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Proposal to propagate uncertainties in ENSDF using Monte Carlo techniques

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Proposal: use Monte Carlo in ENSDF

- Single unsigned or signed number
- Standard symmetric or asymmetric uncertainty
- Limits

Uncertainty propagation in ENSDF codes:

- Taylor expansion, only valid for
  - a) Linear or nearly-linear relations/equations
  - b) small $\Delta X/X$ values; $\Delta X/X < \sim 10\%$
  - c) Correlations neglected

For multi-variant functions uncertainty propagation is difficult

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Solution: Monte Carlo (MC) uncertainty propagation

- ❑ Recognises and express any asymmetry
- ❑ Uses the full distribution, not just the standard deviation
- ❑ Produces valid coverage intervals

1) Evaluation of measurement data — Supplement 1 to the "Guide to the expression of uncertainty in measurement" — Propagation of distributions, JCGM 101:2008 (Joint Committee for Guides in Metrology)
2) M. Cox, A. O`Hagan, Accreditation and Quality Assurance 27 (2022) 19-37
3) A. Possolo, C. Merkatas, O. Bodnar, Metrologia 56 (2019) 045009

Two statistical paradigms

- **Frequentist methods** are based on the frequency definition of probability, where the probability of an event is defined to be the frequency with which that event occurs in the long run, over many repetitions. The Type A procedures given in the GUM are based on frequentist statistical theory, and accordingly the resulting standard uncertainties quantify how variable the estimate of a measurand will be over many repetitions of the measurement process.
- **Bayesian methods** employ a subjective definition of probability, whereby the probability of an event is a subjective judgement representing a person's rational degree of belief that it will occur. Type B evaluation in the GUM is a subjective judgement and the resulting standard uncertainty quantifies the metrologist's uncertainty about the measurand.

Ref: O'Hagan, Anthony, and Maurice Cox. "Simple Informative Prior Distributions for Metrology." (2021).

GUM: **Guide to the expression of uncertainty in measurement**, Working Group 1 of the Joint Committee for Guides in Metrology

Doing Monte Carlo uncertainty propagation in the nutshell

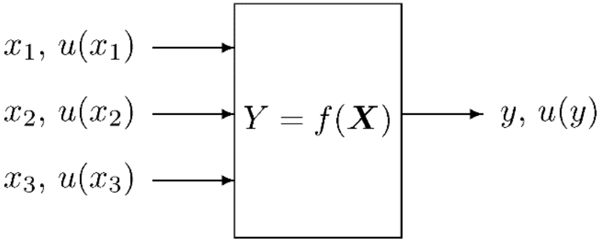
- Develop a model, f(X) relating the output quantity to the input quantities.
- Based on the available knowledge, assign a Probability Density Function (PDF) for each input quantity.
- Evaluate the mathematical model N* times and build the PDF of the output quantity
- Deduce statistical properties of the output quantity from its PDF. NO assumptions on the output UNC from the input.

  Recommended value: central value

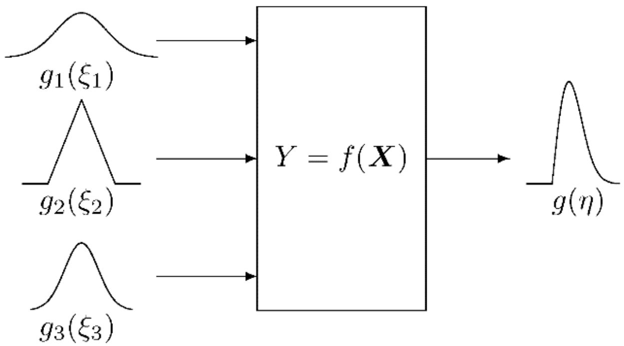
  Left (u_L) and right (u_R) uncertainties from 1s coverage interval

Number of recommended MC trials: 10 k to 1 M

Mathematical model



Monte Carlo using PDF



Existing software tools for Monte Carlo uncertainty propagation

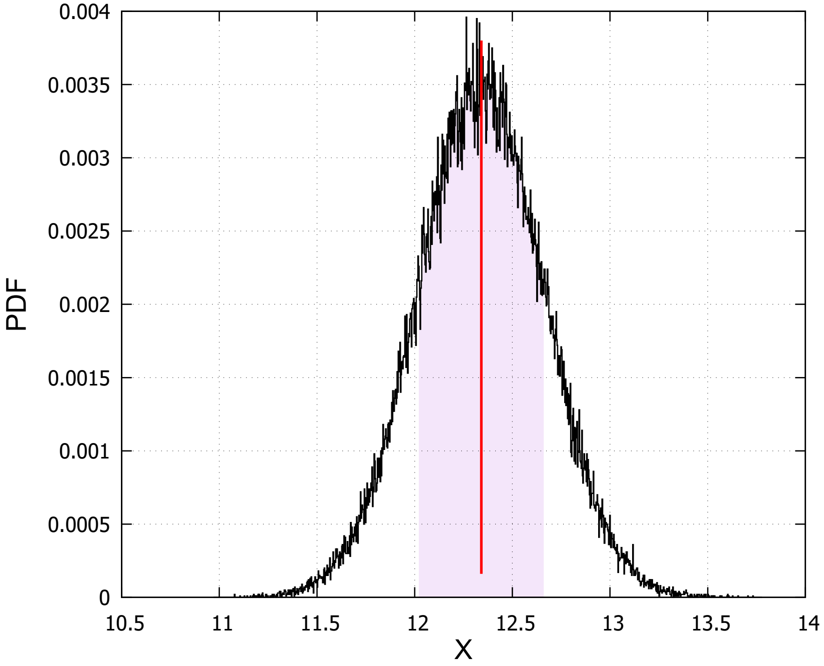
- NIST Uncertainty machine: https://uncertainty.nist.gov
- Error Propagation Calculator (python)
- GUM_MC (application)

Many more at:
https://en.wikipedia.org/wiki/List_of_uncertainty_propagation_software

Some ENSDF tools are already using MC approaches: UncTools, NS_Radlist, java-Ruler

Symmetric uncertainty

Representation in ENSDF: X(u)



X = 12.34(32)

PDF: Normal distribution

$$PDF(x) = \frac{1}{\sigma\sqrt{2\pi}} \times \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

μ = mean = 12.34 mode

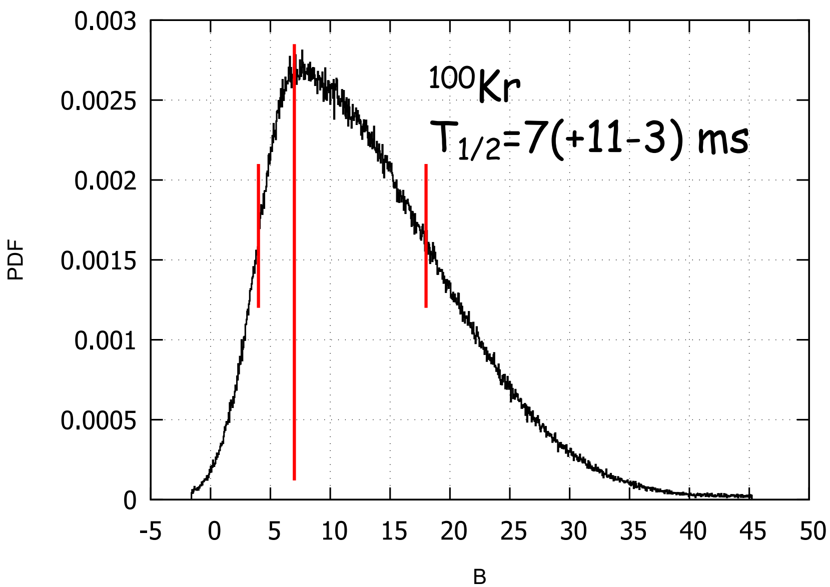
σ = 0.32 standard deviation

Asymmetric uncertainty

<u>Representation in ENSDF:</u> $X(+u_R\ -u_L)$

<u>Symmetrizing:</u> Audi et al, NUBASE2016, *C. Phys. C* Vol. 41, No. 3 (2017) 030001

$X\ (+u_R\ -u_L) \rightarrow$ value: $X+(u_R-u_L)/2$, symmetric uncertainty: $(u_R+u_L)/2$



- 1σ (68%) coverage intervals on the left and right are not equal!
- For best performance: $0.645 < u_R/u_L < 1.55$
- μ is the measured value: μ=7

X = 7(+11,-3)

PDF: Split normal distribution

$$PDF(x) = A \times \exp\left(-\frac{(x-\mu)^2}{2u_L^2}\right) \quad X < \mu$$

$$PDF(x) = A \times \exp\left(-\frac{(x-\mu)^2}{2u_R^2}\right) \quad X \geq \mu$$

$$A = \frac{\sqrt{2}}{\sqrt{\pi}(\sigma_L+\sigma_R)}$$

$\mu = 7$ mode

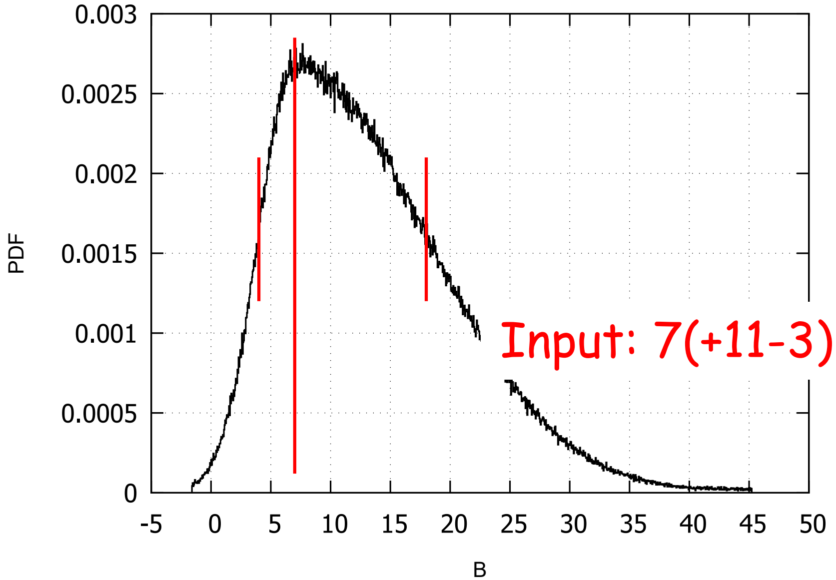
$u_L = 3$ left uncertainty (σ_L)

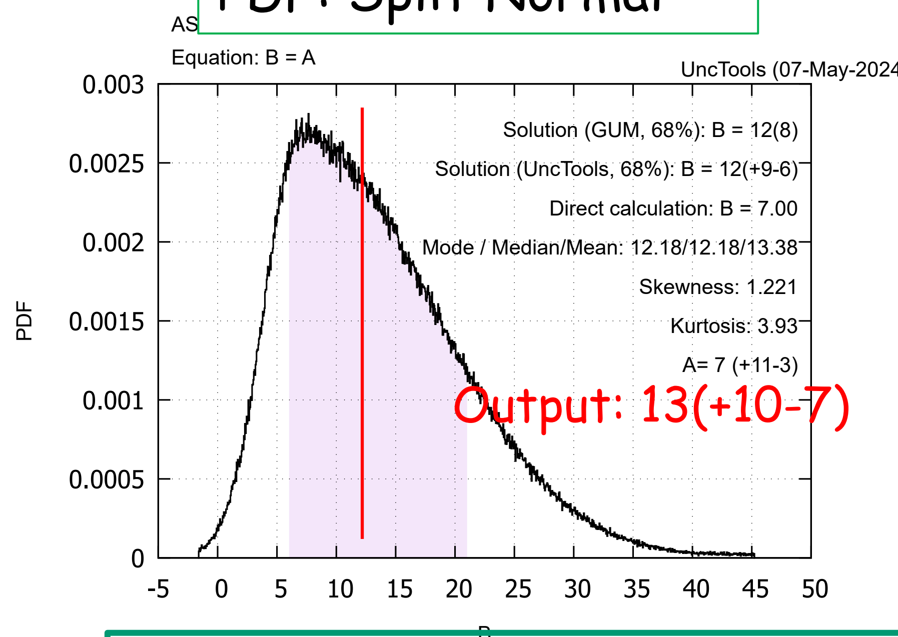
$u_R = 11$ right uncertainty (σ_R)

$$mean = \mu + \sqrt{2/\pi}(u_R - u_L)$$

Asymmetric uncertainty

PDF: Split Normal





MC propagation using Cumulative Density Function:
m – median: p=50%
u_L: p=15.9%; u_R: p=84.1%

<u>MC solution and uL, uR ≠ Measured values!</u>

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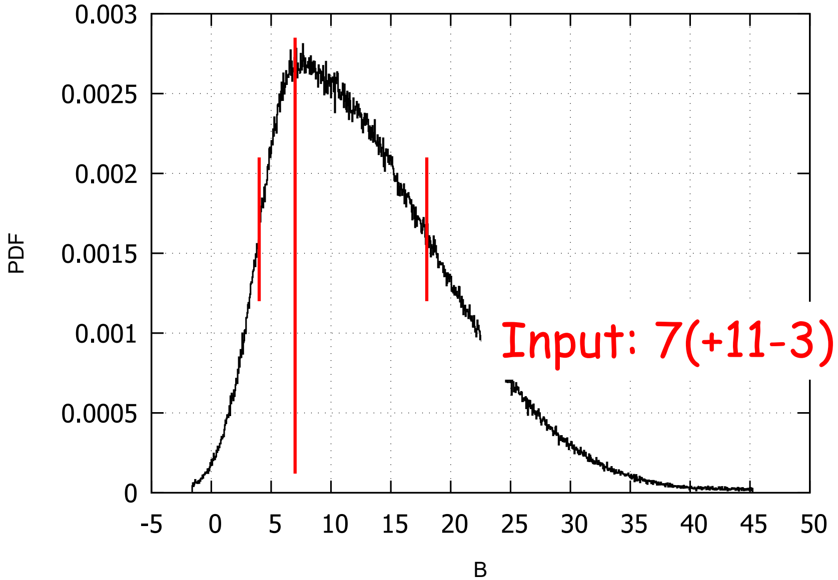
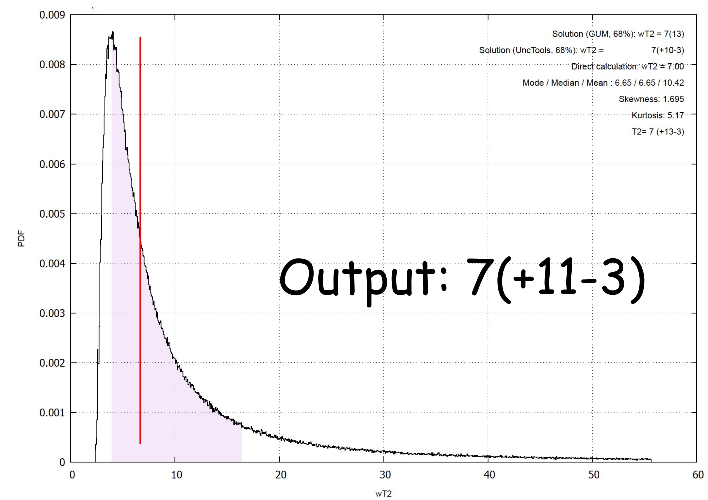
Asymmetric uncertainty



PDF: General Extreme Value (GEV) distribution



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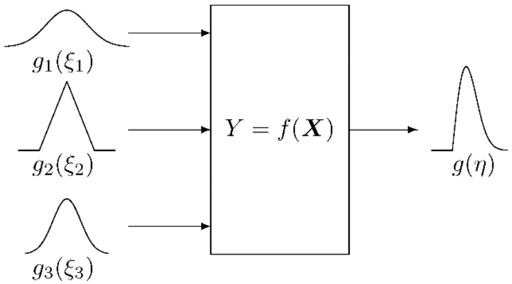
- For best performance: $0.645 < u_R/u_L < 1.55$
- μ is the measured value: μ=7

GEV:
- Valid for broad region of asymmetry
- <u>PDF(x)=f(X,μ,σ,ξ)</u>

A. Possolo, Metrologica 56 (2019) 045009

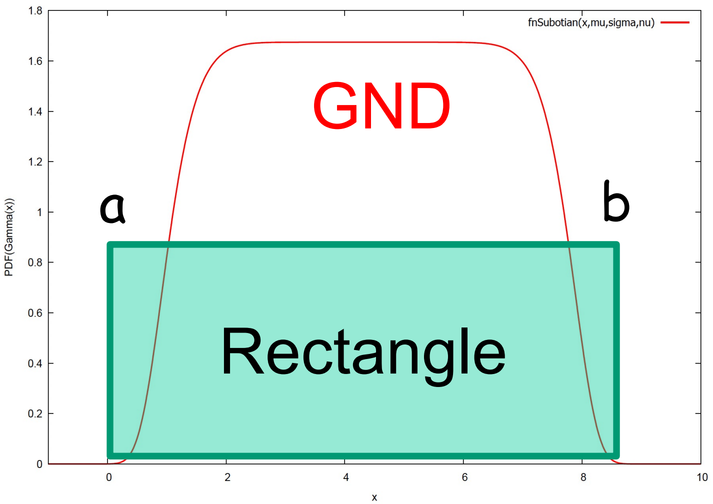
LIMITS

MC: Deduce Output quantity from the PDF



PDF of a limit

- GUM(2008): rectangle distribution: X sampled from [a:b]
  - Expected value: (a+b)/2; variance (b-a)/2
  - Increased weight of very small values f(x)=1/x
- Generalized Normal Distribution (GND, Subbotin 1925)



GENERAL

- Need a policy to propagate Uncertainty in ENSDF

MC Propagation

- Get input from GUM /Metrology community
- What are the DEFAULT Uncertainties for AP, SY
- Which PDF to use
- Derived quantity: MEDIAN, u_L=U_H= 1 s of the PDF
- In some cases, need to be symmetrized
- Provide PDF of the output quantity