Basic statistics, and applications to X-ray spectral fitting

✓ Normal error (Gaussian) distribution

Most important in statistical analysis of data, describes the distribution of random observations for many experiments

✓ Poisson distribution

Generally appropriate for counting experiments related to random processes (e.g., radioactive decay of elementary particles)

✓ Statistical tests: χ^2 and F-test (more on these in the XSPEC tutorial)

Additional specific applications within XSPEC in the X-ray spectral analysis tutorial

All measurements should be provided with errors

• Measurement $X \pm \delta X$ (units of measure)



Error associated with the measurement X

- Significant digits:
- g (gravitational acceleration of an object in a vacuum near the Earth surface)= $=9.82\pm0.02385$ m/s² \rightarrow 9.82 ± 0.02 m/s²

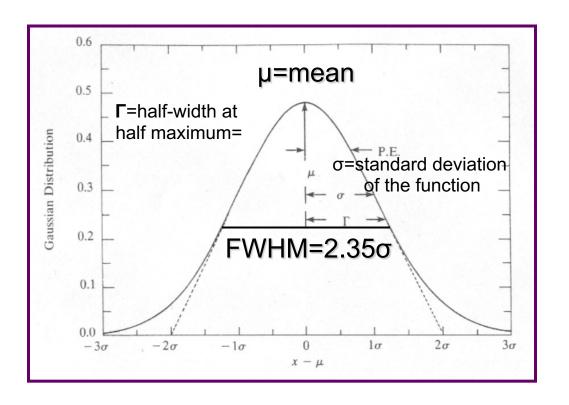
Another example: $v=100.2 \pm 30 \text{ m/s} \rightarrow 100 \pm 30 \text{ m/s}$

Relative (fractionary) uncertainty: δX/X

The Gaussian (normal error) distribution. I

Averages of random variables (sufficiently large in number) independently drawn from independent distributions converge in distribution to the normal Casual errors are above and below the "true" (most "common") value

→ bell-shape distribution if systematic errors are negligible



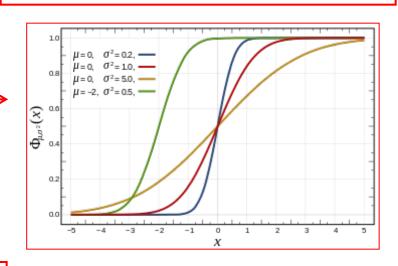
The Gaussian probability function. II

$$P(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

normalization factor, so that $\int f(x) dx = 1$

Probability Density Function (centered on μ)

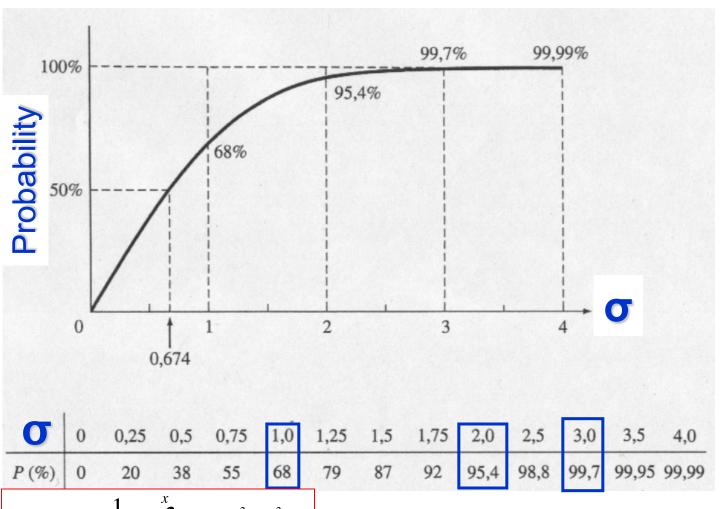
μ=mean (expectation) value
 σ=standard deviation
 σ²=variance



 $a^{-x^2/2\sigma^2}$

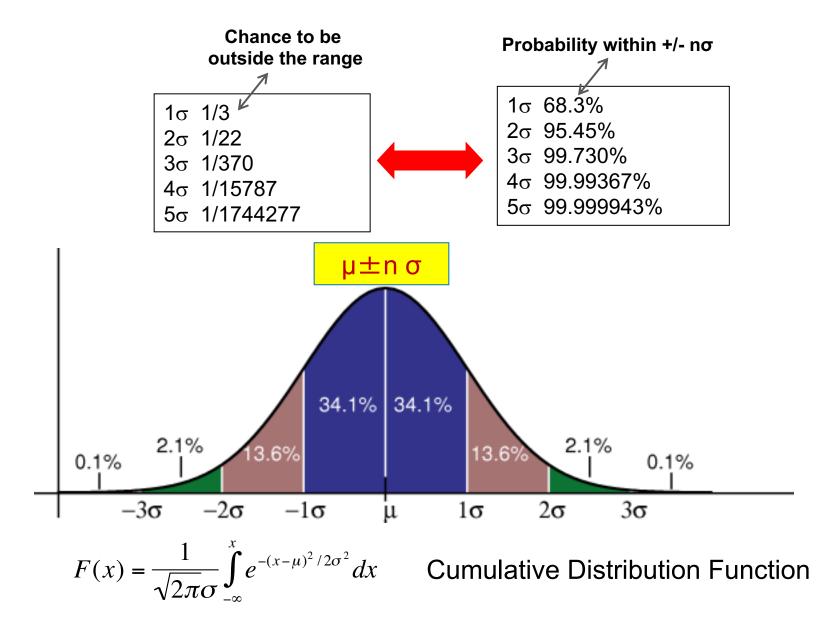
function centered on 0

The Gaussian probability function. III



 $F(x) = \frac{1}{\sqrt{2\pi}\sigma} \int e^{-(x-\mu)^2/2\sigma^2} dx$

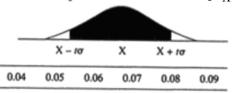
Cumulative Distribution Function



Value ± error at 1σ confidence level: if we make a measurement N times, in 68.3% of the times we obtain such value

Every measurement should be reported and considered along its own error

Percentage probability P within to: $P = \int_{x-t\sigma}^{x+t\sigma} G(x) dx$



Bevington textbook

						$X - \iota \sigma$		X	$X + t\sigma$		
t	0.00	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09	
0.0	0.00	0.80	1.60	2.39	3.19	3.99	4.78	5.58	6.38	7.17	
0.1	7.97	8.76	9.55	10.34	11.13	11.92	12.71	13.50	14.28	15.07	
0.2	15.85	16.63	17.41	18.19	18.97	19.74	20.51	21.28	22.05	22.82	
0.3	23.58	24.34	25.10	25.86	26.61	27.37	28.12	28.86	29.61	30.35	
0.4	31.08	31.82	32.55	33.28	34.01	34.73	35.45	36.16	36.88	37.59	
0.5	38.29	38.99	39.69	40.39	41.08	41.77	42.45	43.13	43.81	44.48	
0.6	45.15	45.81	46.47	47.13	47.78	48.43	49.07	49.71	50.35	50.98	
0.7	51.61	52.23	52.85	53.46	54.07	54.67	55.27	55.87	56.46	57.05	
8.0	57.63	58.21	58.78	59.35	59.91	60.47	61.02	61.57	62.11	62.65	
0.9	63.19	63.72	64.24	64.76	65.28	65.79	66.29	66.80	67.29	67.78	
1.0	68.27	68.75	69.23	69.70	70.17	70.63	71.09	71.54	71.99	72.43	
1.1	72.87	73.30	73.73	74.15	74.57	74.99	75.40	75.80	76.20	76.60	
1.2	76.99	77.37	77.75	78.13	78.50	78.87	79.23	79.59	79.95	80.29	
1.3	80.64	80.98	81.32	81.65	81.98	82.30	82.62	82.93	83.24	83.55	
1.4	83.85	84.15	84.44	84.73	85.01	85.29	85.57	85.84	86.11	86.38	
1.5	86.64	86.90	87.15	87.40	87.64	87.89	88.12	88.36	88.59	88.82	
1.6	89.04	89.26	89.48	89.69	89.90	90.11	90.31	90.51	90.70	90.90	
1.7	91.09	91.27	91.46	91.64	91.81	91.99	92.16	92.33	92.49	92.65	
1.8	92.81	92.97	93.12	93.28	93.42	93.57	93.71	93.85	93.99	94.12	
1.9	94.26	94.39	94.51	94.64	94.76	94.88	95.00	95.12	95.23	95.34	
2.0	95.45	95.56	95.66	95.76	95.86	95.96	96.06	96.15	96.25	96.34	
2.1	96.43	96.51	96.60	96.68	96.76	96.84	96.92	97.00	97.07	97.15	
2.2	97.22	97.29	97.36	97.43	97.49	97.56	97.62	97.68	97.74	97.80	
2.3	97.86	97.91	97.97	98.02	98.07	98.12	98.17	98.22	98.27	98.32	
2.4	98.36	98.40	98.45	98.49	98.53	98.57	98.61	98.65	98.69	98.72	
2.5	98.76	98.79	98.83	98.86	98.89	98.92	98.95	98.98	99.01	99.04	
2.6	99.07	99.09	99.12	99.15	99.17	99.20	99.22	99.24	99.26	99.29	
2.7	99.31	99.33	99.35	99.37	99.39	99.40	99.42	99.44	99.46	99.47	
2.8	99.49	99.50	99.52	99.53	99.55	99.56	99.58	99.59	99.60	99.61	
2.9	99.63	99.64	99.65	99.66	99.67	99.68	99.69	99.70	99.71	99.72	
2.0	00.70)	00 7	700/		1000	

 3σ =99.73%: in 1000 experiments you can get results outside this $\pm 3\sigma$ range only three times $(1000 \times 0.9973 = 997 \text{ times within the } 3\sigma \text{ range})$

 $5\sigma = 99.99994\%$:

6 cases out of 10⁶

The Poisson distribution

Describes experimental results where events are counted and the uncertainty is not related to the measurement but reflects the **intrinsically casual behavior of the process** (e.g., radioactive decay of particles (Geiger counter), X-ray photons, etc.)

$$P(x) = e^{-\mu} \mu^x / x!$$
 (x=0,1,2,...)

Probability of obtaining x events when μ events are expected x=observed number of events in a time interval (frequency of events)

average number of events

$$\frac{1}{x} = \sum_{x=0}^{\infty} xP(x) = \sum_{x=0}^{\infty} xe^{-\mu} \mu^{x} / x! = \mu$$

→ µ=average number of expected events if the experiment is repeated many times

$$\sigma^{2} = \langle (x - \mu)^{2} \rangle =$$

$$= \sum_{x=0}^{\infty} (x - \mu)^{2} \frac{\mu^{x}}{x!} e^{-\mu} = \mu$$

expectation value of the square of the deviations



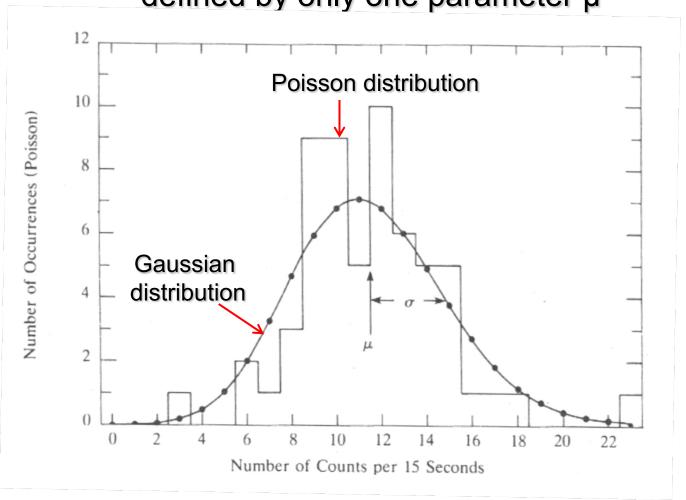
the Poisson distribution with average counts= μ has standard deviation $\sqrt{\mu}$



Example: N_{counts}±√N

High µ: the Poisson distribution is approximated by the Gaussian distribution

defined by only one parameter µ



Statistical test: χ^2 – more on XSPEC tutorial

Test to compare the observed distribution of the results with that expected

$$\chi^2 = \sum_{k=1}^n \frac{(O_k - E_k)^2}{\sigma_k^2}$$

It provides a measure on how much the data differ from the expectations (model), taking into account the errors associated with the measurement (e.g., datapoints)

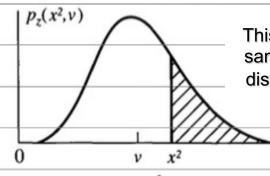
- O_k=observed values (e.g., spectral datapoints)
- E_k=expected values (model, i.e. predicted distribution)
- \circ σ_k =error on the measured values (e.g., error on each spectral bin)
- k=number of datapoints (e.g., bins after rebinning)

$$\chi^2 / dof \approx 1$$



the observed and expected distributions are similar

dof=degrees of freedom = #datapoints - #free parameters



This table gives the probability that a random sample of data, when compared to its parent distribution, would yield values of X²/v larger than the observed value

 x^2

TABLE C.4

Reduced chi-squared distribution

 χ^2 distribution. Values of the reduced chi-square $\chi^2_{\nu} = \chi^2/\nu$ corresponding to the probability $P_{\chi}(\chi^2; \nu)$ of exceeding χ^2 versus the number of degrees of freedom ν_{ν} v=dof=#datapoints - #free parameters

. 4	P=probability of exceeding									
Ψ	0.99	0.98	0.95	0.90	0.80	0.70	0.60	0.50		
1	0.00016	0.00063	0.00393	0.0158	0.0642	0.148	0.275	0.455		
2	0.0100	0.0202	0.0515	0.105	0.223	0.357	0.511	0.693		
3	0.0383	0.0617	0.117	0.195	0.335	0.475	0.623	0.789		
4	0.0742	0.107	0.178	0.266	0.412	0.549	0.688	0.839		
5	0.111	0.150	0.229	0.322	0.469	0.600	0.731	0.870		
6	0.145	0.189	0.273	0.367	0.512	0.638	0.762	0.891		
7	0.177	0.223	0.310	0.405	0.546	0.667	0.785	0.907		
8	0.206	0.254	0.342	0.436	0.574	0.691	0.803	0.918		
9	0.232	0.281	0.369	0.463	0.598	0.710	0.817	0.927		
10	0.256	0.306	0.394	0.487	0.618	0.727	0.830	0.934		
11	0.278	0.328	0.416	0.507	0.635	0.741	0.840	0.940		
12	0.298	0.348	0.436	0.525	0.651	0.753	0.848	0.945		
13	0.316	0.367	0.453	0.542	0.664	0.764	0.856	0.949		
14	0.333	0.383	0.469	0.556	0.676	0.773	0.863	0.953		
15	0.349	0.399	0.484	0.570	0.687	0.781	0.869	0.956		

```
Model phabs<1>*powerlaw<2> Source No.: 1
                                           Active/On
Model Model Component Parameter
                                            Value
par
     comp
           phabs
                                  10^22
                       nH
                                            1.59000E-02
                                                         frozen
                       PhoIndex
           powerlaw
                                            2.72811
           powerlaw
                                            1.51490E-04
                       norm
  Using energies from responses.
Chi-Squared =
                        97.23 using 105 PHA bins.
Reduced chi-squared =
                               0.9440 for
                                              103 degrees of freedom
Null hypothesis probability =
                                 6.417127e-01
```

X²=97.2, 103 d.o.f., Null-hypothesis probability (probability that the model reproduces the data, i.e., no difference between the two distributions)=0.64 (6.4e-01 above)

f(x;k)Table of values of χ^2 in a Chi-Squared Distribution with k degrees of freedom such that p is the area between x^2 and $+\infty$ k=degrees of freedom Probability Content, p, between χ^2 and $+\infty$ 0.995 0.99 0.975 0.95 0.9 0.75 0.5 0.25 0.025 0.01 0.005 0.002 0.1 0.05 0.001 3.927e-5 1.570e-4 9.820e-4 0.00393 0.0157 0.102 0.455 1.323 2.706 3.841 5.024 6.635 7.879 9.550 10.828 0.0100 0.0201 0.0506 0.103 0.211 0.575 1.386 2.773 4.605 5.991 7.378 9.210 10.597 12.429 13.816 0.0717 0.352 0.584 1.213 2.366 4.108 6.251 7.815 9.348 11.345 12.838 14.796 16.266 0.115 0.216 0.207 0.297 0.484 0.711 1.064 1.923 3.357 5.385 7.779 9.488 11.143 13.277 14.860 16.924 18.467 0.412 0.554 0.831 1.145 1.610 2.675 4.351 6.626 9.236 11.070 12.833 15.086 16.750 18.907 20.515 0.676 0.872 1.237 1.635 2.204 3.455 5.348 12.592 14.449 22.458 7.841 10.645 16.812 18.548 20.791 100 67.328 70.065 74.222 77.929 82.358 90.133 99.334 109.141 118,498 124.342 129.561 135.807 140.169 145.577 149.449 101 68.146 70.901 75.083 78.813 83.267 91.085 100.334 110.189 119.589 125.458 130.700 136.971 141.351 146.780 150.667 102 84.177 147.982 68 965 71.737 75 946 79 697 92.038 101 334 111.236 120 679 126 574 131.838 138 134 142 532 151.884 103 69.785 72.575 76.809 80.582 85.088 92.991 102.334 112.284 121.769 127.689 132.975 139.297 143.712 149.183 153.099 70.606 73.413 77.672 81.468 85.998 103.334 113.331 122.858 128.804 134.111 140.459 144.891 150.383 154.314

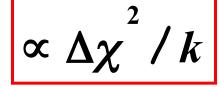
0.01

 10^{-3}

Statistical test: F-test – more on XSPEC tutorial

If two statistics following the χ^2 distribution have been determined, the ratio of the reduced chi-squares is distributed according to the F distribution

$$P_f(f;v_1,v_2) = \frac{\chi_1^2/v_1}{\chi_2^2/v_2}$$



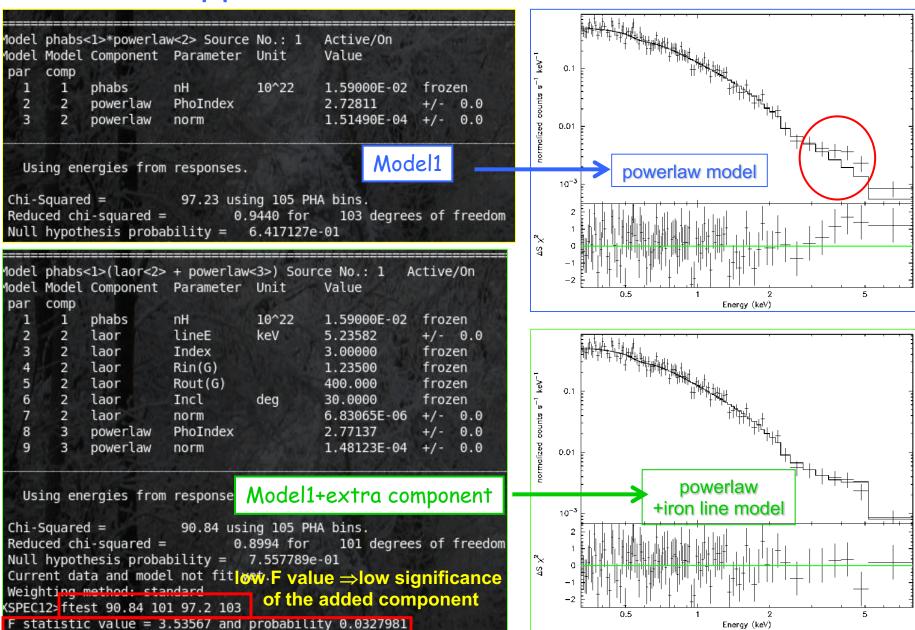
with k=number of additional terms (parameters)



Example: Use the F-test to evaluate the improvement to a spectral fit due to the assumption of a different model, with additional terms

- Conditions: (a) the simpler model is nested within the more complex model;
 - (b) the extra parameters have Gaussian distribution (not truncated by the parameter space boundaries)
 - → see the F-test tables for the corresponding probabilities (specific command in XSPEC)

An application of the F-test within XSPEC



F-test probability in XSPEC: probability of exceeding F (see tabulated values)

Fit
$$(2)$$
 = Fit (1) + one component

xspec> ftest χ^2 (best fit) dof (best fit) χ^2 (previous fit) dof (previous fit)

xspec> ftest 90.8 101 97.2 103 → ftest=3.54 → prob=0.0328

$$F_t = (\frac{\chi^2(dof) - \chi^2(dof - k)}{dof - (dof - k)}) / (\chi^2(dof - k)/(dof - k)) =$$

$$= (\Delta \chi^2/k) / \chi_{\nu}^2$$
Ex: $\chi^2(103) = 97.23$

$$\chi^2(101) = 90.84$$

$$\to \Delta \chi^2 = 6.39, k = 2 \to F_t = (6.39/2)/(90.84/101) = 3.55$$

 F_t follows the F distribution with $v_1=k=\Delta(dof)$ and $v_2=dof-k(-1)$

Search in the F-distribution tables for the probability of the null hypothesis (H_0) for v_1 =2 and v_2 ~100

The significance of the improvement is given by P=1-prob=1-0.032=96.8% (i.e., not particularly significant)

Note of caution: F-test is an approximation (BUT quick); optimal solution would be running simulations (ses Protassov+2002)

You simulate N times (1000, 10000 trials) within XSPEC (command *fakeit*) data (source and background) of the same quality as that of your original data (including also response matrices ARF and RMF) and fit them with the same modeling without the line (e.g., a powerlaw); you then verify how many times your feature is found purely by chance

If you find it X times, the significance of the line =(1-X)/(number of trials)

						X-to		х	X+tσ		
t	0.00	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09	
0.0	0.00	0.80	1.60	2.39	3.19	3.99	4.78	5.58	6.38	7.17	
0.1	7.97	8.76	9.55	10.34	11.13	11.92	12.71	13.50	14.28	15.07	
0.2	15.85	16.63	17.41	18.19	18.97	19.74	20.51	21.28	22.05	22.82	
0.3	23.58	24.34	25.10	25.86	26.61	27.37	28.12	28.86	29.61	30.35	
0.4	31.08	31.82	32.55	33.28	34.01	34.73	35.45	36.16	36.88	37.59	
0.5	38.29	38.99	39.69	40.39	41.08	41.77	42.45	43.13	43.81	44.48	
0.6	45.15	45.81	46.47	47.13	47.78	48.43	49.07	49.71	50.35	50.98	
0.7	51.61	52.23	52.85	53.46	54.07	54.67	55.27	55.87	56.46	57.05	
8.0	57.63	58.21	58.78	59.35	59.91	60.47	61.02	61.57	62.11	62.65	
0.9	63.19	63.72	64.24	64.76	65.28	65.79	66.29	66.80	67.29	67.78	
1.0	68.27	68.75	69.23	69.70	70.17	70.63	71.09	71.54	71.99	72.43	- i
1.1	72.87	73.30	73.73	74.15	74.57	74.99	75.40	75.80	76.20	76.60	
1.2	76.99	77.37	77.75	78.13	78.50	78.87	79.23	79.59	79.95	80.29	
1.3	80.64	80.98	81.32	81.65	81.98	82.30	82.62	82.93	83.24	83.55	(
1.4	83.85	84.15	84.44	84.73	85.01	85.29	85.57	85.84	86.11	86.38	
1.5	86.64	86.90	87.15	87.40	87.64	87.89	88.12	88.36	88.59	88.82	
1.6	89.04	89.26	89.48	89.69	89.90	90.11	90.31	90.51	90.70	90.90	
1.7	91.09	91.27	91.46	91.64	91.81	91.99	92.16	92.33	92.49	92.65	
1.8	92.81	92.97	93.12	93.28	93.42	93.57	93.71	93.85	93.99	94.12	
1.9	94.26	94.39	94.51	94.64	94.76	94.88	95.00	95.12	95.23	95.34	
2.0	95.45	95.56	95.66	95.76	95.86	95.96	96.06	96.15	96.25	96.34	_
2.1	96.43	96.51	96.60	96.68	96.76	96.84	96.92	97.00	97.07	97.15	3
2.2	97.22	97.29	97.36	97.43	97.49	97.56	97.62	97.68	97.74	97.80	_
2.3	97.86	97.91	97.97	98.02	98.07	98.12	98.17	98.22	98.27	98.32	
2.4	98.36	98.40	98.45	98.49	98.53	98.57	98.61	98.65	98.69	98.72	
2.5	98.76	98.79	98.83	98.86	98.89	98.92	98.95	98.98	99.01	99.04	
2.6	99.07	99.09	99.12	99.15	99.17	99.20	99.22	99.24	99.26	99.29	
2.7	99.31	99.33	99.35	99.37	99.39	99.40	99.42	99.44	99.46	99.47	
2.8	99.49	99.50	99.52	99.53	99.55	99.56	99.58	99.59	99.60	99.61	
2.9	99.63	99.64	99.65	99.66	99.67	99.68	99.69	99.70	99.71	99.72	
3.0	99.73										
3.5	99.95										

shaded region

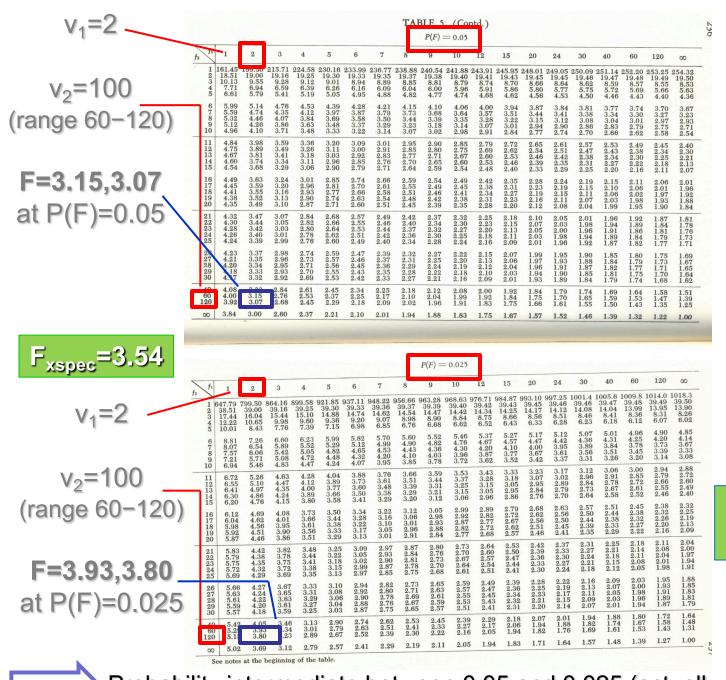
X between -tσ and +tσ

(t means # in units of σ)

Compute the significance of the improvement in terms of σ given P=0.0328, hence (1-P)=0.968

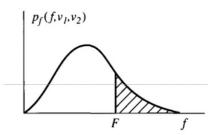
P=96.8% **→**≈2.1σ

Gaussian probability table



P(F) = 0.05

F-test probability in XSPEC: probability of exceeding F (see tabulated values)



P(F)=0.025

F-test probability table



Probability intermediate between 0.05 and 0.025 (actually, **0.0323**)