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An Initial Comparison of Methods for Representing and Aggregating Experimental Uncertainties involving Sparse Data

Vicente Romero, Laura Swiler, Angel Urbina

Sandia National Laboratories*

Albuquerque, NM

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Introduction and Motivation

- **This talk discusses characterization and treatment of uncertainty associated with random variability of stochastic materials, systems, and processes when limited samples of the randomness are available.**
  - pervasive and important problem in experimental data UQ and model validation or calibration to experimental data
- **Sparse sampling introduces epistemic uncertainty that undermines accurate characterization of the quantity's aleatory uncertainty (i.e., of its randomness as represented by a probability density function (PDF) or "variability distribution")**
- **The view is therefore here taken that:**
  - One should not endeavor for the impossible (accurate estimation of the underlying variability distribution from which the sparse samples come)
  - Rather, a pragmatic goal is that the uncertainty representation should be conservative so as to bound a specified percentage of the underlying PDF
  - An opposing goal (making this a difficult problem) is that the uncertainty representation not be overly conservative—i.e., should minimally over-estimate the specified variability range of the true PDF.

Four Methods Tried for Sparse-Data Uncertainty Representation

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- **<u>Method 1</u>: Fit the data with a Normal distribution**
  - An easy and very common approach used in engineering practice.
  - But how well does it work?

- **<u>Method 2</u>: Tolerance Intervals from classical statistics**

- **<u>Method 3</u>: PDF estimation by Pradlwarter-Schueller KDE (kernel density estimation) approach to fitting the data (slide follows)**

- **<u>Method 4</u>: PDF estimation by Sankararaman-Mahadevan "Non-Parametric" PDF fit to the data (slides follow)**

- **Evaluation criteria:**
  - how well the approaches perform on the two stated objectives:
    - conservative ⇔ but not overly conservative
    - <u>assess on illustrative problem</u>:
      - estimate 95% PDF coverage range (central 0.95 percentile) of exact PDFs from which data samples are drawn
  - ease of implementation and use for engineering practice

Classical Tolerance Interval Method for Dealing with Sparse Data

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- **Approach**
  - calculate the standard deviation σ of the data
  - multiply σ by appropriate factor *f* from statistical tables
  - create interval bars of extent $f\sigma$ about the mean μ of the data: $\mu \pm f\sigma$
  - 0.9/0.95 Tolerance Intervals — in this study, the factors *f* correspond to approximate 90% confidence that the produced tolerance interval encompasses the central 95-percentile range (between the 0.025 and 0.975 percentiles) of the true PDF

# samples	$f_{0.9/0.95}$
2	18.80
4	4.94
8	3.26
12	2.86
20	2.56
30	2.41
40	2.33
∞	1.96

- **Very simple to use in practice**

Pradlwarter-Schueller KDE Method for Dealing with Sparse Data

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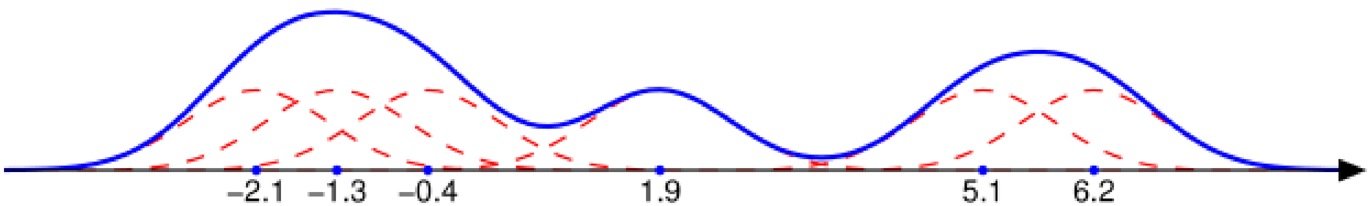
Pradlwarter, H.J., and G.I. Schuëller, "The use of kernel densities and confidence intervals to cope with insufficient data in validation experiments," *Computer Methods in Applied Mechanics and Engineering*. Vol. 197, Issues 29-32, May 2008, pp. 2550-2560.

- **Kernel Density Estimation (KDE) is a technique used to estimate the density of a random variable *X* given *n* independent samples $X_1, \ldots, X_n$ of it.[1]**



$$f_n^{\{KDE\}}(x;h) = \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right)$$

- **We used a Gaussian Kernel**
- **KDE is very sensitive to the bandwidth, *h*. Bandwidth estimation typically involves optimization (e.g. maximize a cross-validation likelihood)**
- **For small samples, we used the approach in Pradlwarter and Schuëller: find *h* to satisfy a fixed probability:** $\int_{-\infty}^{a} f(x;h)dx + \int_{b}^{+\infty} f(x;h)dx = P(\alpha, n)$

1. Figure taken from http://en.wikipedia.org/wiki/Kernel_density_estimation

Sankararaman-Mahadevan Method for constructing a PDF from Sparse Data

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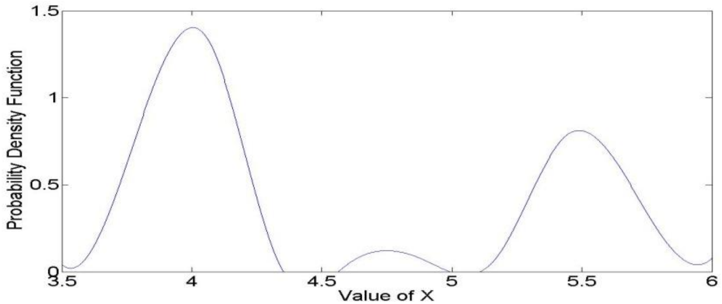
Shankar Sankararaman & Sankaran Mahadevan, "Likelihood-based representation of epistemic uncertainty due to sparse point data and/or interval data," *Reliability Engineering and System Safety*, doi:10.1016/j.ress.2011.02.003.

- **Discretize the domain of $X \rightarrow \theta_i$, i = 1 to Q**
- **PDF values at each of these Q points**
  - **$f_X(x=\theta_i)=p_i$ for i = 1 to Q**
- **Interpolation technique (cubic splines used here)**
- **Construct likelihood as a function of:**
  - Discretization points θ_i selected, i = 1 to Q
  - Corresponding probability density function values p_i
  - Type of interpolation technique

$$L \propto \left(\prod_{i=1}^{n} \int_{a_i}^{b_i} f_X(x)dx \right) \left(\prod_{i=1}^{m} f_X(x_i) \right)$$

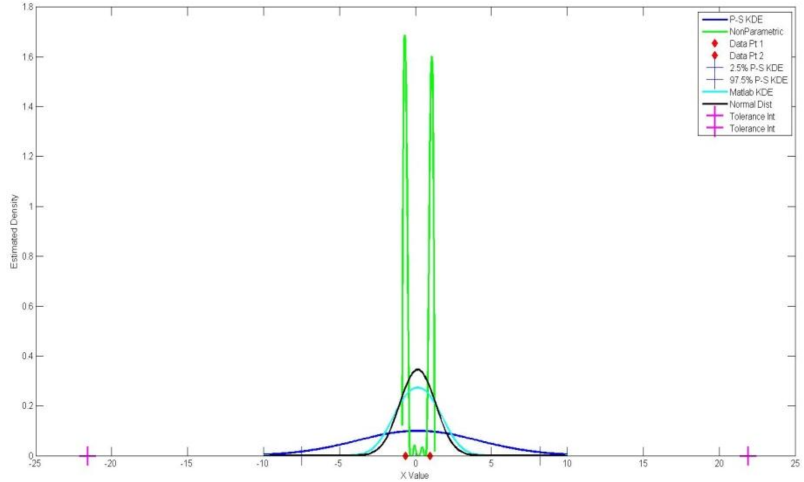
- **Maximize Likelihood $L(p)$ where p = {p_i ; i = 1 to Q) subject to applicable constraints**
  - **Estimate $f(x)$**

Probability Density Function



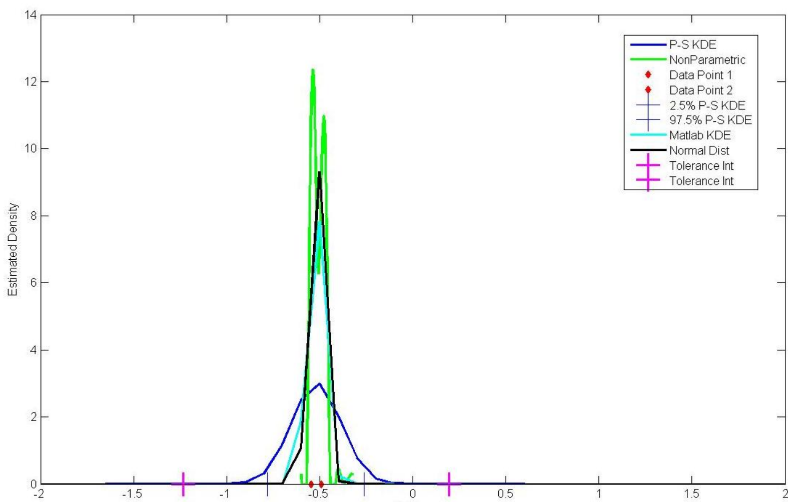
Illustrative PDFs or 95% Intervals from the Four Methods + a Matlab-KDE Method

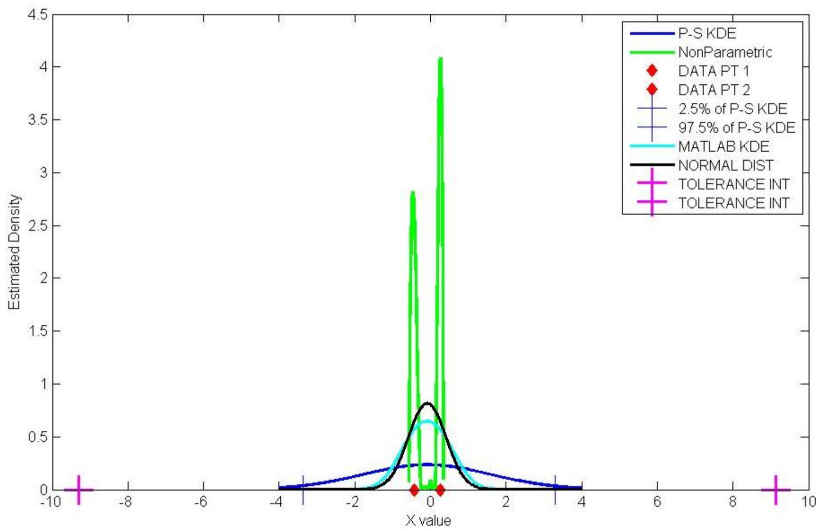
- **Three instances of 2 samples from a Normal PDF**
  - **2 samples "close" together**
  - **2 samples "far" apart**
  - **2 "intermediately" spaced**



far

close

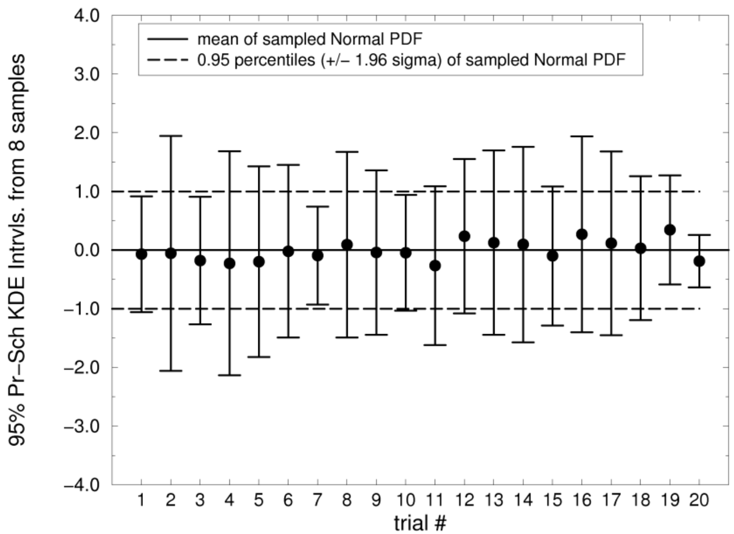


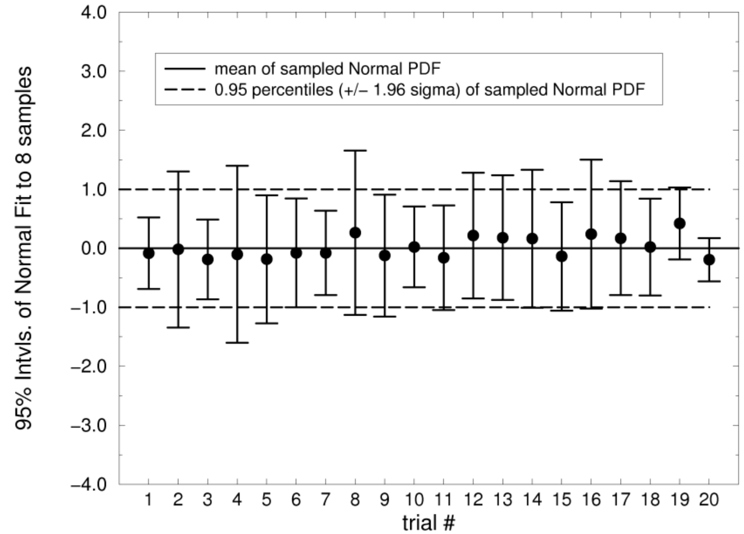


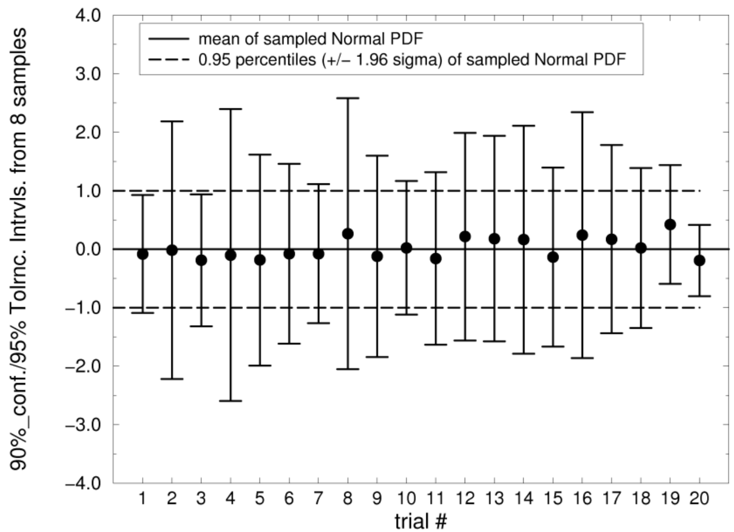
inter med.

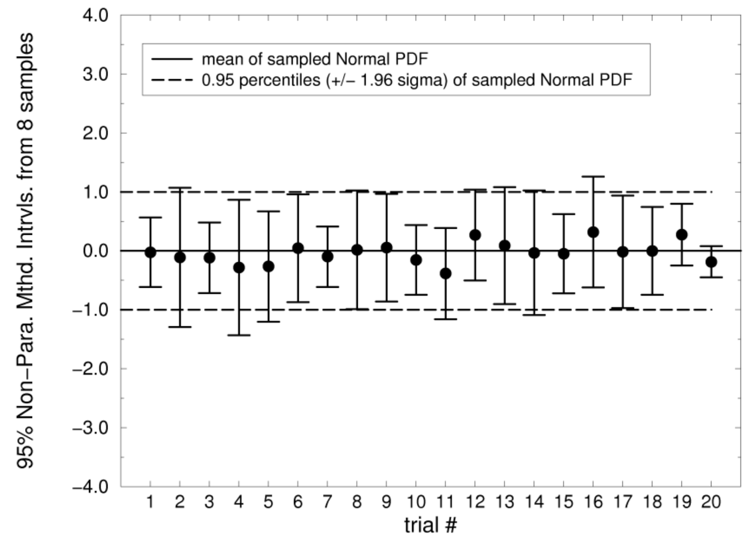
Illustrative 95% Intervals from the Four Methods

– 20 trials per method, 8 random samples of a Normal PDF per trial









- **Tol. Intvls. most conservative, then Pr-Sch, Normal Fit, and Non-Para.**

The Larger Test Matrix

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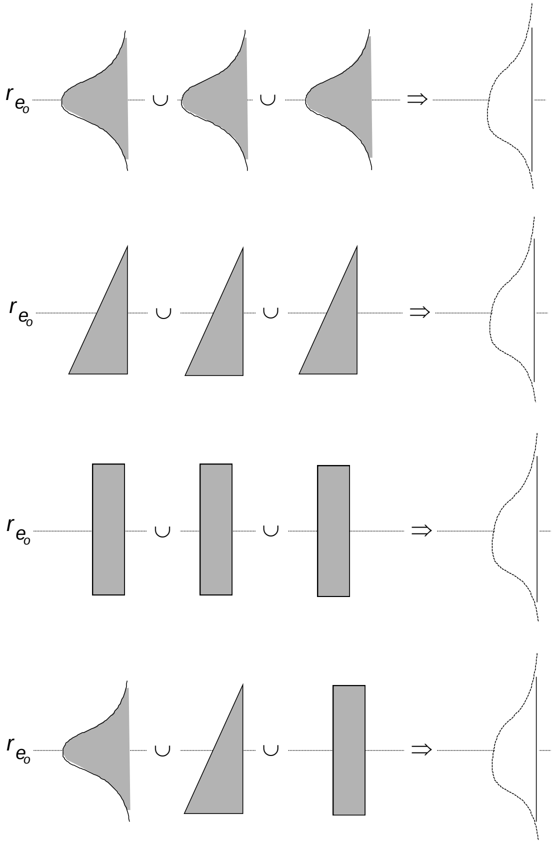
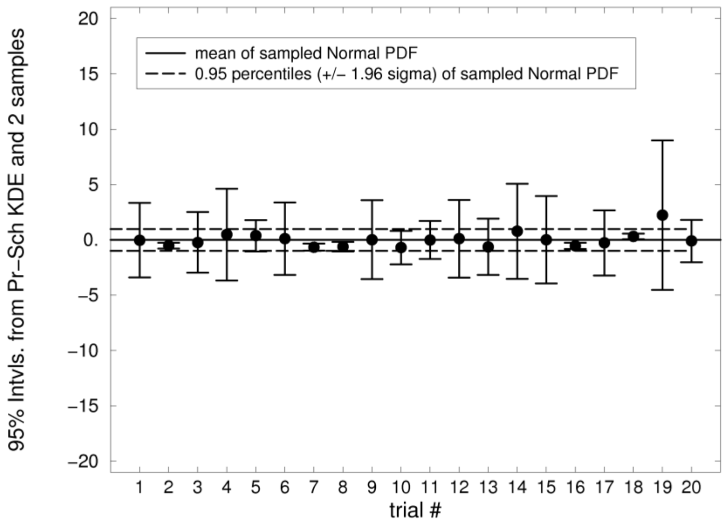
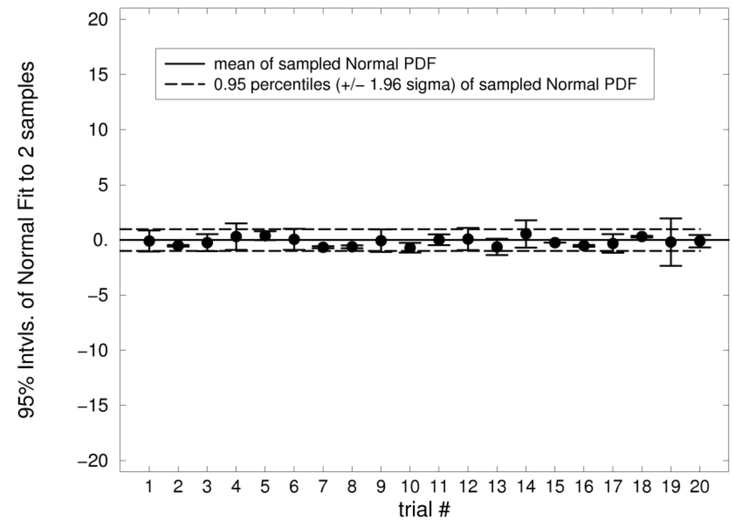
- **1000 trials of each method for fitting sample data from each of:**
  - normal PDF
  - right-triangular PDF
  - uniform PDF
  - Convolutions of these PDF types (figure at right) acting as three equally dominant sources of random uncertainty in a linear system.
    - Answer question: does the presence of multiple sources of uncertainty smooth or mitigate the errors in representing the individual PDFs?
- **Fit the data for sample sizes of *n* = 2, 8, 32 for each PDF**
- **Initial results reported here and in the paper are for Top Row of figure only**

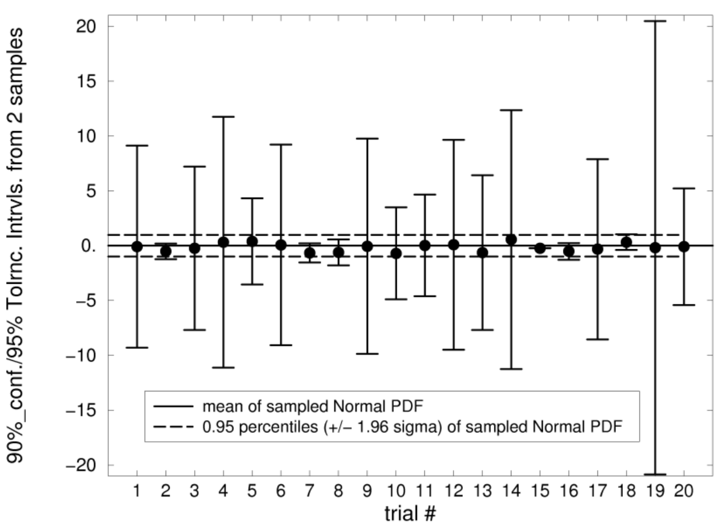


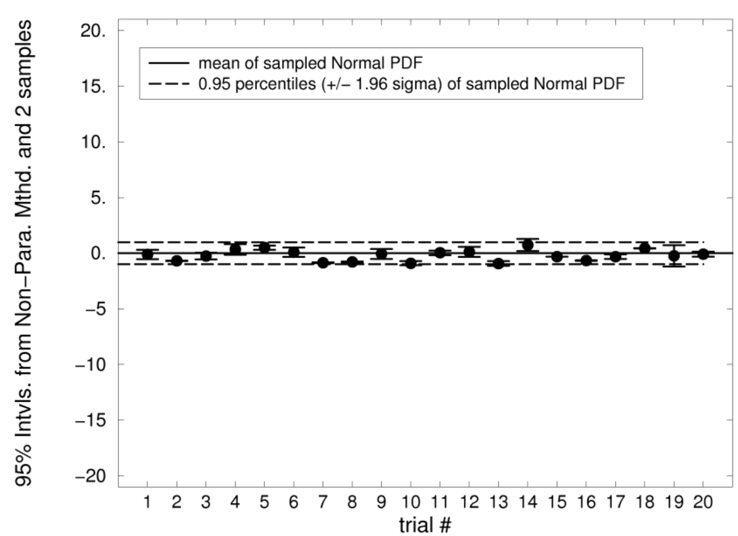
Glimpse of 95% Intervals from the Four Methods

– 20 trials per method, 2 random samples of a Normal PDF per trial





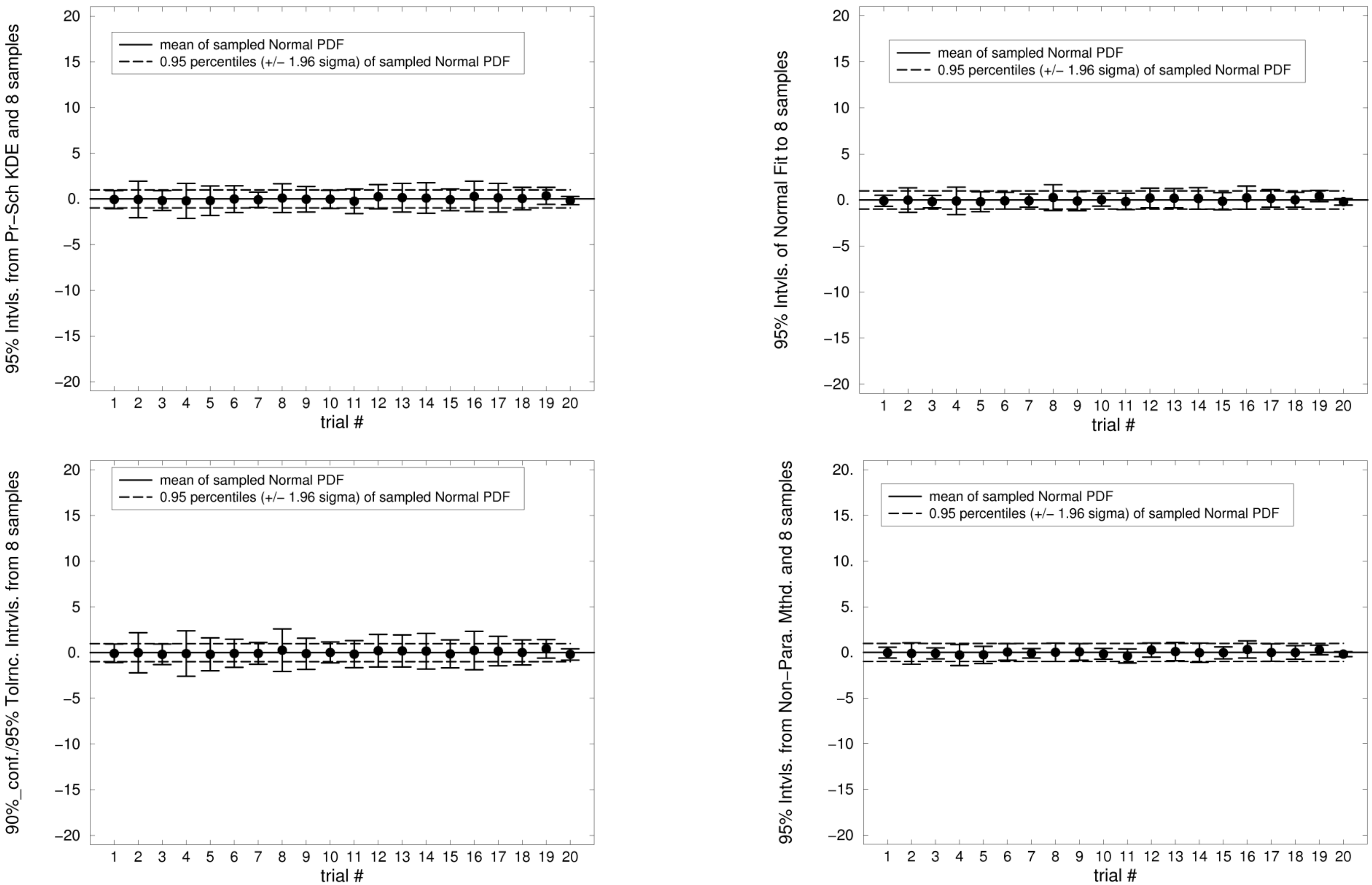




- **Method results differ greatly for low numbers of samples.**

Glimpse of 95% Intervals from the Four Methods

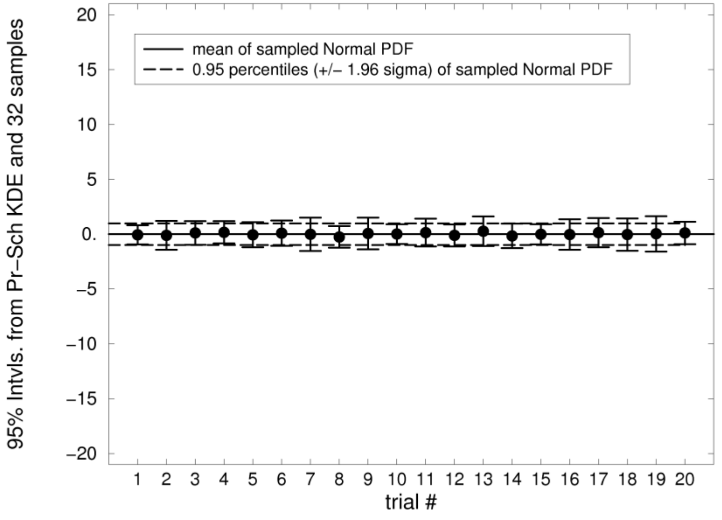
– 20 trials per method, 8 random samples of a Normal PDF per trial

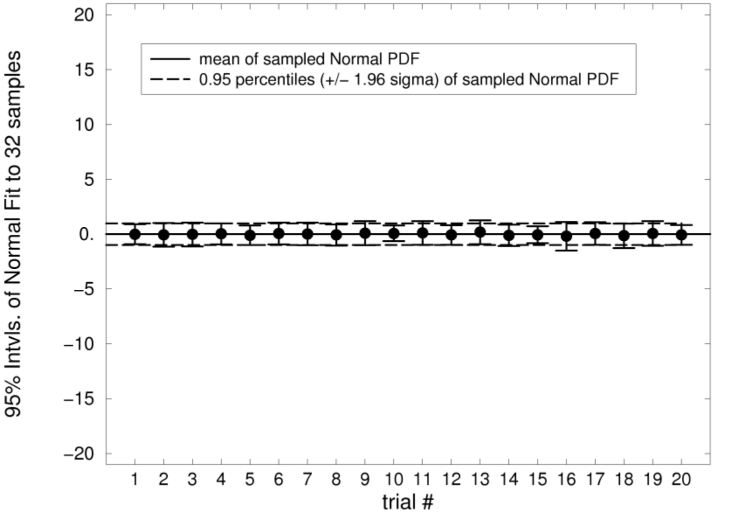


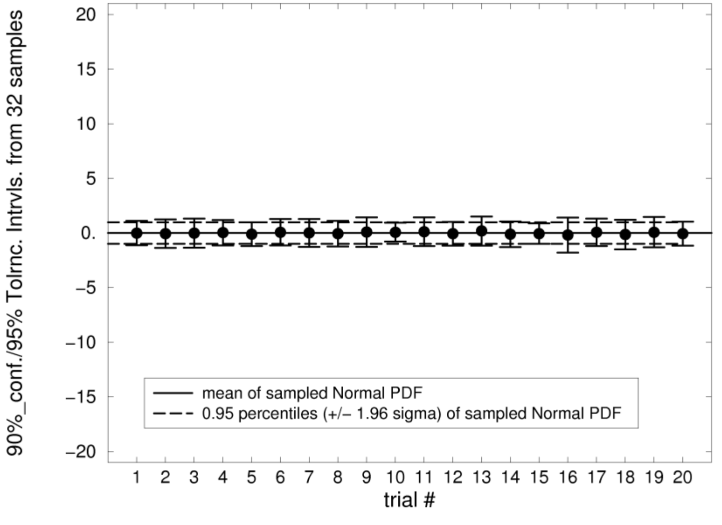
- **Interval estimation improves markedly as # of samples increases to 8.**

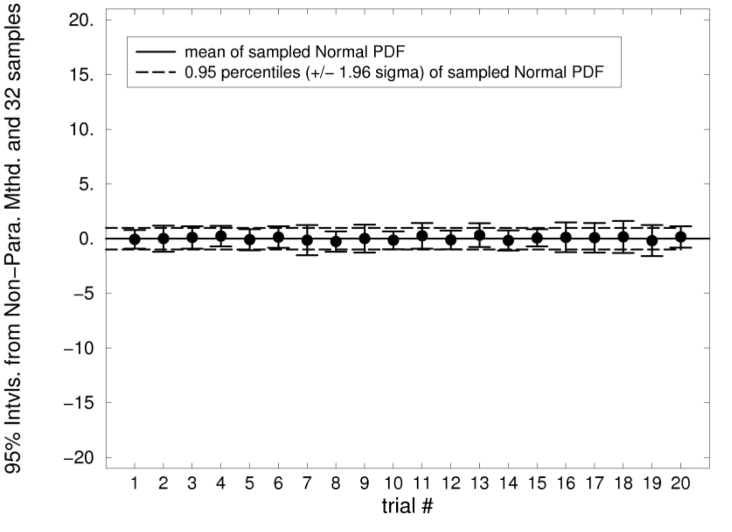
Glimpse of 95% Intervals from the Four Methods

– 20 trials per method, <u>32</u> random samples of a Normal PDF per trial









- **Differences in method performance diminish for “large” # of samples.**

Quantification of Error of 95% Intervals produced by the various methods

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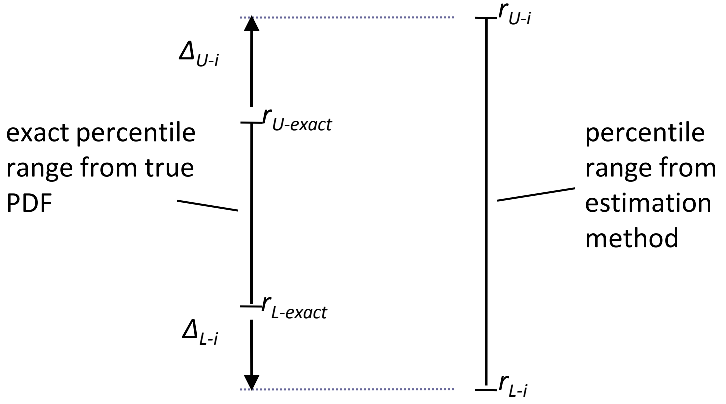
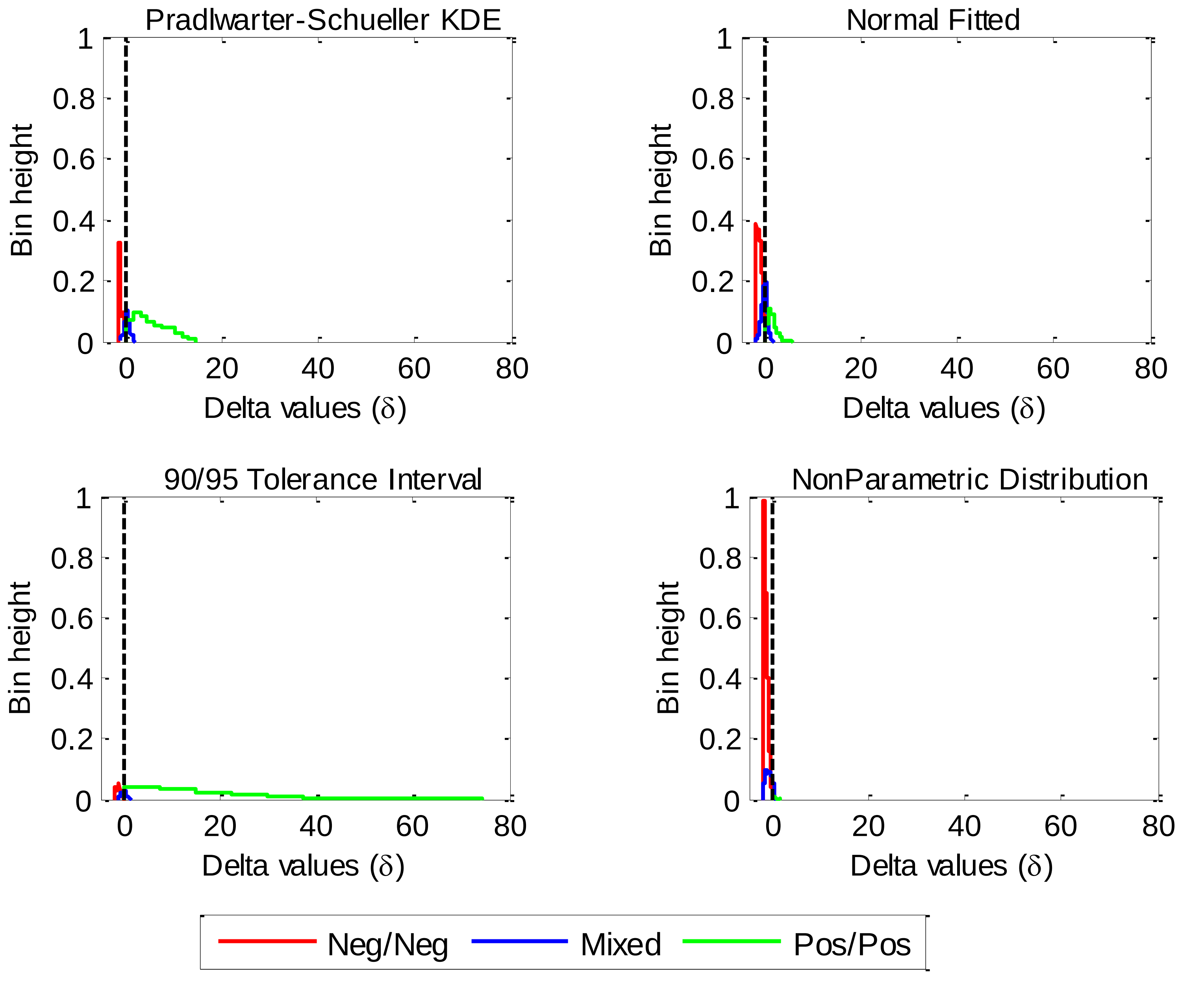
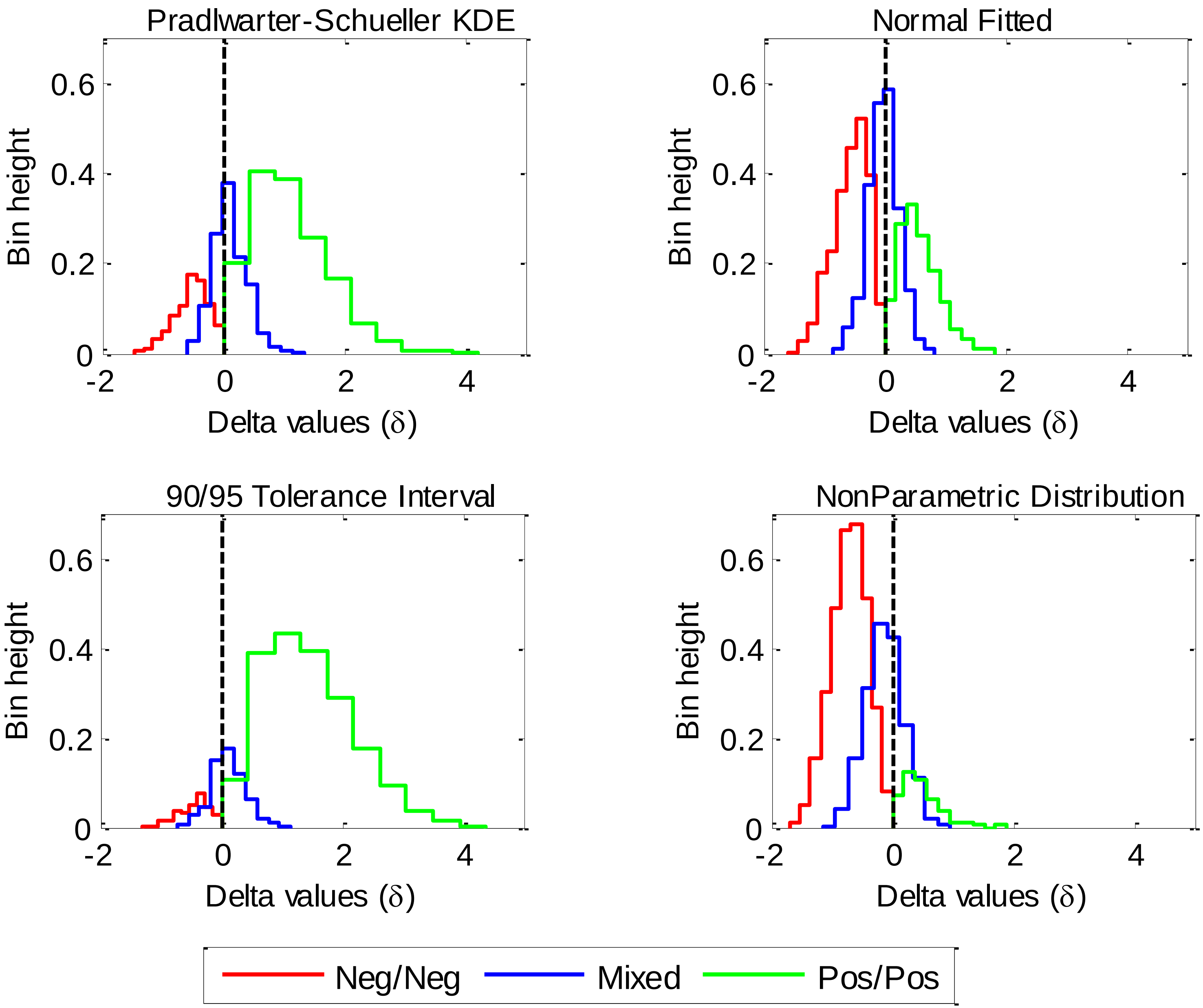
- **Interval estimation error is quantified and put into one of three bins as follows:**
  - **+/+** *or* **pos/pos error (**both Δ_U and Δ_L in schematic at right are positive**)**
    - **estimated interval exceeds true 95% range at both top and bottom (estimated interval encompasses true interval)**
    - **most desirable according to objective**
  - **+/− *or* −/+ "mixed" error (**Δ_U and Δ_L are of opposite sign**)**
    - **estimated interval encompasses true 95% range at one end, but falls short at other end**
    - **less desirable**
  - **−/−** *or* **neg/neg error (**both Δ_U and Δ_L are negative**)**
    - **estimated interval falls short of true 95% range at both top and bottom**
    - **least desirable**



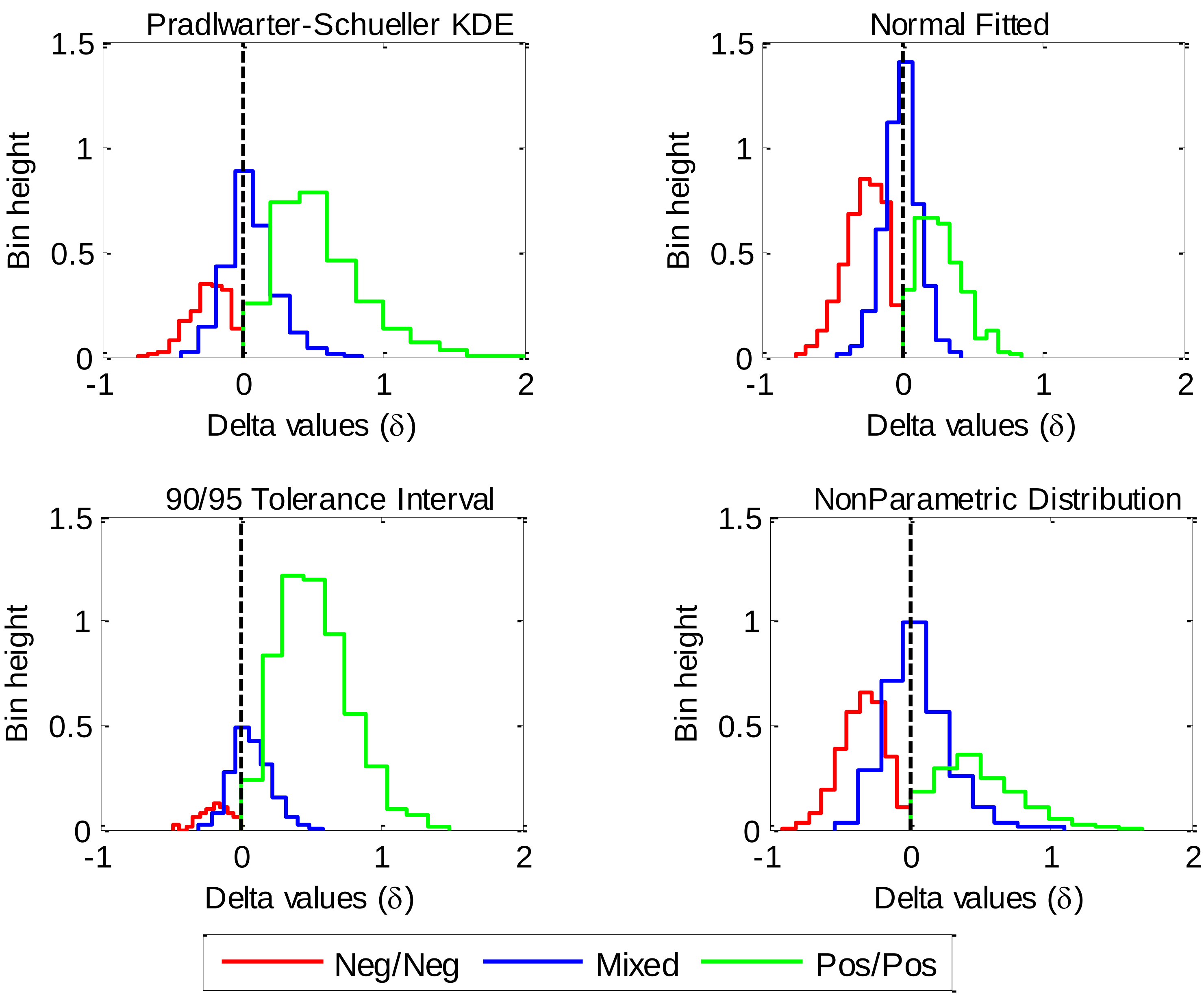
Error histograms — Normal PDF, 2 samples



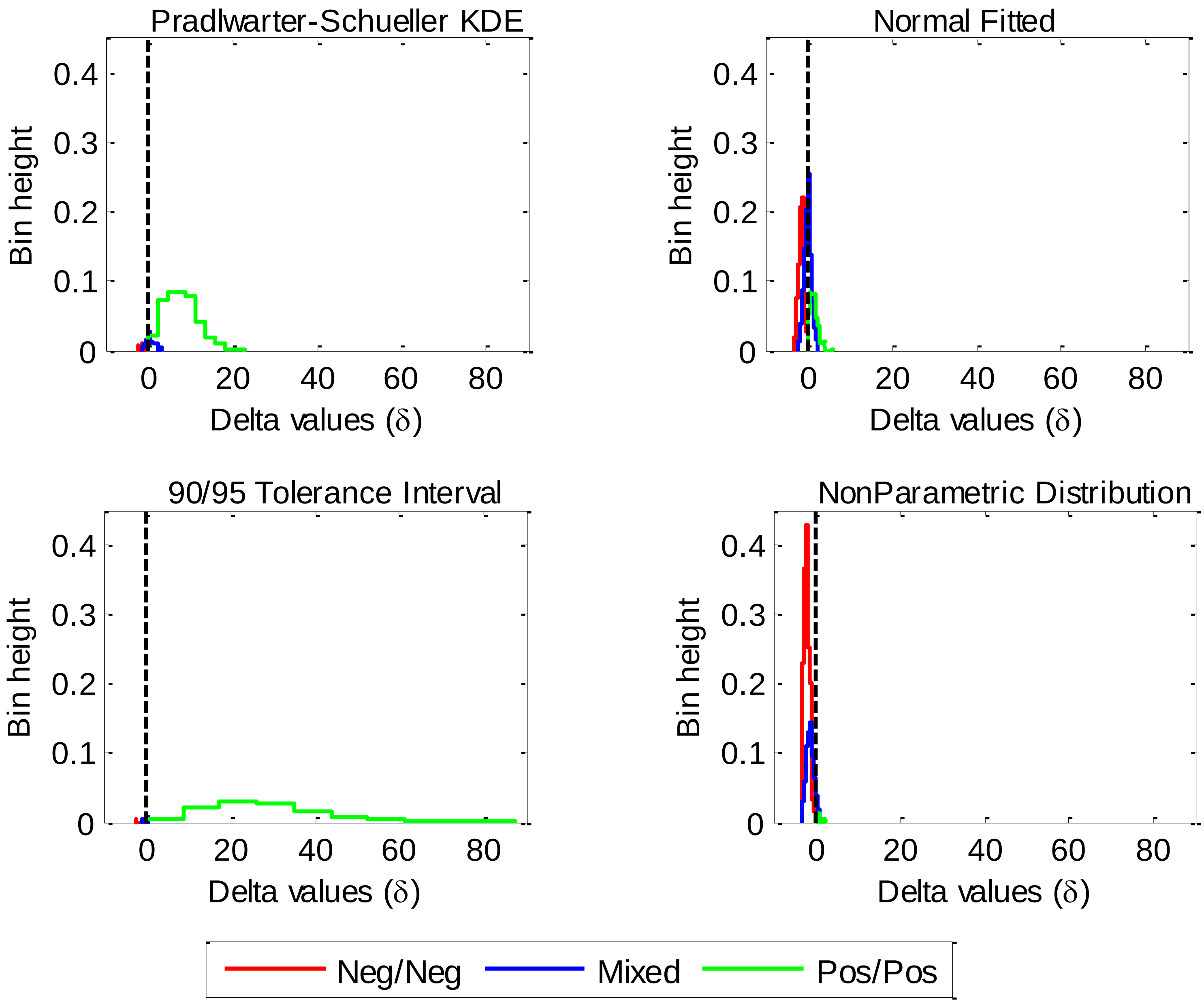
Error histograms — Normal PDF, 8 samples



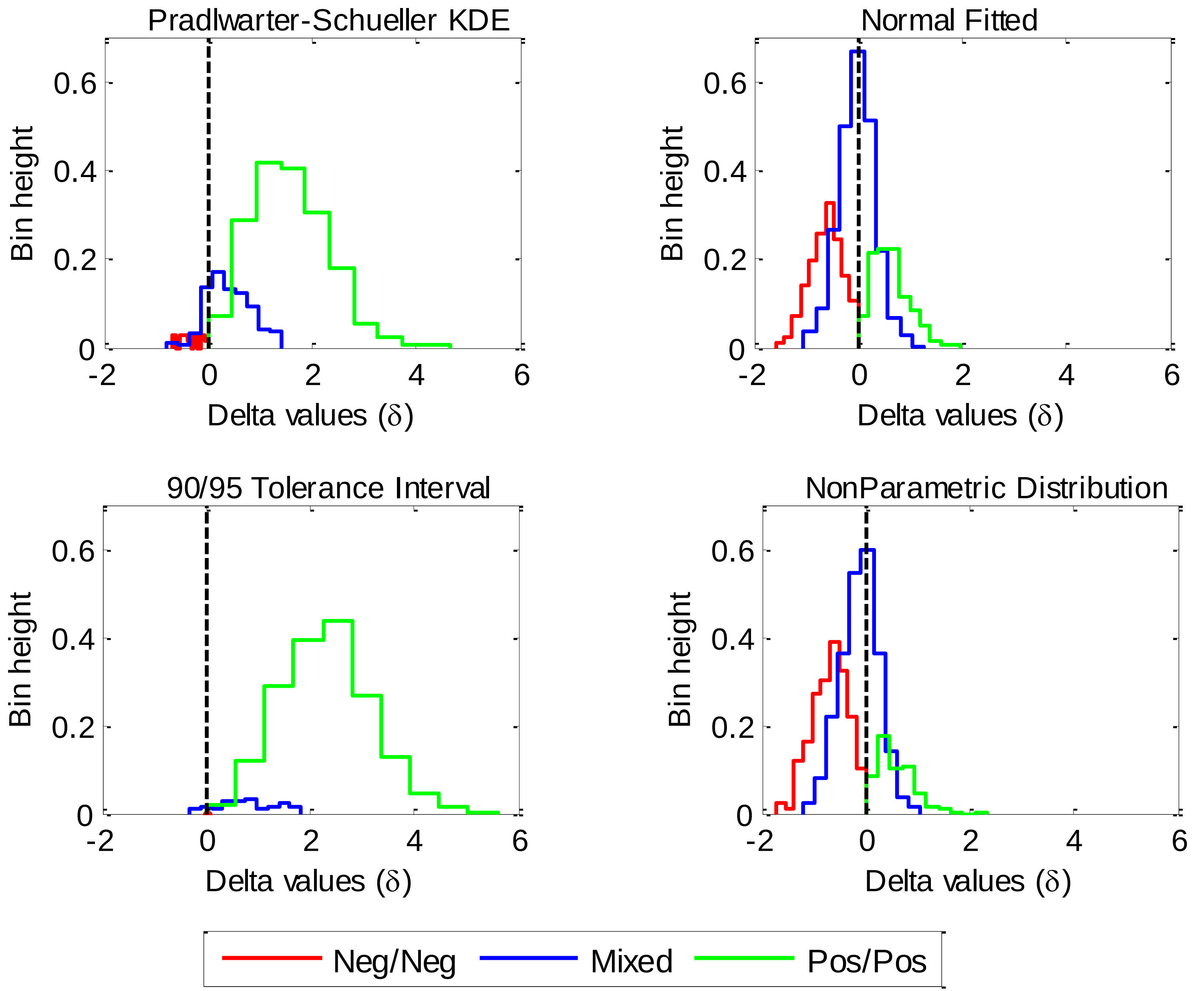
Error histograms — Normal PDF, 32 samples



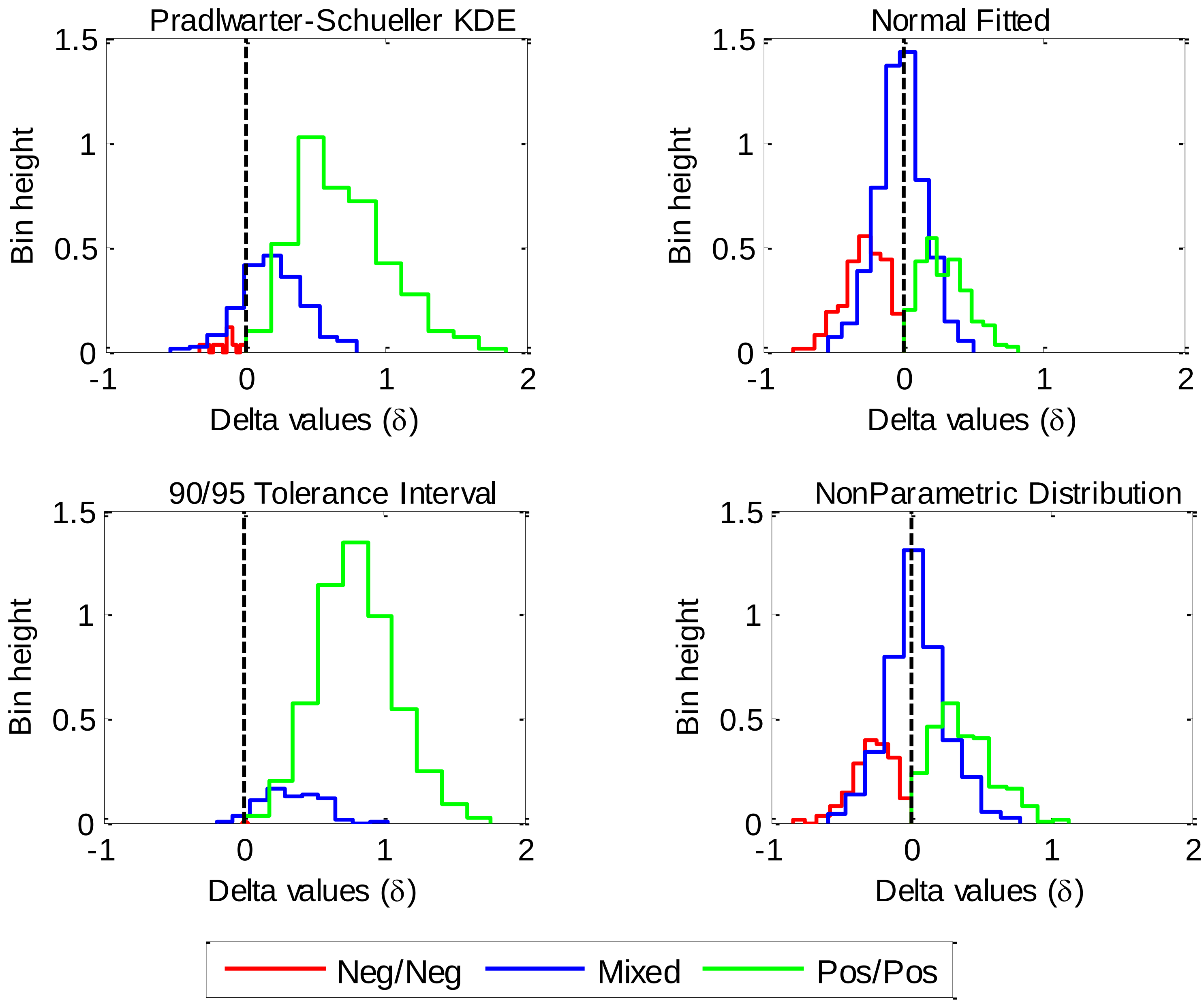
Error histograms — Convolution, 2 samples



Error histograms — Convolution, 8 samples



Error histograms — Convolution, 32 samples



% of Errors in +/+, −/−, and mixed categories for each Method

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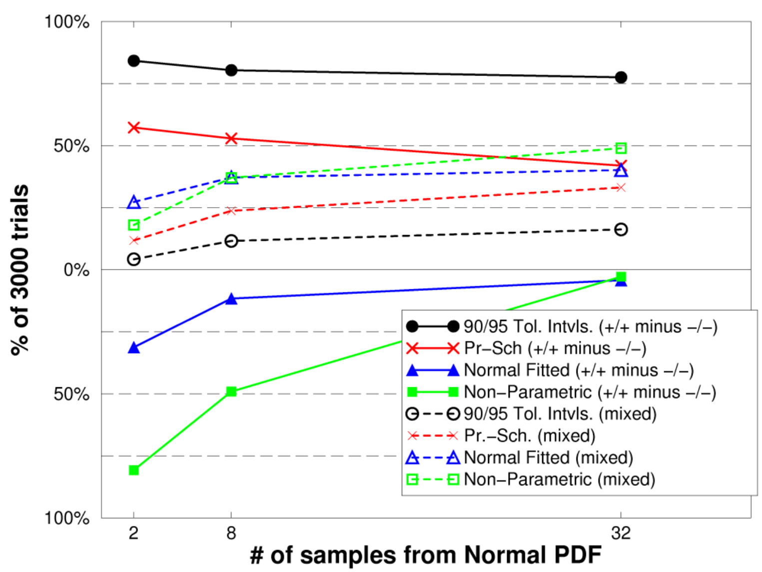
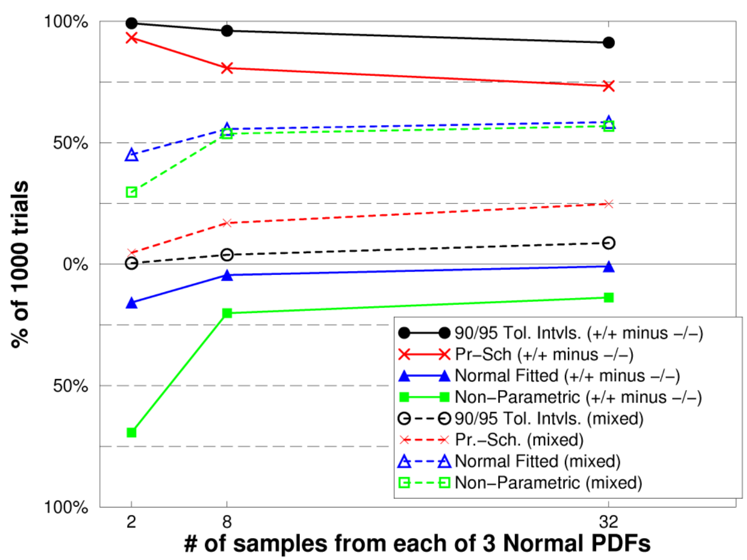
Performance in Fitting Normal PDF



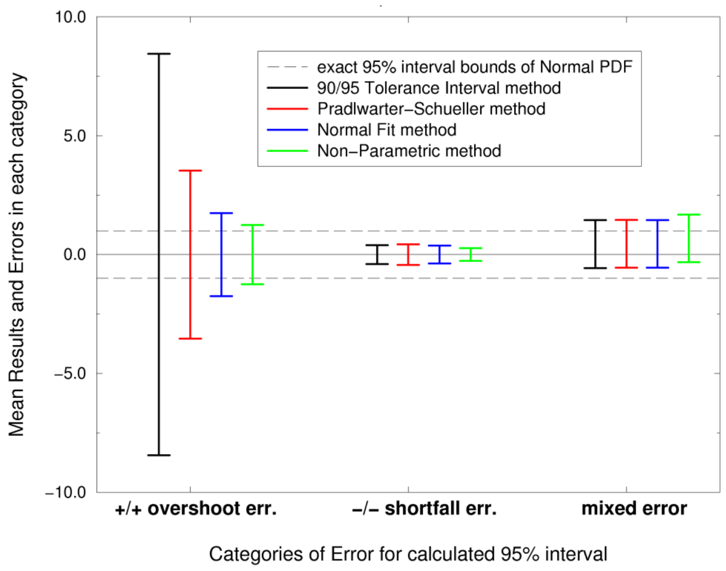
Performance in Convolution



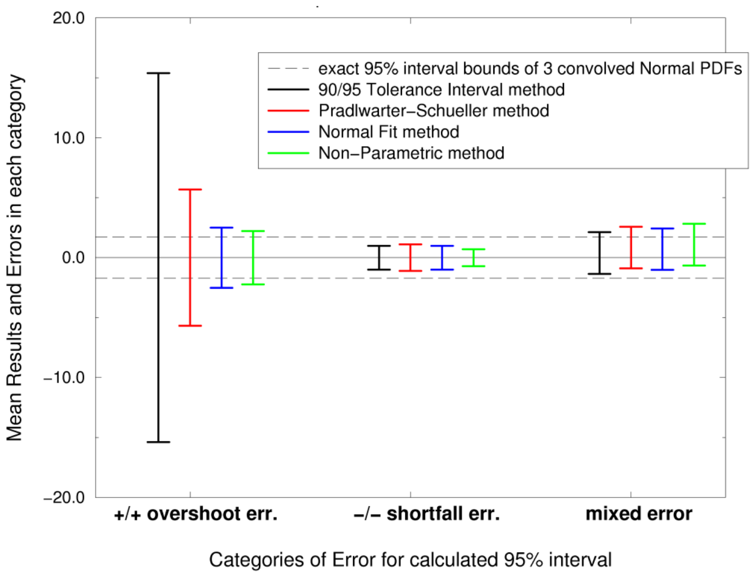
- **The higher the solid lines in the graphs, the more net desirable results (%pos/pos results minus %neg/neg results) occurred.**
- **This desirability measure falls slowly for the better performers (Tol. Intervals and Pr-Sch) with increasing # of samples as the % of less desirable mixed results rises slowly (dashed lines). Proportions of +/+, −/−, and mixed results for Normal-Fit and Non-Para. mthds. improve w/ #samples but still net-undesirable even at 32 samples.**
- **These trends persist for performance in convolution, with slight improvement generally in desirability of percentages of results in the +/+, −/−, and mixed bins.**

Mean Results and Error Magnitudes in each Category for each Method at n=2 samples

Performance in Fitting Normal PDF



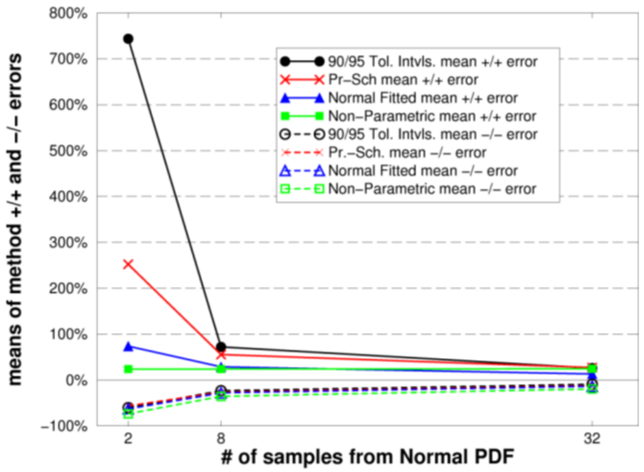
Performance in Convolution

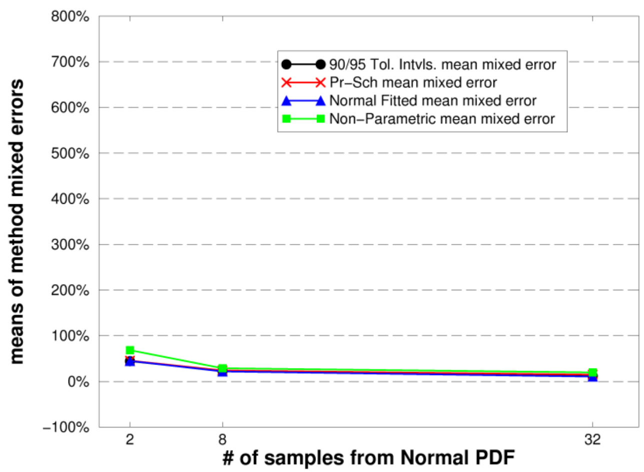


- **Tol. Interval method has much larger average overshoot errors (in +/+ category) than all other methods, with Pr-Sch next largest, then Normal-Fit and Non-Para. Mthds.**
- **Tol. Interval method is least desirable in this performance objective, then Pr-Sch, then the Normal-Fit method, with the Non-Parametric method being most desirable.**
- **Method differences much smaller for −/− shortfall errors and mixed +/− and −/+ errors.**
- **Conclusions same for performance in convolution, where +/+ overshoot errors are generally slightly larger %wise, but the −/− and mixed errors are generally smaller %wise (see next slide).**

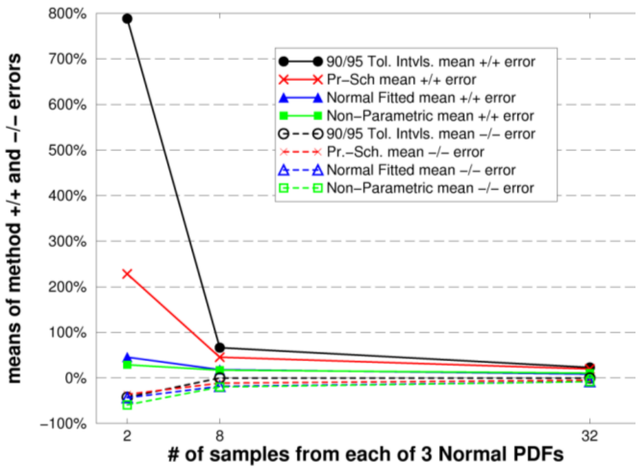
Mean %Error Magnitudes for each method vs. # of samples

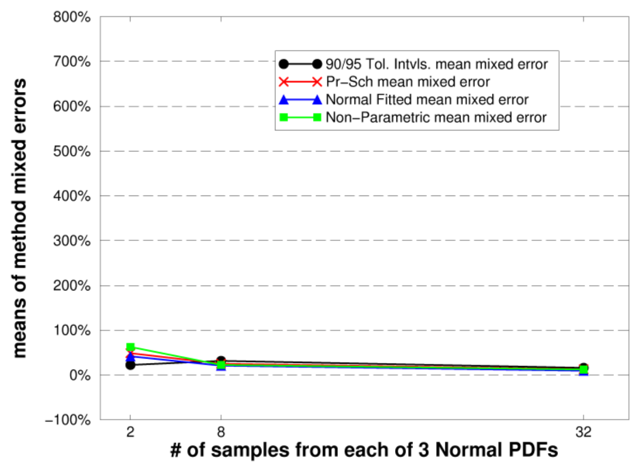
Performance in Fitting Normal PDF



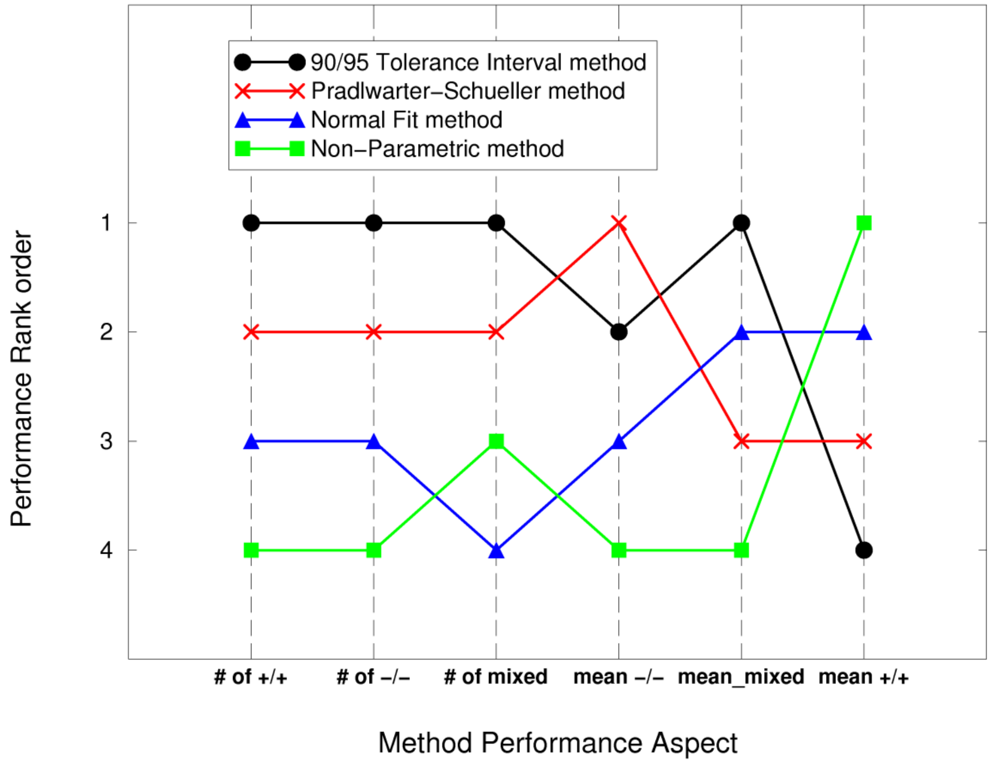


Performance in Convolution





Zeroth-Order Ranking Scheme for Method Performance



- **No method consistently best for all six performance attributes.**
- **Total score across all six attributes yields the following ranking:** **1**-Tol. Intervals, **2**-Pr-Sch, **3**-Normal Approximation, **4**-Non-Parametric mthd.
- **Method ranking on total score is robust whether maximum instead of mean errors are considered, or Normal PDF or Convol., or n=2,8,32.**

Tentative Conclusions based on this Initial Partial Study (Normal PDFs)

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- **Tolerance Interval method performed best on balance according to the simple ranking scheme employed. The method is also very simple to use.**
- **However, the Zeroth-Order ranking scheme used is very simplistic:**
  - weights all six attributes equally
  - only considers performance order in each attribute, not *how much better* one method performs vs. another.
- **A different ranking could occur with a more sophisticated performance scoring system and when the other aspects of the fuller study are performed.**
  - In particular, Pradlwarter-Schueller KDE general performed well and at low # of samples has less egregious +/+ overshoot errors than Tol. Intvls., but also has significantly less desirable +/+ results and significantly more undesirable −/− & mixed results than Tol. Intvls. Implementation of the Pr-Sch method is also considerably more involved.
- **The disadvantage of large Tol. Intvl. +/+ overshoot errors relative to the other methods diminishes by 8 samples, but the advantage in terms % of net desirable results remains through 32 samples.**
- **The common practice of fitting a Normal distribution to the data underperforms even if the underlying PDF being sampled is Normal!**
  - This common practice is inadequate for dealing with sparse data and should be abandoned in favor of the Tolerance Interval or Pradlwarter-Schueller KDE approaches.
- **The presence of multiple sources of uncertainty in aggregation (convolution) does not substantially lessen the effect of method approximation errors in representation of the individual contributing PDFs.**