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Whisper updates

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Motivation

- Demonstrate that Whisper calculates the calculational margin as described in Brian Kiedrowski's NSE paper[1]
- Educate community of Whisper users and provide visualization of a significant component of the upper subcritical limit (USL) calculation
- Pursuant to porting Whisper capabilities to modular library structure

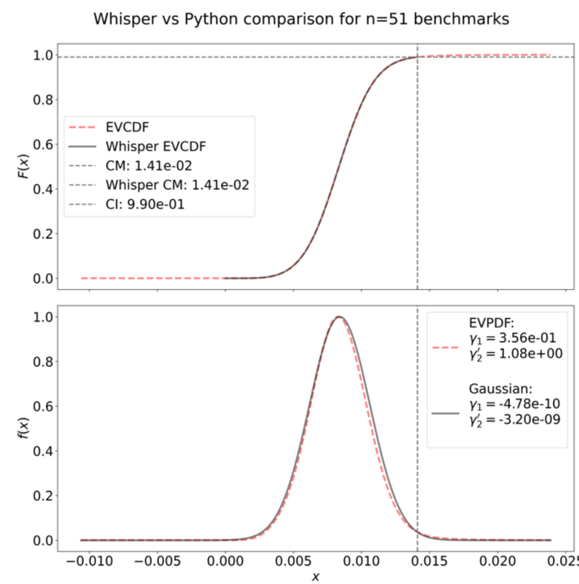
```
Calculating application nuclear data uncertainties ...
   application                                  adjusted     prior
   pu-met-fast-001-001.i                        0.00058      0.01388

Calculating upper subcritical limits ...
                                                calc         data unc     baseline     k(calc)
   application                                  margin       (1-sigma)    USL          > USL
   pu-met-fast-001-001.i                        0.01412      0.00058      0.97937      0.02138

   Benchmark population   =   51
   Population weight      =  25.00877
   Maximum similarity     =   0.99994

   Bias                   =   0.00840
   Bias uncertainty       =   0.00572
   Nuc Data uncert margin =   0.00058
   Software/method margin =   0.00500
   Non-coverage penalty   =   0.00000
```

Snippet from a Whisper output file of the USL computed for an application.



Comparison of the Extreme-Value PDF and CDF computed by Whisper vs Python.

1. B. Kiedrowski et. al, "Whisper: Sensitivity/Uncertainty-Based Computational Methods and Software for Determining Baseline Upper Subcritical Limits", Nucl. Sci. and Eng., 181:1, 17-47 (2015), DOI: 10.13182/NSE14-99

Computing the calculational margin

- Bias β_i, variance σ_i^2, and weight w_i are computed for each benchmark-calculation pair

$$\beta_i = k_{i,b} - k_{i,c}$$

$$\sigma_i^2 = \sigma_{i,b}^2 + \sigma_{i,c}^2$$

$$c_{k,i} = \frac{\mathrm{cov}\left(k_{i,a}, k_{i,b}\right)}{\mathrm{stdev}\left(k_{i,a}\right)\mathrm{stdev}\left(k_{i,b}\right)}$$

$$w_i = \max\left\{0, \frac{c_{k,i} - c_{k,acc}}{c_{k,max} - c_{k,acc}}\right\}$$

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Computing the calculational margin

- Each benchmark-calculation pair is treated as being sampled from a weighted normal distribution, where the PDF and the CDF are denoted as $f(x_i)$ and $F(x_i)$, respectively.

$$f(x_i) = \frac{w_i}{\sqrt{2\pi}\sigma_i} \exp\left[-\left(\frac{x-\beta_i}{\sqrt{2}\sigma_i}\right)^2\right]$$

$$F(x_i) = (1 - w_i) + \frac{w_i}{2}\left[1 + \operatorname{erf}\left(\frac{x-\beta_i}{\sqrt{2}\sigma}\right)\right]$$

- Extreme-Value CDF is defined as the product of the benchmark-calculation pair CDFs[a]

$$F(x) = \prod_{i=1}^{N} F(x_i)$$

- Extreme-Value PDF is the derivative of the Extreme-Value CDF

$$f(x) = F(x) \sum_{i=1}^{N} \frac{f(x_i)}{F(x_i)}$$

[a]The classic Extreme-Value CDF is defined in terms of IID samples (i.e. sampled from the same CDF). Whisper takes a more conservative approach in computing the Extreme-Value CDF via single samples from different CDFs, such that the calculational margin is bounded by the maximum product of bias and weight.

Computing the calculational margin

- Calculational margin is bias m such that the Extreme-Value CDF value is above an arbitrary confidence interval q

$$F(m) = q$$

- The mean bias β is computed as the mean of the Extreme-Value PDF and used to conservatively bound the calculational margin

$$\beta = \int_{-\infty}^{\infty} x f(x) dx$$

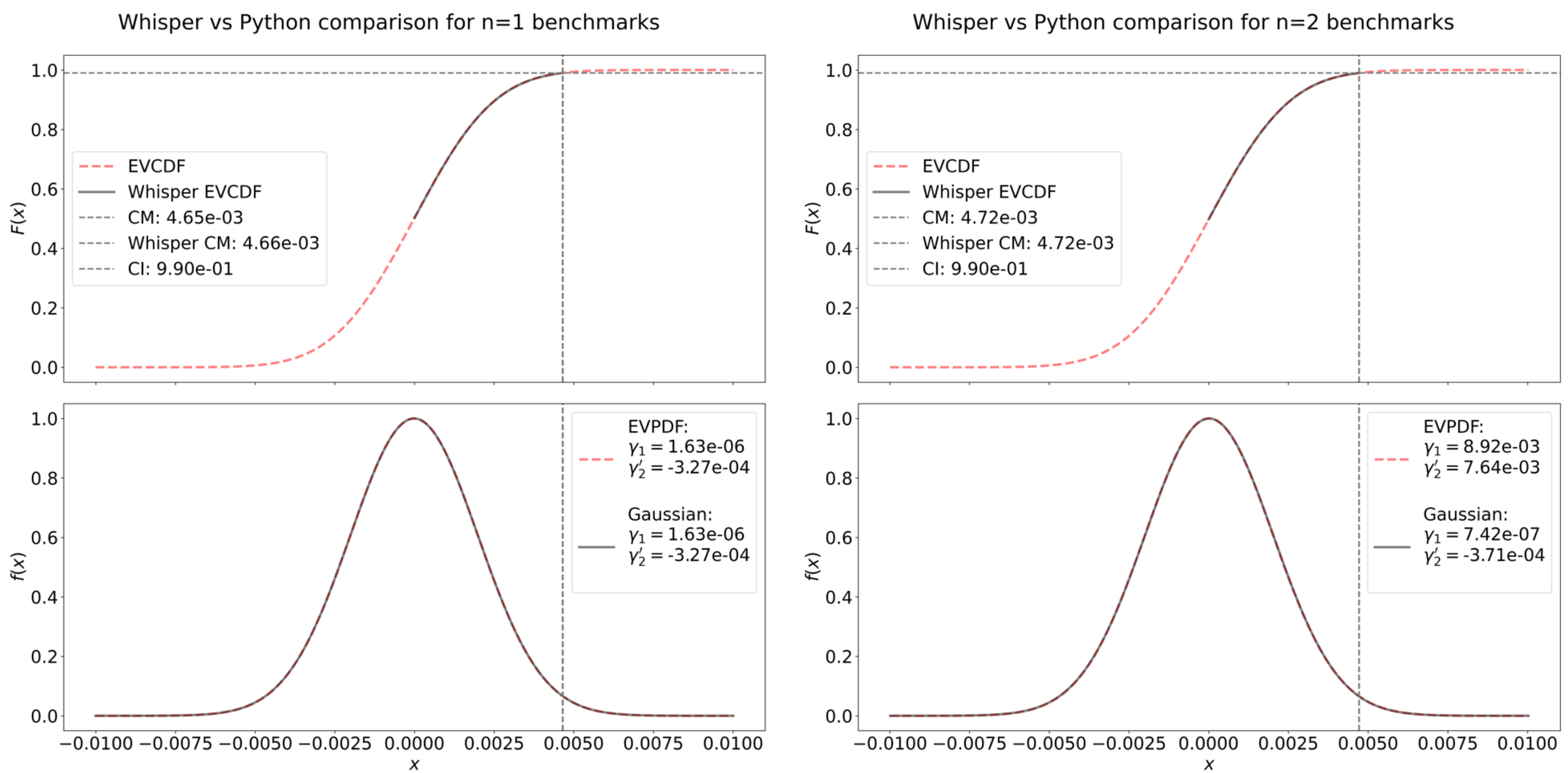
$$\Delta m = \max\{0, \beta\}$$

$$\begin{aligned} \mathrm{CM} &= m + \Delta m \\ &= F^{-1}(q) + \max\{0, \beta\} \end{aligned}$$

Visualizing Extreme-Value CDF and corresponding calculational margin

- Defined the following variables using the “user options” -u flag
  - MinimumWeightSum
    - Changes the number of benchmarks that Whisper selects
    - Smaller values result in fewer selected benchmarks and vice versa.
    - Set to arbitrary values
  - WeightSumPenalty
    - Takes effect when the benchmarks are not similar to the application
    - Used in tandem with MinimumWeightSum to ensure a large enough population size
    - WeightRequired = MinimumWeightSum + (1 - MaxSimilarity) * WeightSumPenalty
    - Set to zero
  - MinimumNonCoveragePenalty
    - Takes effect if there aren’t enough benchmarks to obtain a large enough calculational margin
    - UnweightedData%CalcMargin = max(UnweightedData%CalcMargin, MinimumNonCoveragePenalty)
    - Set to zero
- Write Whisper-calculated Extreme-Value CDF to file
- Parse calculational margin from the Whisper.out file

Extreme-Value CDF for single benchmark is Gaussian

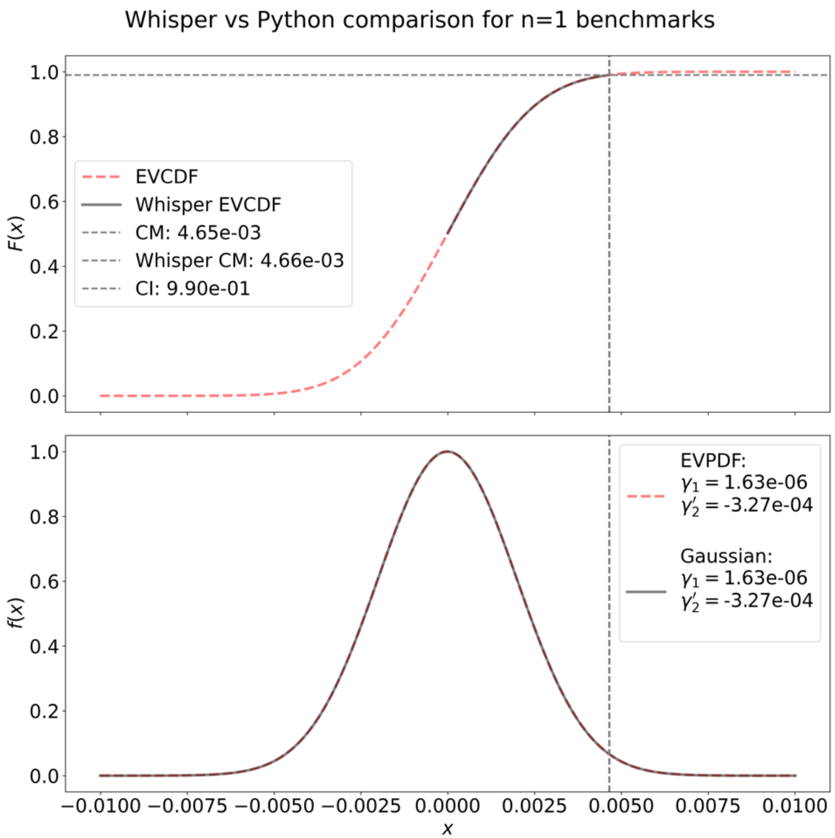


MinimumWeightSum 1.00000

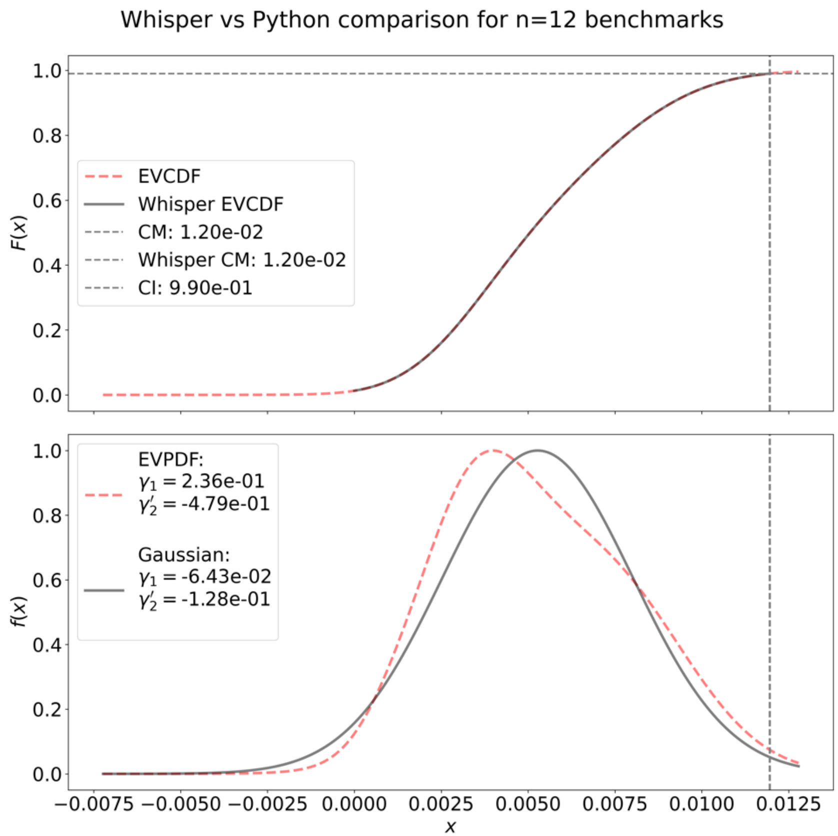
MinimumWeightSum 1.00001

Both Whisper- and Python-calculated calculational margins match what is described by B. Kiedrowski's NSE paper

Deviation of Extreme-Value CDF from Gaussian increases with additional benchmarks



MinimumWeightSum 1.00000



MinimumWeightSum 5.00000

Gaussian defined with same mean and standard deviation as Extreme-Value PDF.

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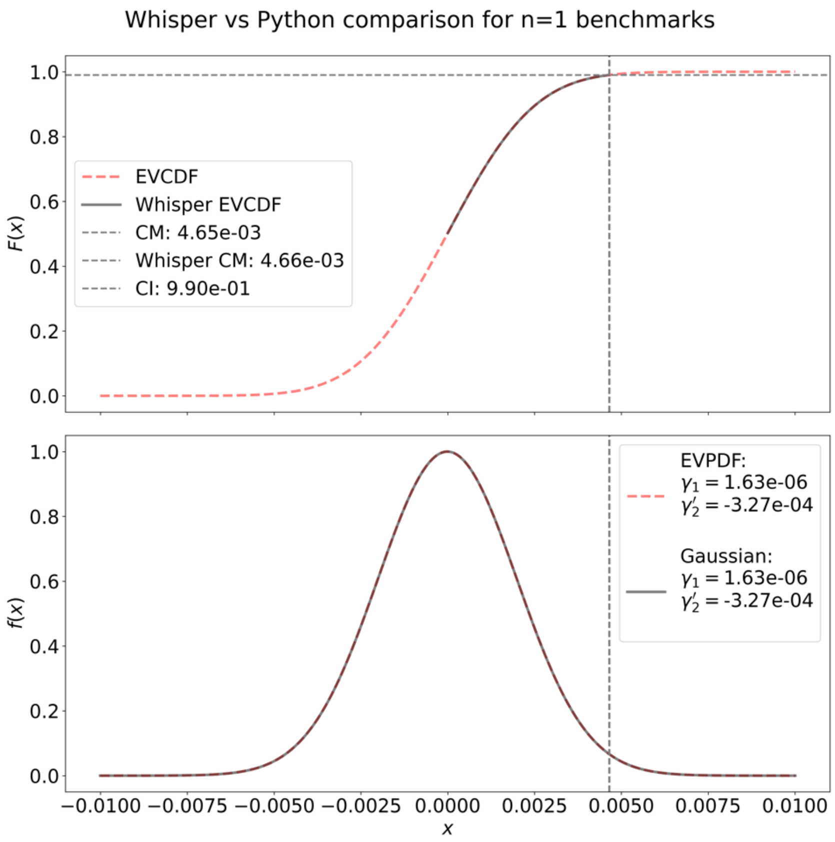
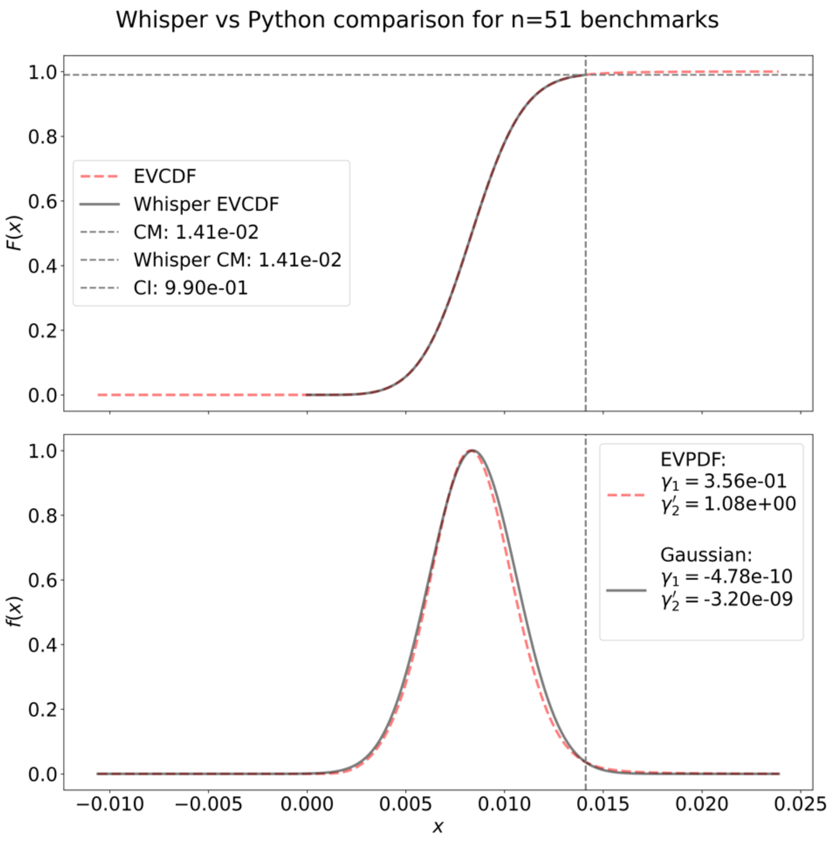
Artifacts in Extreme-Value CDF are washed out with increasing benchmarks



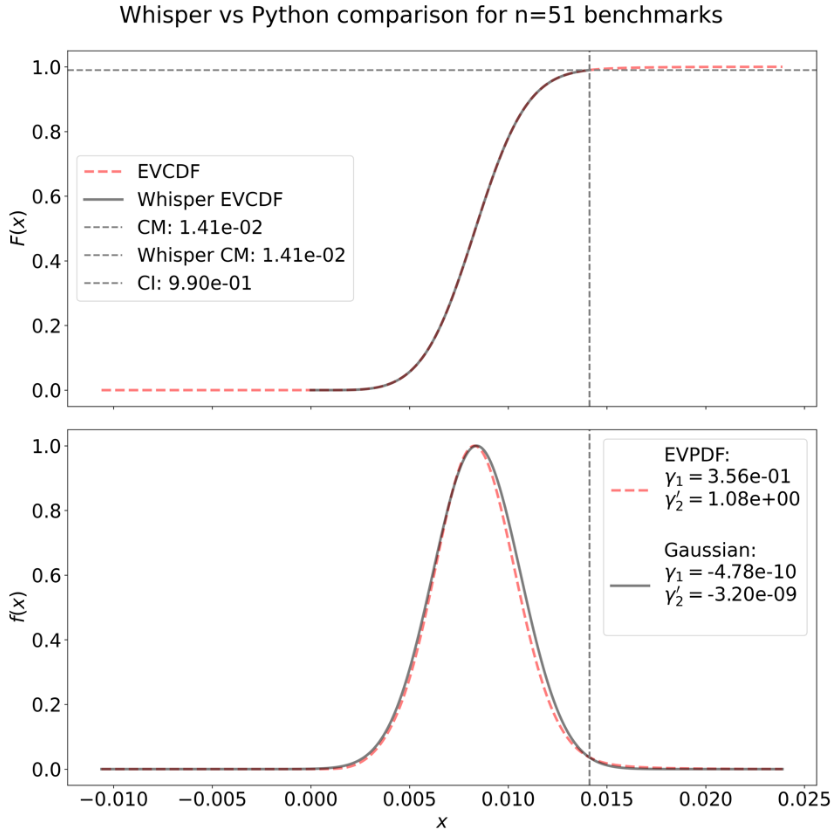
MinimumWeightSum 1.00000



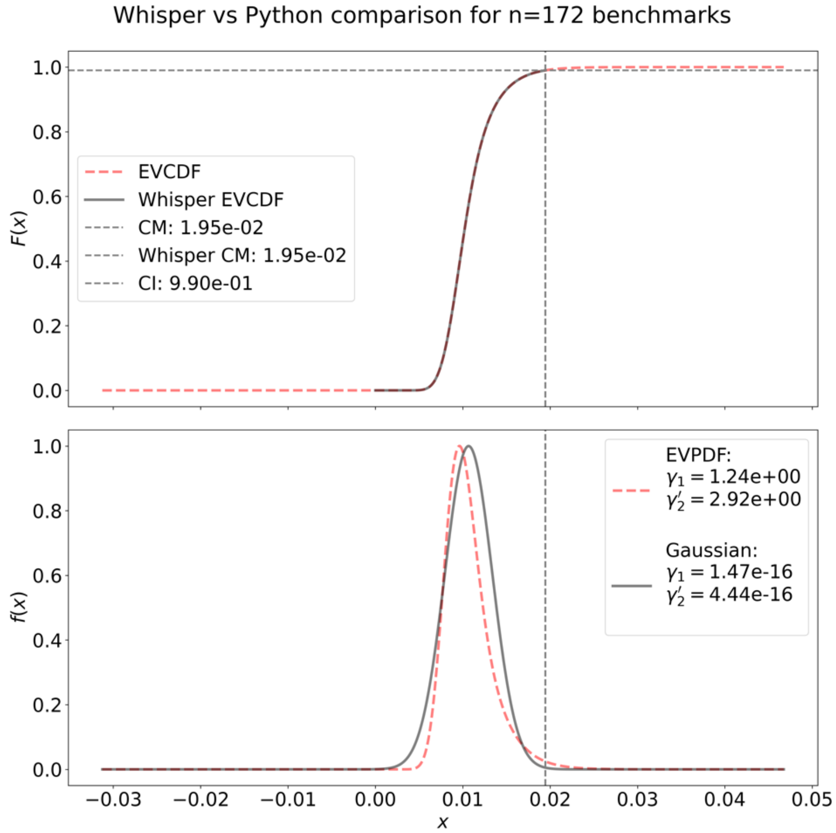
MinimumWeightSum 25.0000 (default)

n=51 benchmarks is what Whisper selects by default.

Allowing for more benchmarks to be selected than the default can be more conservative…



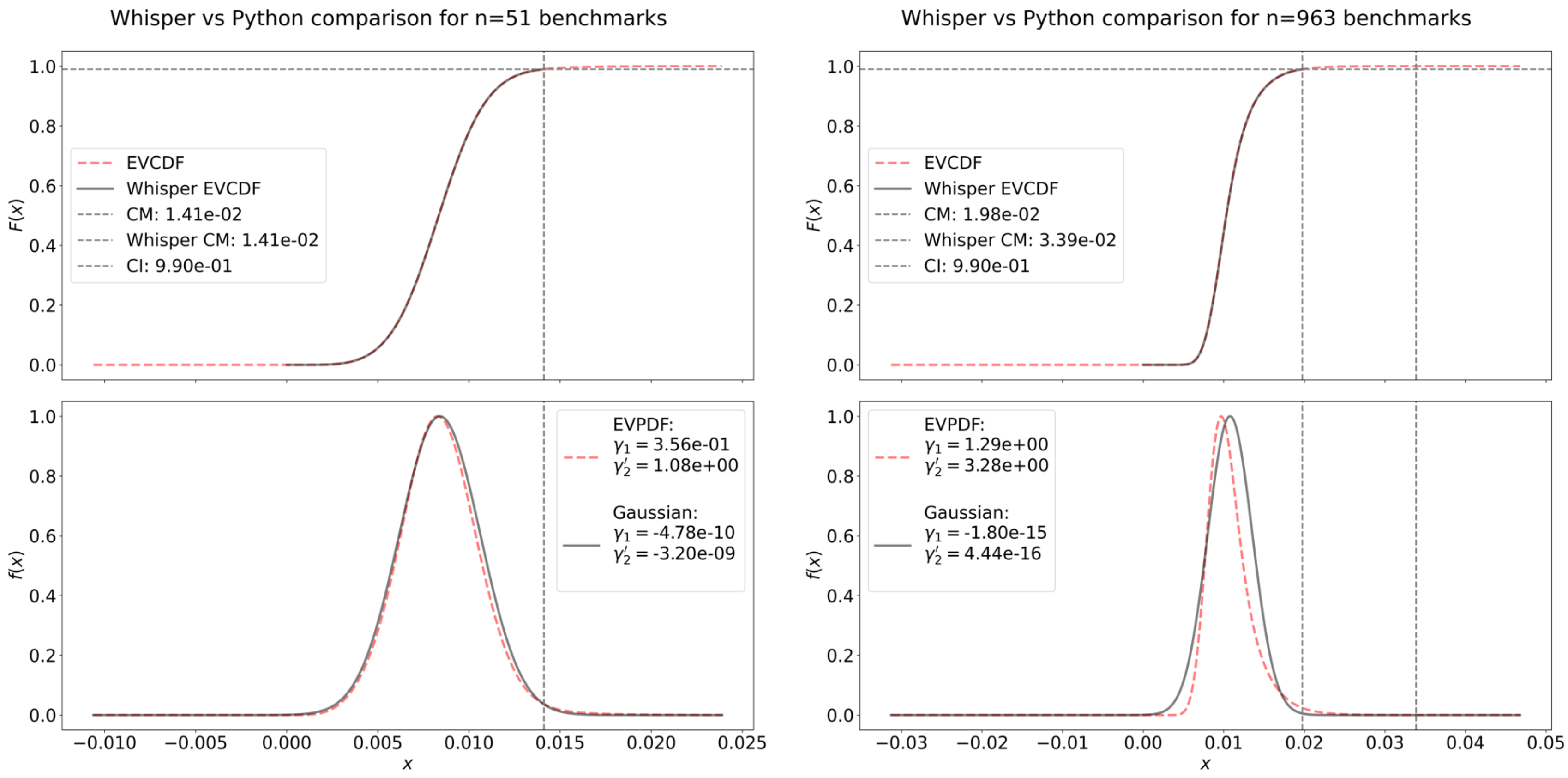
MinimumWeightSum 25.0000 (default)



MinimumWeightSum 100.00000

Going from n=51 to n=172 results in a nearly 500 pcm increase in the calculational margin!

…but will eventually result in a penalty being applied



MinimumWeightSum 25.0000 (default)

MinimumWeightSum 200.00000

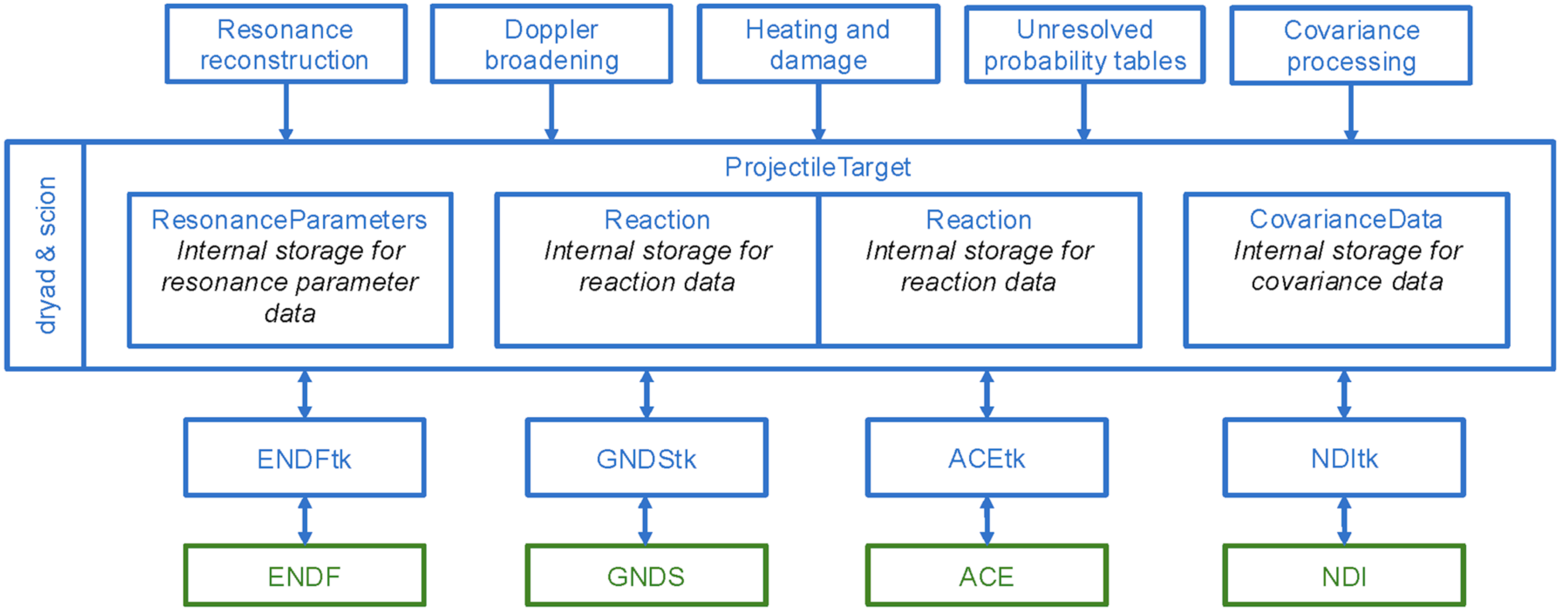
CoveragePenalty (not MinimumNonCoveragePenalty) is applied when the MinimumWeightSum can't be met.

Conclusions

- Whisper computes the calculational margin as described in B. Kiedrowski's NSE paper
- The computed Extreme-Value CDF and corresponding calculational margin are conservative
  - Bounded by largest product of weight and bias
  - Extreme-Value CDF grows monotonically
  - Significant penalty when MinimumWeightSum isn't met
- Implementing a verbose flag in Whisper for outputing distribution information, enabling users to visualize these results
- Happy for feedback on what kinds of outputs would be most useful for users: please email us at whisper_help@lanl.gov

Future outlook

- The LANL Nuclear Data team is working toward a “format-agnostic data interface” called DRYAD[1]



- Will allow Whisper to interact with nuclear-data-team-supported covariances
- Currently integrating ACEtk into Whisper port to demonstrate feasibility

1. W. Haeck, N. A. Gibson, P. Talou, C. J. Josey. **The Road to a Modernized NJOY**. Los Alamos National Laboratory Presentation LA-UR-24-28898. Los Alamos, NM, USA. August 2024.

Acknowledgements

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