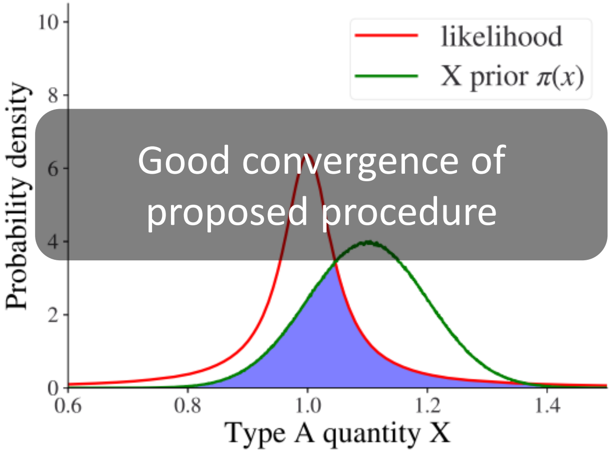
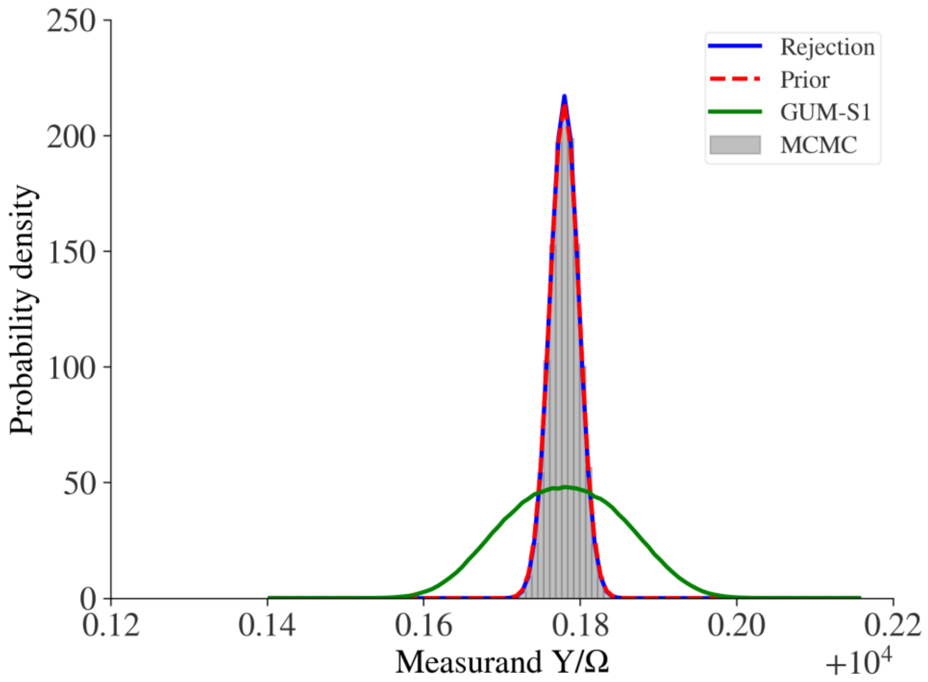






Example: calibration of a standard resistor

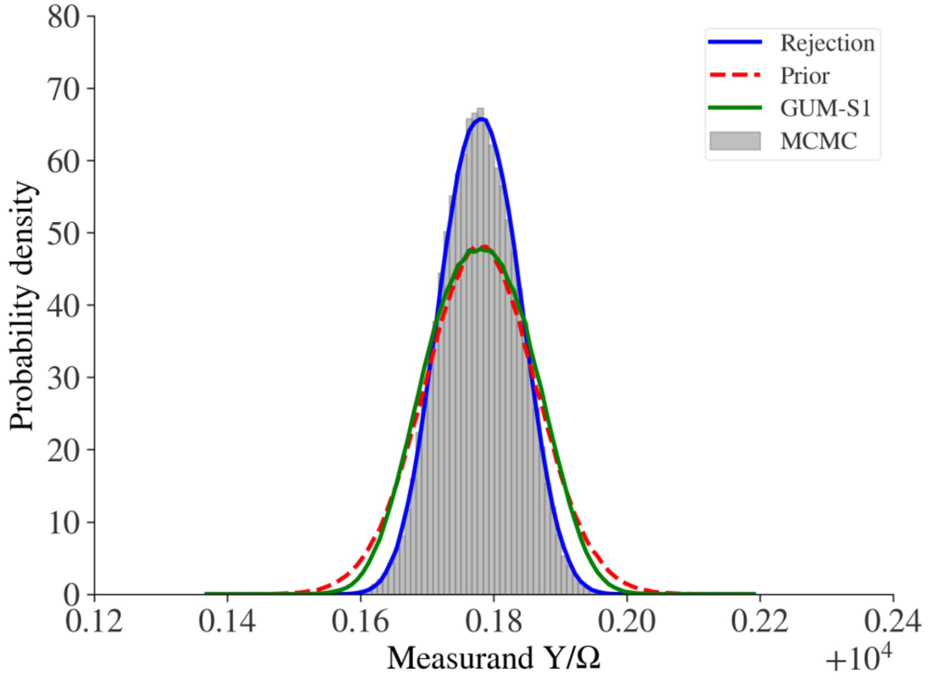


Prior dominates posterior

Observed acceptance rate: 9.1%

EA-04/02 M: 2013, Example S3 modified by artificial prior knowledge about the measurand

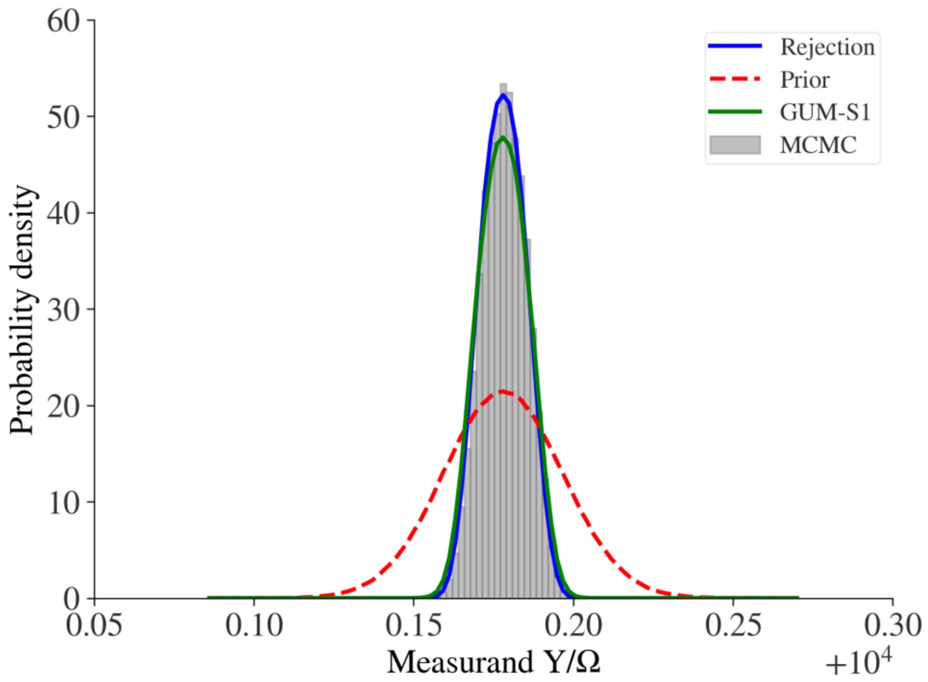
Example: calibration of a standard resistor



Observed acceptance rate: 6.7%

EA-04/02 M: 2013, Example S3 modified by artificial prior knowledge about the measurand

Example: calibration of a standard resistor



Data dominates posterior

Observed acceptance rate: 3.7%

EA-04/02 M: 2013, Example S3 modified by artificial prior knowledge about the measurand

Example: calibration of a standard resistor

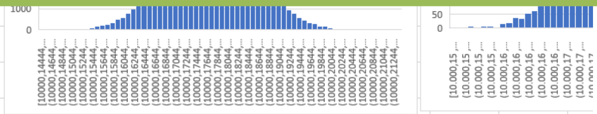
As described in the article, the measurement model reads

$$Y = (R_S + \delta R_D + \delta R_{TS}) r_C X \; - \delta R_{TX}.$$

The corresponding type-B distributions of the input parameter can be found in Table 2. of the manuscript. Samples according to the independent distributions, together with the recordings for the type-A quantity X are given below.

Drawing samples can be done for example using Matlab© or Python. Alternatively, platforms like the NIST Uncertainty Machine https://uncertainty.nist.gov/ can easily generate the sample lists below.

Informative Bayesian uncertainty evaluation in a spreadsheet



Row I collects the recordings/observations of the type-A quantity X

Row N to L computes the number of observations, the mean and standard deviation of the recordings

Row M implements the unnormalized likelihood function, cf. Equation (4) of the manuscript

Row N then applies the rejection by simply ignoring samples that do not meet the requirement $row\ G_i < row\ M_i \Leftrightarrow u_i < \ell_i$

Row O repeats row A but replaces every not-accepted samples with a #NV (no-value) to allow easy plotting of the posterior of Y

Y	RS	dRD	dRTX	dRTS	rC	uniform sample	X prior	recordings of X	N	xbar	s	likelihood	Accepted?	Y - Posterior samples
10000,18938	10000,05196	0,015752933	-0,00515313	0,002164417	1,000001893	0,530407232	1,000009542	1,0000104	5	1,0000105	1,58114E-07	0,073787287	0	#NV
10000,17331	10000,05298	0,020892988	0,005315236	-0,002347245	1,0000043	0,037437183	1,00000641	1,0000107				0,000143419	0	#NV
10000,18101	10000,04847	0,011941781	-0,001781145	0,001186094	0,999992853	0,580359894	1,000018912	1,0000106				4,12487E-06	0	#NV
10000,18325	10000,05096	0,021752049	0,000991231	0,000323266	1,000001237	0,34235587	1,000009883	1,0000103				0,242917154	0	#NV
10000,18136	10000,05218	0,026649064	0,001140843	-0,002663944	0,999998127	0,338925172	1,000012506	1,0000105				0,004059968	0	#NV
10000,17712	10000,05467	0,015725017	0,00415067	0,002276073	0,999993216	0,2890839	1,000017643					9,27484E-06	0	#NV
10000,19055	10000,04966	0,024157765	-0,00254126	-0,002314641	0,999995768	0,645948394	1,000015883					3,74881E-05	0	#NV

Conclusions

- Assignment of an informative Type-A PDF and subsequent naive application of GUM-S1 differs from a truly informative Bayesian inference.
    - A simple counterexample shows the reason: ignorance of dependency.

- In metrological relevant cases, the techniuqes of GUM-S1 can be applied for rejection sampling to efficiently generate i.i.d. samples from the Bayesian posterior.

Marschall, M., Wübbeler, G., and Elster, C, “Rejection sampling for Bayesian uncertainty evaluation using the Monte Carlo techniques of GUM-S1,” ***Metrologia***, *2021*

Link to software repository: https://gitlab1.ptb.de/marsch02/gums1-rejection-sampler

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Appendix: Type-A uncertainty evaluation

GUM-S1 pure Type-A uncertainty evaluation (6.4.9.2)

Statistical model $\mathbf{X} \mid X, \sigma^2 \sim N(X, \sigma^2)$

(Reference prior) $X, \sigma^2 \sim \pi(X, \sigma^2) \propto \sigma^{-2}$

Marginal posterior $X \mid \mathbf{X} = x_1, \ldots, x_n \sim t_{n-1}(\bar{x}, s^2/n)$

Prior knowledge from Y to X

$$Y = X + Z$$

- X indication quantity with single recording — x_1 drawn from $N(X, \sigma^2)$
- Z type-B with assigned PDF of — $N(z_0, u_{z_0}^2)$
- Y measurand with prior knowledge PDF of — $N(y_0, u_{y_0}^2)$

A possible informative GUM-S1 procedure (Bayes for X only):

Use this for MC propagation?

A priori

$$X \sim N(y_0 - z_0, u_{y_0}^2 + u_{z_0}^2)$$

A posteriori

$$X \mid x_1 \sim N\left(x_p = u_{x_p}^2 \left(\frac{y_0 - z_0}{u_{z_0}^2 + u_{y_0}^2} + \frac{x_1}{\sigma^2}\right), u_{x_p}^2 = \left(\frac{1}{u_{z_0}^2 + u_{y_0}^2} + \frac{1}{\sigma^2}\right)^{-1}\right)$$

A simple counterexample (Appendix)

$$Y = X + Z$$

- X indication quantity with single recording x_1 drawn from $N(X, \sigma^2)$
- Z type-B with assigned PDF of $N(z_0, u_{z_0}^2)$

$$X \mid x_1 \sim N\left(x_p = u_{x_p}^2\left(\frac{y_0 - z_0}{u_{z_0}^2 + u_{y_0}^2} + \frac{x_1}{\sigma^2}\right), u_{x_p}^2 = \left(\frac{1}{u_{z_0}^2 + u_{y_0}^2} + \frac{1}{\sigma^2}\right)^{-1}\right)$$

Then, GUM-S1 yields output PDF

$$Y_G \sim N\left(y_G, u_{y_G}^2\right)$$

$$y_G = z_0 + \left(\frac{1}{u_{z_0}^2 + u_{y_0}^2} + \frac{1}{\sigma^2}\right)^{-1}\left(\frac{y_0 - z_0}{u_{z_0}^2 + u_{y_0}^2} + \frac{x_1}{\sigma^2}\right), \quad u_{y_G}^2 = u_{z_0}^2 + \left(\frac{1}{u_{z_0}^2 + u_{y_0}^2} + \frac{1}{\sigma^2}\right)^{-1}$$

A simple counterexample (Appendix)

$$Y = X + Z$$

- X indication quantity with single recording x_1 drawn from $N(X, \sigma^2)$
- Z type-B with assigned PDF of $N\left(z_0, u_{z_0}^2\right) = \pi(z)$
- Y measurand with prior knowledge PDF of $N\left(y_0, u_{y_0}^2\right) = \pi(y)$
- Joint prior $\pi(y, z) = \pi(y)\pi(z)$

Then, the Bayesian approach yields output PDF

$$Y_B |\, x_1 \sim N\left(y_B, u_{y_B}^2\right)$$

$$y_B = u_{y_B}^2 \left(\frac{z_0 + x_1}{u_{z_0}^2 + \sigma^2} + \frac{y_0}{u_{y_0}^2} \right), \quad u_{y_B}^2 = \left(\frac{1}{u_{y_0}^2} + \frac{1}{u_{z_0}^2 + \sigma^2} \right)^{-1}$$

A simple counterexample (Appendix)

$$y_G = z_0 + \left(\frac{1}{u_{z_0}^2 + u_{y_0}^2} + \frac{1}{\sigma^2}\right)^{-1}\left(\frac{y_0 - z_0}{u_{z_0}^2 + u_{y_0}^2} + \frac{x_1}{\sigma^2}\right), \quad u_{y_G}^2 = u_{z_0}^2 + \left(\frac{1}{u_{z_0}^2 + u_{y_0}^2} + \frac{1}{\sigma^2}\right)^{-1}$$

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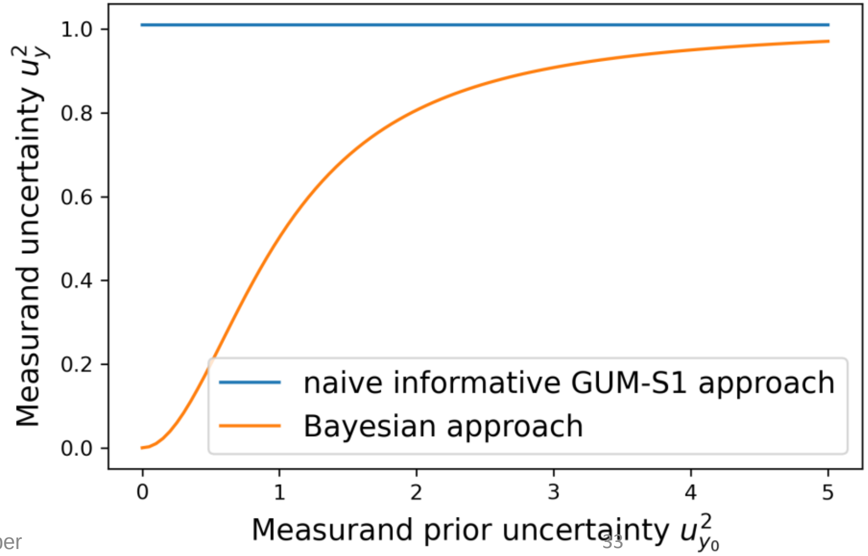

$u_{z_0}^2$