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Title: Statistical Testing for MCNP

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LA-UR-YY-NNNNN

Statisitical Testing for MCNP

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Background - Ideology

- Statistical testing is used when exact answers cannot be replicated
- The sampling distribution of the mean of a variable will be normally distributed
- Compare tallies from two random number sequeneces (rand card)
- Use a specific tally as ensemble via bins

Testing

Tally bins should be well converged

- Valid Confidence Intervals
- Regular Tallies: Std. err $<=$ 0.05
- Point detectors: Std. err $<=$ 0.1
- VOV $<$ 0.1 recommended but not always available.

StatsTools

Ideology encapsulated into two Python tools

- Python Dependencies: MCNPTools, scipy
- do_mctal_stats.py
- do_meshtal_stats.py

do_mctal_stats.py

```
bash-4.2$ do_mctal_stats.py --help
usage: do_mctal_stats.py [-h] --new NEW --ref REF
       --tally TALLY [--err ERR] [--pcrit PCRIT] [--report]

optional arguments:
  -h, --help      show this help message and exit
  --new NEW       New mctal file
  --ref REF       Reference mctal file
  --tally TALLY   Tally number to process
  --err ERR       Allow values equal or less than this relative error
         ( default: 0.05 )
  --pcrit PCRIT   Critical pvalue to use for statistical tests
         ( default: 0.005 )
  --report        Report bin by bin analysis
```

Statisical Significance

- Statistically probable measurements
- Validation ”Good”=”Not Bad”
- Critical levels for probability 0.05, 0.01, 0.005

Statisical Tests

- Z^2, $\log P$ summed (both follow χ^2 distributions)
- Z, P binned (Std. normal vs uniform)
- Z, P Kolmogorov Smirnov (erf vs linear)

Z-Values

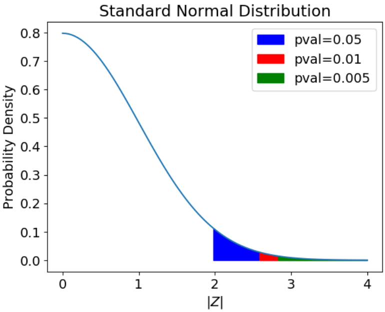
The Z-value statistic of normally distributed values follow a standard normal distribution.

- $Z_i = \frac{x_i - y_i}{\sqrt{s_{x_i}^2 + s_{y_i}^2}}$
- x_i is the tally result obtained via one random number sequence
- y_i is the tally result obtained via a different sequence
- s_{x_i, y_i} is the standard deviation
- $Z_i \approx 0$ values are thrown away (not statisticaly different)

The standard deviation is computed from the MCNP estimated standard error

P-Values

- *P*-value defines the probability of a measured *Z* or higher
- $P = \frac{1}{2}(1 - erf(\frac{|Z|}{2}))$



P-Values

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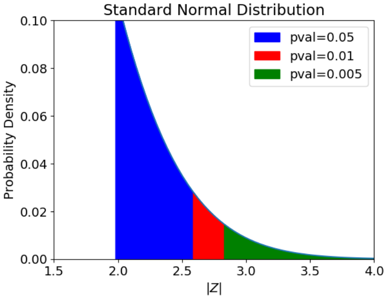
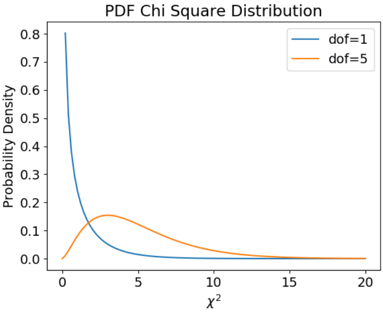


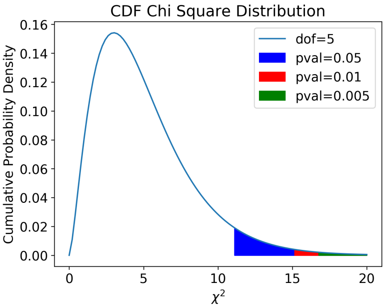
Chi squared background

- Z_i is normally distributed
- $\chi^2 = \sum_{i=1}^{N} Z_i^2$
- $dof = NN =$ number of bins
- Then χ^2 follows a chisquare distribution



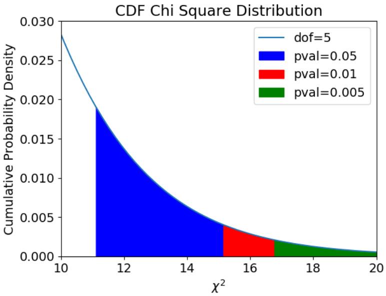
Chi squared background

- p-values define the probability of a measured χ^2 or higher



Chi squared background

- *p*-values define the probability of a measured χ^2 or higher



Chi squared summed testing

- $\chi^2 = \sum_i^N Z_i^2$
- $\chi^2 = -2 \sum_i^N \log(2 * P_i)$
- From each computed and χ^2 a p-value can be computed with respect to the χ^2 distribution

Chi squared binned testing

- specify a number of bins (nbins=21,20) for Z,P
- prepare histogram bins for Z,P
- Compute bin boundaries such that the volumes of the bins are equal.

Chi squared binned testing

- O_j is the number of Z, P within bin j
- $\chi_j = \frac{(O_j - E_{exp})^2}{E_{exp}}$
- $\chi^2 = \sum_j^{nbins} \chi_j$
- A p-value can be computed for this χ^2

Kolmogorov-Smirnov Z,P values testing

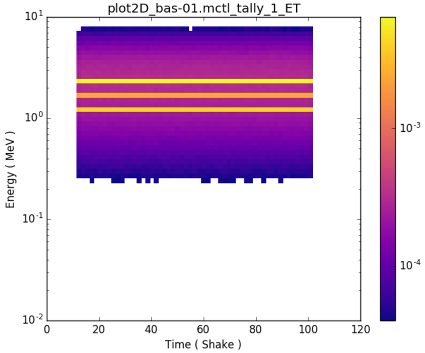
- Construct CDF of sorted Z, P values
- Construct corresponding CDF
  - CDF for Z is $\frac{1}{2}erf(\frac{Z}{\sqrt{2}})$
  - CDF for P is P (linear).
- Look for largest separation between the two
- This distance is the d-value
- Compute corresponding p-value

Test Problem bas-01

```
SDEF POS=0 0 0 RAD=D1 ERG=D2 TME=D3
c
SI1    0 1              $ RAD distribution
SP1  -21 2
c
SI2  S 21  22           $ ERG distribution
SP2      1  2.
SP21 -3                 $ Watt spectrum
SI22 L  1.1  1.5  2.0   $ Discrete lines
SP22     2    1   3.
c
SI3  H  10   100          $ Pulse
SP3    0    1
c
F1:N 1                    $ ERG and TME tallies
E1  1E-2 63ilog 10
T1  5 63i 110
c
F11:N 1                     $ ERG Only
E11  1E-2 255ilog 20
```

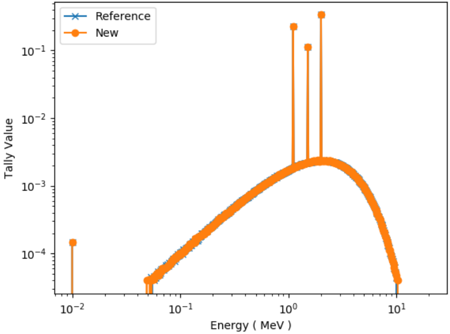
Test Problem bas-01 - Surface Tally 1

- Time - Uniform pulse distribution
- Energy - 3 lines + Watt Spectrum
- Space - Spherical Volue $r = 1cm$



Test Problem bas-01 - Surface Tally 11

- Energy - 3 lines + Watt Spectrum



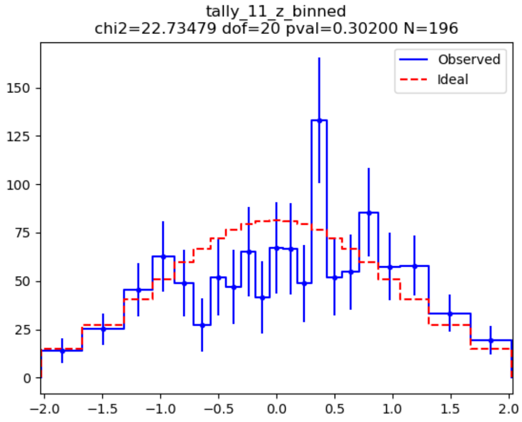
Test Problem bas-01

```
Processing tally: 11
Nonzero scores: 256 Z Critcal: 2.6600674686174592
Warning! LargeZ: 2.815806122121412 valref: 0.0029065 valnew: 0.002975 errref: 0.0059 errnew: 0.00
Warning! LargeZ: 2.829843781428351 valref: 0.0011837 valnew: 0.0012276 errref: 0.0092 errnew: 0.0
Total scores                  : 257
Usable scores                 : 196
Unusable scores               : 60
Unusable matching zero scores    : 1
Unusable matching nonzero scores: 0
```

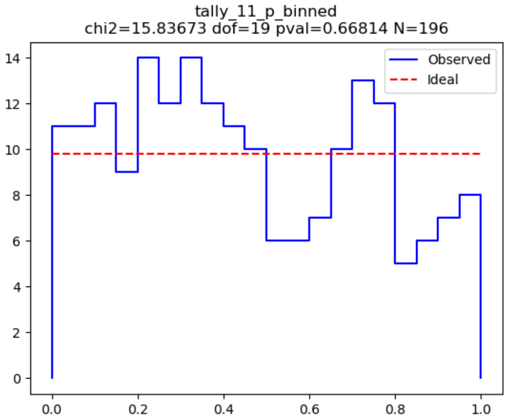
Test Problem bas-01

```
Ref scores with errors <= 0.05   : 196
New scores with errors <= 0.05   : 197
Errors outside crit ratio        : 3.0  count:  0
Minimum non zero error over all ref data: 0.0004
Minimum non zero error over all new data: 0.0004
zspace_binned: scores: 196 chisq: 22.73479444149072 dof: 20 pvalue: 0.30200355809947327
z_summed_test: chisq: 225.5458350589523  dof: 196  pvalue: 0.07261966846939263
zspace_ks: scores: 196 D: 0.11914784582184068 pvalue: 0.006993056520287106
pspace_binned: scores: 196 chisq: 15.836734693877549 dof: 19 pvalue: 0.6681419596523805
pspace_summed: scores: 196 chisq: 440.42402210482635 dof: 392 pvalue: 0.04584767913524263
pspace_ks: scores: 196 D: 0.10042705348936298 pvalue: 0.03572416809095569
```

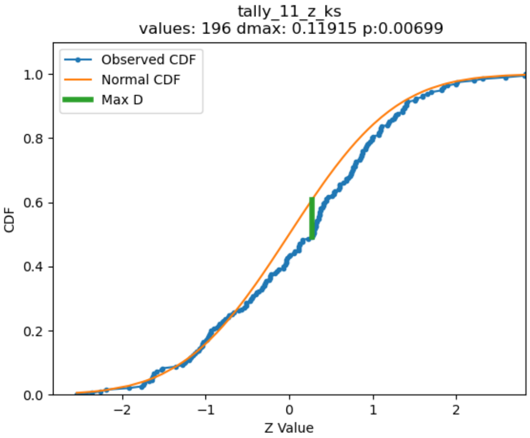
Test Problem bas-01
Surface Tally 11 - *Z* binned



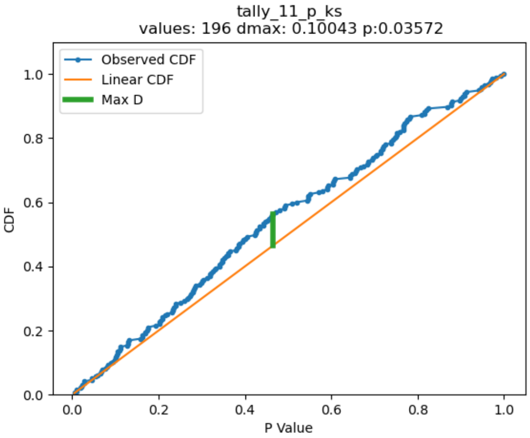
Test Problem bas-01
Surface Tally 11 - *P* binned



Test Problem bas-01
Surface Tally 11 - Kolmogorov Smirnov



Test Problem bas-01
Surface Tally 11 - Kolmogorov Smirnov



Test Problem bas-01 modified

```
Basic Source in a Sphere
100     0     -1     IMP:N=1   $  inside sphere
999     0      1     IMP:N=0   $  outside world

1  SO  1

print
MODE N
NPS 1E7
PRDMP 2J +1
c
SDEF POS=0 0 0 RAD=D1 ERG=D2 TME=D3
c
SI1   0 1               $ RAD distribution
SP1 -21 2
c
SI2  S 21  22           $ ERG distribution
SP2     1.01  2
SP21 -3                 $ Watt spectrum
SI22 L  1.1 1.5 2.0     $ Discrete lines
SP22     2   1  3.05
c
SI3  H  10  100          $ Pulse
SP3     0    1
c
F1:N 1                   $ ERG and TME tallies
E1  1E-2 63ilog 10
T1  5 63i 110
c
F11:N 1                   $ ERG Only
E11  1E-2 255ilog 20
```

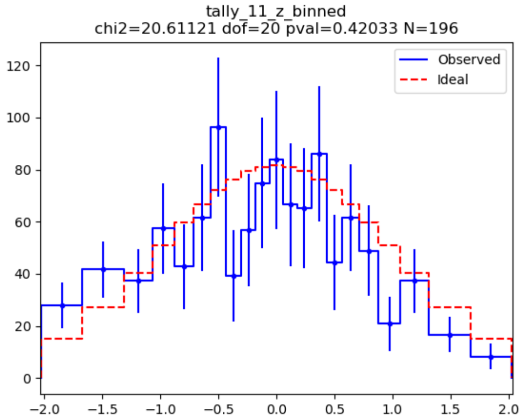
Test Problem bas-01 modified

```
Total scores                    : 257
Usable scores                   : 196
Unusable scores                 : 60
Unusable matching zero scores   : 1
Unusable matching nonzero scores: 0
Ref scores with errors <= 0.05  : 196
New scores with errors <= 0.05  : 197
Errors outside crit ratio       : 3.0  count: 0
Minimum non zero error over all ref data: 0.0004
Minimum non zero error over all new data: 0.0004
```

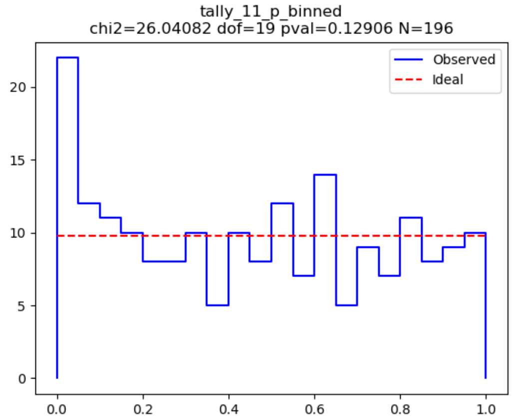
Test Problem bas-01 modified

```
Minimum non zero error over all new data: 0.0004
zspace_binned: scores: 196 chisq: 20.61121148274366 dof: 20 pvalue: 0.4203251973217062
z_summed_test: chisq: 298.8060630841057  dof: 196  pvalue: 3.0624173630059094e-06
 Failure! Z Summed pvalue < pcrit 3.0624173630059094e-06 0.005
zspace_ks: scores: 196 D: 0.13856774091732865 pvalue: 0.000958291677962661
 Failure! KS normal pvalue < pcrit 0.000958291677962661 0.005
pspace_binned: scores: 196 chisq: 26.04081632653061 dof: 19 pvalue: 0.12905571066264981
pspace_summed: scores: 196 chisq: 521.3030690394801 dof: 392 pvalue: 1.2590408950300071e-05
 Failure! P Summed pvalue < pcrit: 1.2590408950300071e-05 0.005
pspace_ks: scores: 196 D: 0.1034116844159888 pvalue: 0.0280643749049152
```

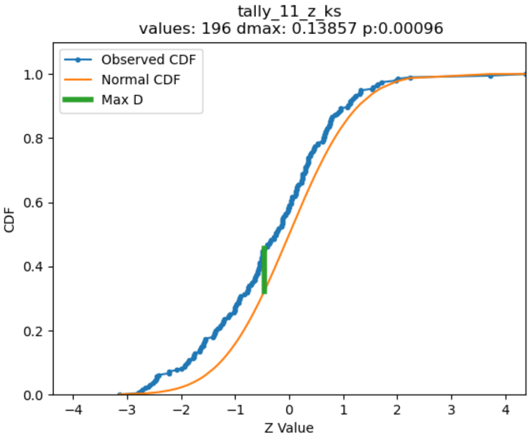
Test Problem bas-01 modified Surface Tally 11 - *Z* binned



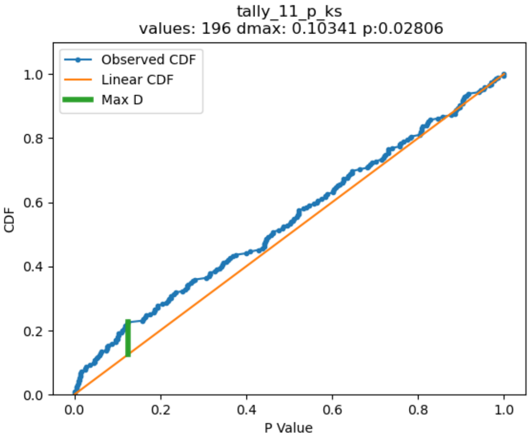
Test Problem bas-01 modified Surface Tally 11 - *P* binned



Test Problem bas-01 modified
Surface Tally 11 - *Z* Kolmogorov Smirnov



Test Problem bas-01 modified
Surface Tally 11 - *P* Kolmogorov Smirnov



Test Problem bas-01 –report option

```
Processing tally: 11
...
Binname   Ref Val  Ref Err   New Val  New Err   Z-Value  P-Value  CI Analysis
---------------------------------------------------------------------------------
     E0 1.495e-04 0.02590 1.489e-04 0.02590  -0.10979 0.91258  ValidCIs
     E1 6.400e-06 0.12500 6.700e-06 0.12220                    Both invalid
    E20 1.520e-05 0.08110 1.520e-05 0.08110                    Exact Nonzero
    E41 4.050e-05 0.04970 4.120e-05 0.04930   0.24479 0.80662  ValidCIs
    E42 3.970e-05 0.05020 4.240e-05 0.04860                    Valid new, invalid ref
    E62 1.021e-04 0.03130 1.021e-04 0.03130                    ValidCI Exact Values
    E74 1.777e-04 0.02370 1.618e-04 0.02490  -2.72811 0.00637  ValidCIs LargeZ
```

Future work

- Is *P* sensitive enough?
- Added statistical tests
- Distribute with MCNPTools
- Variance reduction testing
- Particle physics testing