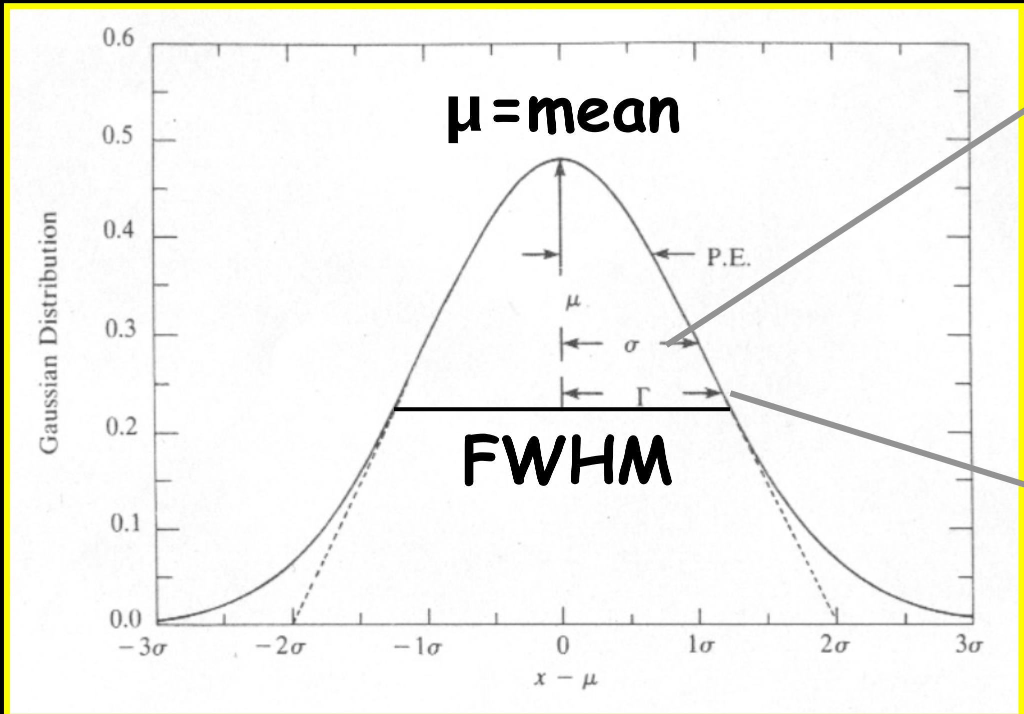
A taste of statistics and applications to X-ray spectral fitting

- ✓ 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
- ✓ Statistical errors and contour plots
- ✓ Low-count regime: the C-statistic
- ✓ Applications to X-ray spectral fitting

The Gaussian (normal error) distribution

Casual errors are above and below the "true" (most "common") value
→ bell-shape distribution if systematic errors are negligible



σ=standard deviation of the function

Γ=half-width at half maximum=1.17σ

FWHM=2.35σ

Gaussian probability function

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

Probability Density Function
(centered on μ)

μ=mean value
σ=standard deviation

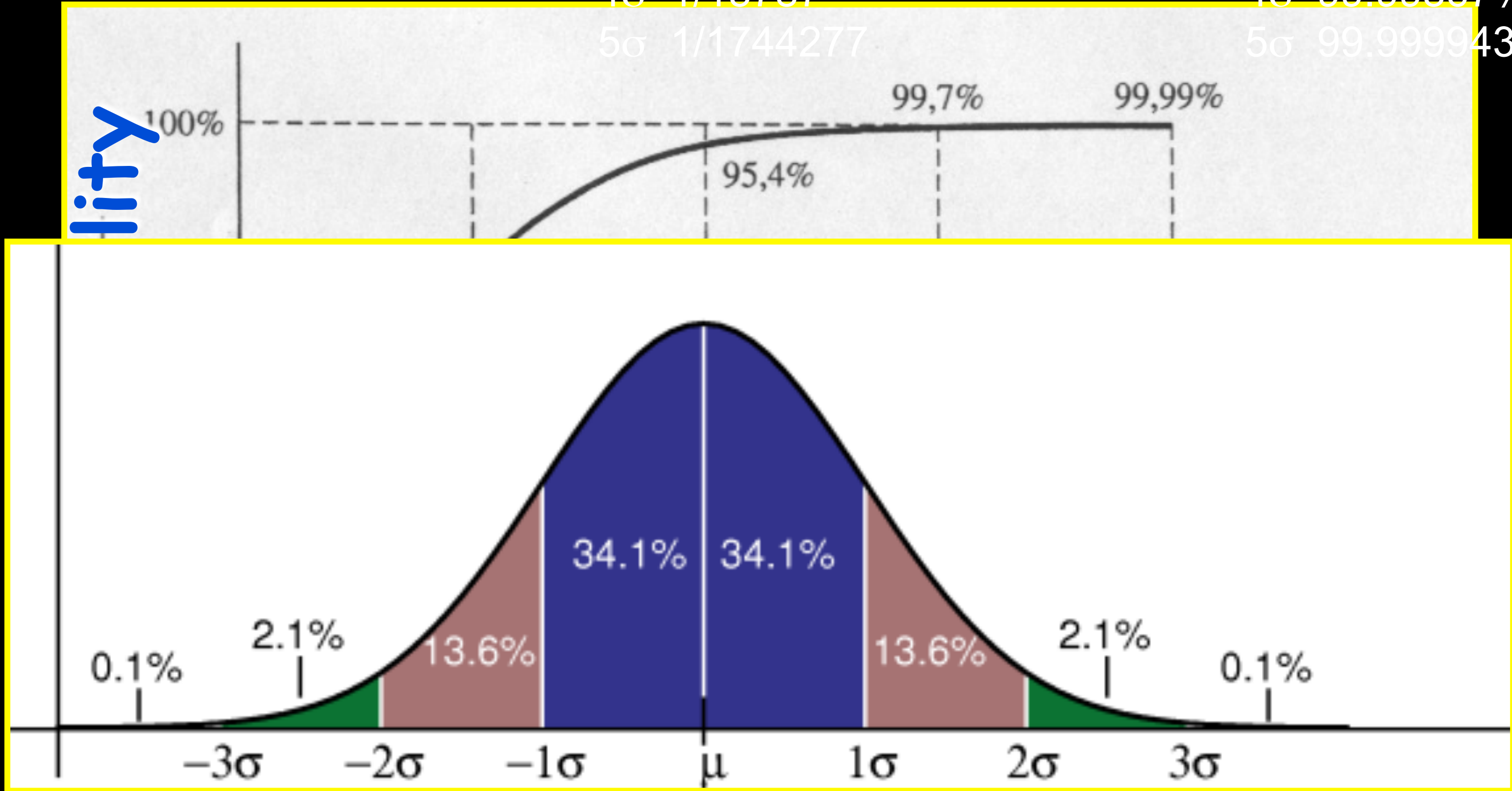
normalization factor, so that ∫f(x) dx=1

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

function centered on 0

1σ 1/3
2σ 1/22
3σ 1/370
4σ 1/15787
5σ 1/1744277

1σ 68.3%
2σ 95.45%
3σ 99.730%
4σ 99.99367%
5σ 99.999943%



t σ	0	0,25	0,5	0,75	1,0	1,25	1,5	1,75	2,0	2,5	3,0	3,5	4,0
P (%)	0	20	38	55	68	79	87	92	95,4	98,8	99,7	99,95	99,99

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

Cumulative Distribution Function

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, X-ray photons, etc.)

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

Probability of obtaining x events when the expected number is μ

μ>0: main parameter of the Poisson distribution

x=observed number of events in a time interval (frequency of events)

average number of events

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

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

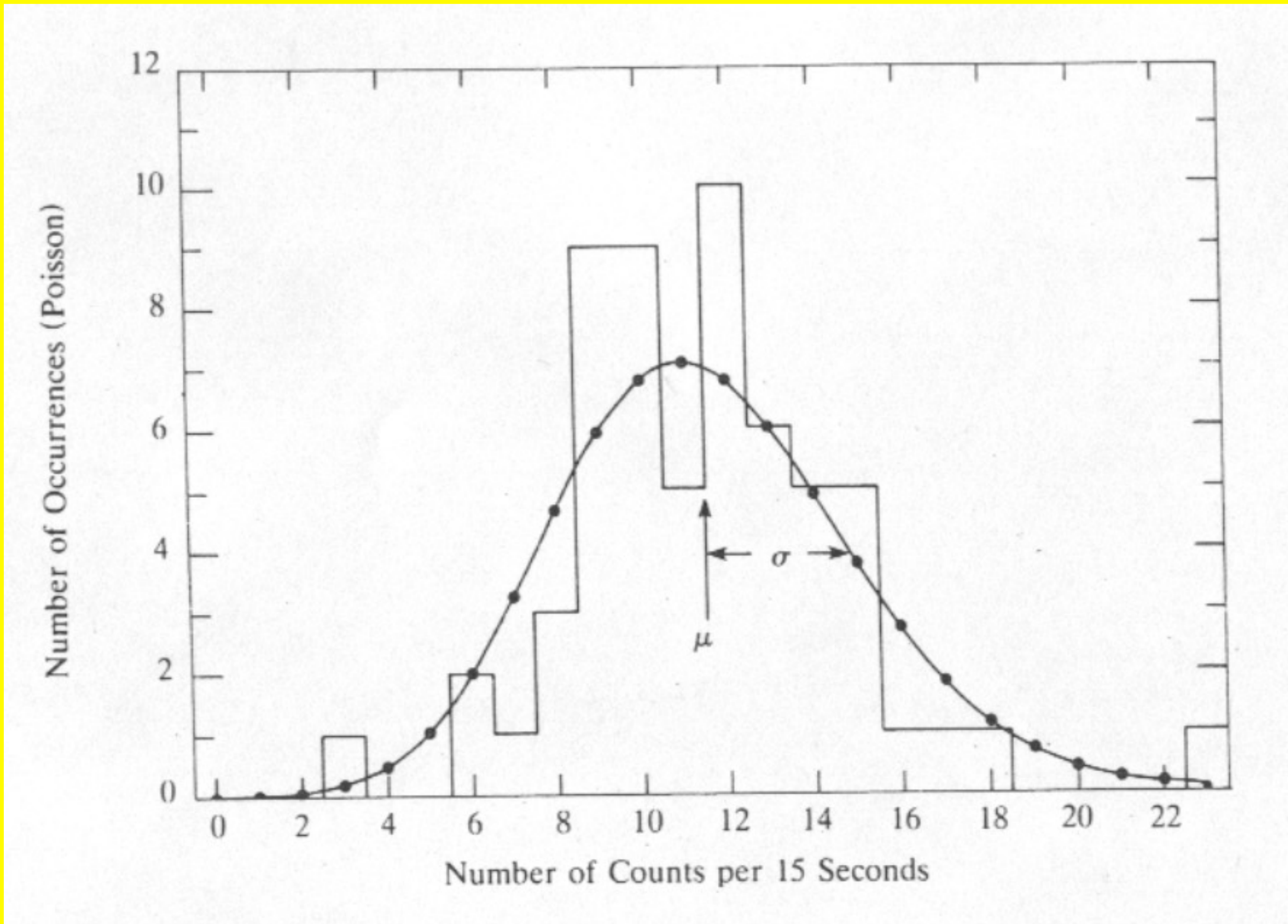
$$\sigma^2 = \langle (x-\mu)^2 \rangle = \sum_{x=0}^{\infty} (x-\mu)^2 \frac{\mu^x}{x!} e^{-\mu} = \mu$$

expectation value of the square of the deviations

the Poisson distribution with average counts=μ has standard deviation √μ

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

defined by only one parameter μ



Statistical tests: χ^2

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

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

O_k=observed values
E_k=expected values
σ_k=error on the measured values
k=number of intervals

$\chi^2 \leq n$ ⇒ the observed and expected distributions are similar

Degrees of freedom

Degrees of freedom (d.o.f.)=number of observed data – number of parameters computed from the data and used in the calculation

d.o.f.=n-c

where

n=number of data (e.g., spectral bins)

c=number of parameters which must be computed from the data to obtain the expected E_k

↓

X-ray spectral fits

d.o.f.=number of spectral data points – number of free parameters

```
1 file 1 spectrum
Spectrum 1  Spectral Data File: CXOJ033238.93-275700.6_c30.pi
Net count rate (cts/s) for Spectrum:1  1.692e-03 +/- 3.064e-05 (87.7 % total)
 Assigned to Data Group 1 and Plot Group 1
  Noticed Channels:  2-118
  Telescope: CHANDRA Instrument: ACIS  Channel Type: PI
  Exposure Time: 2.156e+06 sec
 Using fit statistic: chi
 Using Background File                CXOJ033238.93-275700.6_bkg.pi
  Background Exposure Time: 2.156e+06 sec
 Using Response (RMF) File            CXOJ033238.93-275700.6.rmf for Source 1
 Using Auxiliary Response (ARF) File  CXOJ033238.93-275700.6.arf

 Spectral data counts: 4158
 Model predicted rate: 1.64776E-03


Current model list:

========================================================================
Model phabs<1>(zbbody<2> + zphabs<3>*powerlaw<4>) Source No.: 1   Acti
Model Model Component  Parameter  Unit     Value
 par  comp
   1    1   phabs      nH         10^22    8.90000E-03  frozen
   2    2   zbbody     kT         keV      0.213162     +/-  0.0
   3    2   zbbody     Redshift            0.298000     frozen
   4    2   zbbody     norm                1.66494E-08  +/-  0.0
   5    3   zphabs     nH         10^22    3.44911      +/-  0.0
   6    3   zphabs     Redshift            0.298000     frozen
   7    4   powerlaw   PhoIndex            1.70660      +/-  0.0
   8    4   powerlaw   norm                1.18377E-05  +/-  0.0
________________________________________________________________________

   Using energies from responses.

 Chi-Squared =          117.48 using 117 PHA bins.
 Reduced chi-squared =          1.0489 for    112 degrees of freedom
 Null hypothesis probability =    3.429318e-01
 Current data and model not fit yet.
 Weighting method: standard
```

d.o.f.=

channels (PHA bins)

–

free parameters

$$\text{reduced } \chi^2 = \chi^2 / d.o.f.$$

channels=117
#free param=5
dof=112
X^2/dof=1.05
Pnull=0.34

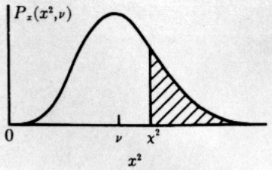


TABLE C.4

χ^2 **distribution. Values of the reduced chi-square $\chi_\nu^2 = \chi^2/\nu$ corresponding to the probability $P_\chi(\chi^2;\nu)$ of exceeding χ^2 vs. the number of degrees of freedom ν**

	P							
ν	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
16	0.363	0.413	0.498	0.582	0.697	0.789	0.874	0.959
17	0.377	0.427	0.510	0.593	0.706	0.796	0.879	0.961
18	0.390	0.439	0.522	0.604	0.714	0.802	0.883	0.963
19	0.402	0.451	0.532	0.613	0.722	0.808	0.887	0.965
20	0.413	0.462	0.543	0.622	0.729	0.813	0.890	0.967
22	0.434	0.482	0.561	0.638	0.742	0.823	0.897	0.970
24	0.452	0.500	0.577	0.652	0.753	0.831	0.902	0.972
26	0.469	0.516	0.592	0.665	0.762	0.838	0.907	0.974
28	0.484	0.530	0.605	0.676	0.771	0.845	0.911	0.976
30	0.498	0.544	0.616	0.687	0.779	0.850	0.915	0.978
32	0.511	0.556	0.627	0.696	0.786	0.855	0.918	0.979
34	0.523	0.567	0.637	0.704	0.792	0.860	0.921	0.980
36	0.534	0.577	0.646	0.712	0.798	0.864	0.924	0.982
38	0.545	0.587	0.655	0.720	0.804	0.868	0.926	0.983
40	0.554	0.596	0.663	0.726	0.809	0.872	0.928	0.983
42	0.563	0.604	0.670	0.733	0.813	0.875	0.930	0.984
44	0.572	0.612	0.677	0.738	0.818	0.878	0.932	0.985
46	0.580	0.620	0.683	0.744	0.822	0.881	0.934	0.986
48	0.587	0.627	0.690	0.749	0.825	0.884	0.936	0.986
50	0.594	0.633	0.695	0.754	0.829	0.886	0.937	0.987
60	0.625	0.662	0.720	0.774	0.844	0.897	0.944	0.989
70	0.649	0.684	0.739	0.790	0.856	0.905	0.949	0.990
80	0.669	0.703	0.755	0.803	0.865	0.911	0.952	0.992
90	0.686	0.718	0.768	0.814	0.873	0.917	0.955	0.993
100	0.701	0.731	0.779	0.824	0.879	0.921	0.958	0.993
120	0.724	0.753	0.798	0.839	0.890	0.928	0.962	0.994
140	0.743	0.770	0.812	0.850	0.898	0.934	0.965	0.995
160	0.758	0.784	0.823	0.860	0.905	0.938	0.968	0.996
180	0.771	0.796	0.833	0.868	0.910	0.942	0.970	0.996
200	0.782	0.806	0.841	0.874	0.915	0.945	0.972	0.997

TABLE C.4

χ^2 **distribution** (*continued*)

probability →

dof ↓

	P							
ν	0.40	0.30	0.20	0.10	0.05	0.02	0.01	0.001
1	0.708	1.074	1.642	2.706	3.841	5.412	6.635	10.827
2	0.916	1.204	1.609	2.303	2.996	3.912	4.605	6.908
3	0.982	1.222	1.547	2.084	2.605	3.279	3.780	5.423
4	1.011	1.220	1.497	1.945	2.372	2.917	3.319	4.617
5	1.026	1.213	1.458	1.847	2.214	2.678	3.017	4.102
6	1.035	1.205	1.426	1.774	2.099	2.506	2.802	3.743
7	1.040	1.198	1.400	1.717	2.010	2.375	2.639	3.475
8	1.044	1.191	1.379	1.670	1.938	2.271	2.511	3.266
9	1.046	1.184	1.360	1.632	1.880	2.187	2.407	3.097
10	1.047	1.178	1.344	1.599	1.831	2.116	2.321	2.959
11	1.048	1.173	1.330	1.570	1.789	2.056	2.248	2.842
12	1.049	1.168	1.318	1.546	1.752	2.004	2.185	2.742
13	1.049	1.163	1.307	1.524	1.720	1.959	2.130	2.656
14	1.049	1.159	1.296	1.505	1.692	1.919	2.082	2.580
15	1.049	1.155	1.287	1.487	1.666	1.884	2.039	2.513
16	1.049	1.151	1.279	1.471	1.644	1.852	2.000	2.453
17	1.048	1.148	1.271	1.457	1.623	1.823	1.965	2.399
18	1.048	1.145	1.264	1.444	1.604	1.797	1.934	2.351
19	1.048	1.142	1.258	1.432	1.586	1.773	1.905	2.307
20	1.048	1.139	1.252	1.421	1.571	1.751	1.878	2.266
22	1.047	1.134	1.241	1.401	1.542	1.712	1.831	2.194
24	1.046	1.129	1.231	1.383	1.517	1.678	1.791	2.132
26	1.045	1.125	1.223	1.368	1.496	1.648	1.755	2.079
28	1.045	1.121	1.215	1.354	1.476	1.622	1.724	2.032
30	1.044	1.118	1.208	1.342	1.459	1.599	1.696	1.990
32	1.043	1.115	1.202	1.331	1.444	1.578	1.671	1.953
34	1.042	1.112	1.196	1.321	1.429	1.559	1.649	1.919
36	1.042	1.109	1.191	1.311	1.417	1.541	1.628	1.888
38	1.041	1.106	1.186	1.303	1.405	1.525	1.610	1.861
40	1.041	1.104	1.182	1.295	1.394	1.511	1.592	1.835
42	1.040	1.102	1.178	1.288	1.384	1.497	1.576	1.812
44	1.039	1.100	1.174	1.281	1.375	1.485	1.562	1.790
46	1.039	1.098	1.170	1.275	1.366	1.473	1.548	1.770
48	1.038	1.096	1.167	1.269	1.358	1.462	1.535	1.751
50	1.038	1.094	1.163	1.263	1.350	1.452	1.523	1.733
60	1.036	1.087	1.150	1.240	1.318	1.410	1.473	1.660
70	1.034	1.081	1.139	1.222	1.293	1.377	1.435	1.605
80	1.032	1.076	1.130	1.207	1.273	1.351	1.404	1.560
90	1.031	1.072	1.123	1.195	1.257	1.329	1.379	1.525
100	1.029	1.069	1.117	1.185	1.243	1.311	1.358	1.494
120	1.027	1.063	1.107	1.169	1.221	1.283	1.325	1.446
140	1.026	1.059	1.099	1.156	1.204	1.261	1.299	1.410
160	1.024	1.055	1.093	1.146	1.191	1.243	1.278	1.381
180	1.023	1.052	1.087	1.137	1.179	1.228	1.261	1.358
200	1.022	1.050	1.083	1.130	1.170	1.216	1.247	1.338

χ^2 test in a nutshell

Reduced χ^2 large ⇐⇒ $P(\chi^2)$ small:

(a)errors are under-estimated
(b)F(x) does not describe the data very well (bad fit)

Reduced χ^2 small ⇐⇒ $P(\chi^2)$ large:

(a)errors are over-estimated
(b)data specially selected?

Real case when limited photon statistics applies (too many channels with 0−1 counts)

F-test

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

$$P_f(f;\upsilon_1,\upsilon_2) = \frac{\chi_1^2/\upsilon_1}{\chi_2^2/\upsilon_2}$$

$$\propto \Delta\chi^2/k$$

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)

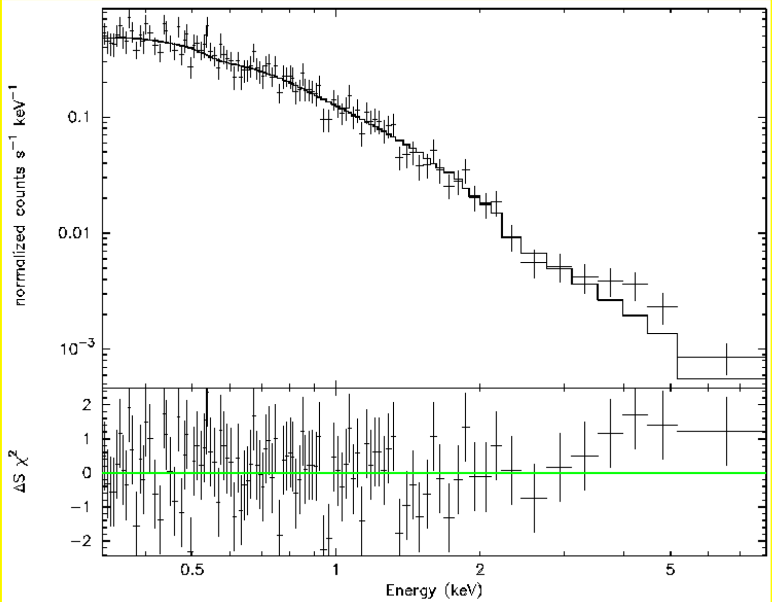
An application of the F-test

```
========================================================================
Model phabs<1>*powerlaw<2> Source No.: 1   Active/On
Model Model Component  Parameter  Unit     Value
 par  comp
   1    1   phabs      nH         10^22    1.59000E-02  frozen
   2    2   powerlaw   PhoIndex            2.72811      +/-  0.0
   3    2   powerlaw   norm                1.51490E-04  +/-  0.0
________________________________________________________________________

   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
```

Model1



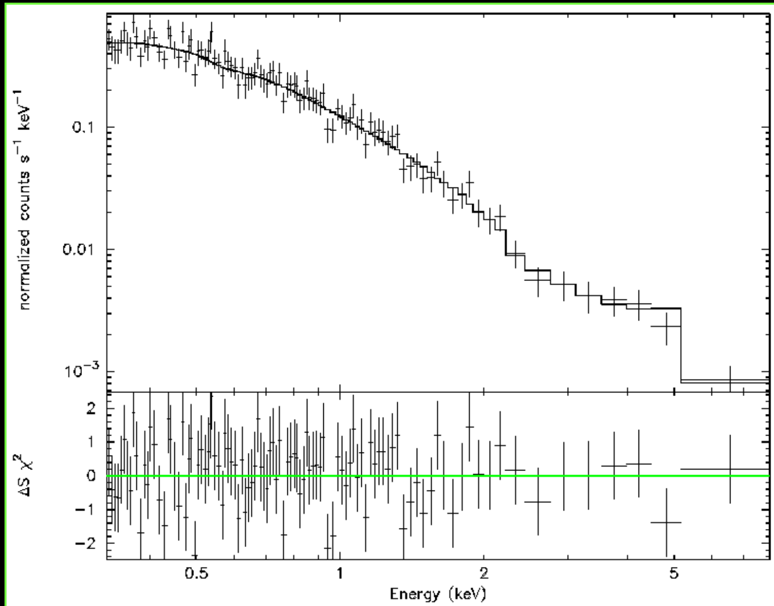

```
========================================================================
Model phabs<1>(laor<2> + powerlaw<3>) Source No.: 1   Active/On
Model Model Component  Parameter  Unit     Value
 par  comp
   1    1   phabs      nH         10^22    1.59000E-02  frozen
   2    2   laor       lineE      keV      5.23582      +/-  0.0
   3    2   laor       Index               3.00000      frozen
   4    2   laor       Rin(G)              1.23500      frozen
   5    2   laor       Rout(G)             400.000      frozen
   6    2   laor       Incl       deg      30.0000      frozen
   7    2   laor       norm                6.83065E-06  +/-  0.0
   8    3   powerlaw   PhoIndex            2.77137      +/-  0.0
   9    3   powerlaw   norm                1.48123E-04  +/-  0.0
________________________________________________________________________

   Using energies from responses.

 Chi-Squared =          90.84 using 105 PHA bins.
 Reduced chi-squared =         0.8994 for    101 degrees of freedom
 Null hypothesis probability =   7.557789e-01
 Current data and model not fit yet.
 Weighting method: standard
XSPEC12>ftest 90.84 101 97.2 103
 F statistic value = 3.53567 and probability 0.0327981
```

Model1+extra component

low F value ⇒ likely low signif. of add. comp



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

$$=(\Delta\chi^2/k)/\chi^2_\nu$$

Ex: $\chi^2(103) = 97.23$

$\chi^2(101) = 90.84$

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

F_t follows the F distribution with v_1=k=Δ(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

v_1=2
v_2=100
(60−120)

F=3.15,3.07
at P(F)=0.05

F=3.93,3.80
at P(F)=0.025

F_{xspec}=3.55

⇩

Prob interm. between 0.05 and 0.025 (actually, 0.0323)

TABLE 5 (Contd.)

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$P(F) = 0.05$

P(F)=0.05

f_2 \ f_1	1	2	3	4	5	6	7	8	9	10	12	15	20	24	30	40	60	120	∞
1	161.45	199.50	215.71	224.58	230.16	233.99	236.77	238.88	240.54	241.88	243.91	245.95	248.01	249.05	250.09	251.14	252.20	253.25	254.32
2	18.51	19.00	19.16	19.25	19.30	19.33	19.35	19.37	19.38	19.40	19.41	19.43	19.45	19.45	19.46	19.47	19.48	19.49	19.50
3	10.13	9.55	9.28	9.12	9.01	8.94	8.89	8.85	8.81	8.79	8.74	8.70	8.66	8.64	8.62	8.59	8.57	8.55	8.53
4	7.71	6.94	6.59	6.39	6.26	6.16	6.09	6.04	6.00	5.96	5.91	5.86	5.80	5.77	5.75	5.72	5.69	5.66	5.63
5	6.61	5.79	5.41	5.19	5.05	4.95	4.88	4.82	4.77	4.74	4.68	4.62	4.56	4.53	4.50	4.46	4.43	4.40	4.36
6	5.99	5.14	4.76	4.53	4.39	4.28	4.21	4.15	4.10	4.06	4.00	3.94	3.87	3.84	3.81	3.77	3.74	3.70	3.67
7	5.59	4.74	4.35	4.12	3.97	3.87	3.79	3.73	3.68	3.64	3.57	3.51	3.44	3.41	3.38	3.34	3.30	3.27	3.23
8	5.32	4.46	4.07	3.84	3.69	3.58	3.50	3.44	3.39	3.35	3.28	3.22	3.15	3.12	3.08	3.04	3.01	2.97	2.93
9	5.12	4.26	3.86	3.63	3.48	3.37	3.29	3.23	3.18	3.14	3.07	3.01	2.94	2.90	2.86	2.83	2.79	2.75	2.71
10	4.96	4.10	3.71	3.48	3.33	3.22	3.14	3.07	3.02	2.98	2.91	2.84	2.77	2.74	2.70	2.66	2.62	2.58	2.54
11	4.84	3.98	3.59	3.36	3.20	3.09	3.01	2.95	2.90	2.85	2.79	2.72	2.65	2.61	2.57	2.53	2.49	2.45	2.40
12	4.75	3.89	3.49	3.26	3.11	3.00	2.91	2.85	2.80	2.75	2.69	2.62	2.54	2.51	2.47	2.43	2.38	2.34	2.30
13	4.67	3.81	3.41	3.18	3.03	2.92	2.83	2.77	2.71	2.67	2.60	2.53	2.46	2.42	2.38	2.34	2.30	2.25	2.21
14	4.60	3.74	3.34	3.11	2.96	2.85	2.76	2.70	2.65	2.60	2.53	2.46	2.39	2.35	2.31	2.27	2.22	2.18	2.13
15	4.54	3.68	3.29	3.06	2.90	2.79	2.71	2.64	2.59	2.54	2.48	2.40	2.33	2.29	2.25	2.20	2.16	2.11	2.07
16	4.49	3.63	3.24	3.01	2.85	2.74	2.66	2.59	2.54	2.49	2.42	2.35	2.28	2.24	2.19	2.15	2.11	2.06	2.01
17	4.45	3.59	3.20	2.96	2.81	2.70	2.61	2.55	2.49	2.45	2.38	2.31	2.23	2.19	2.15	2.10	2.06	2.01	1.96
18	4.41	3.55	3.16	2.93	2.77	2.66	2.58	2.51	2.46	2.41	2.34	2.27	2.19	2.15	2.11	2.06	2.02	1.97	1.92
19	4.38	3.52	3.13	2.90	2.74	2.63	2.54	2.48	2.42	2.38	2.31	2.23	2.16	2.11	2.07	2.03	1.98	1.93	1.88
20	4.35	3.49	3.10	2.87	2.71	2.60	2.51	2.45	2.39	2.35	2.28	2.20	2.12	2.08	2.04	1.99	1.95	1.90	1.84
21	4.32	3.47	3.07	2.84	2.68	2.57	2.49	2.42	2.37	2.32	2.25	2.18	2.10	2.05	2.01	1.96	1.92	1.87	1.81
22	4.30	3.44	3.05	2.82	2.66	2.55	2.46	2.40	2.34	2.30	2.23	2.15	2.07	2.03	1.98	1.94	1.89	1.84	1.78
23	4.28	3.42	3.03	2.80	2.64	2.53	2.44	2.37	2.32	2.27	2.20	2.13	2.05	2.00	1.96	1.91	1.86	1.81	1.76
24	4.26	3.40	3.01	2.78	2.62	2.51	2.42	2.36	2.30	2.25	2.18	2.11	2.03	1.98	1.94	1.89	1.84	1.79	1.73
25	4.24	3.39	2.99	2.76	2.60	2.49	2.40	2.34	2.28	2.24	2.16	2.09	2.01	1.96	1.92	1.87	1.82	1.77	1.71
26	4.23	3.37	2.98	2.74	2.59	2.47	2.39	2.32	2.27	2.22	2.15	2.07	1.99	1.95	1.90	1.85	1.80	1.75	1.69
27	4.21	3.35	2.96	2.73	2.57	2.46	2.37	2.31	2.25	2.20	2.13	2.06	1.97	1.93	1.88	1.84	1.79	1.73	1.67
28	4.20	3.34	2.95	2.71	2.56	2.45	2.36	2.29	2.24	2.19	2.12	2.04	1.96	1.91	1.87	1.82	1.77	1.71	1.65
29	4.18	3.33	2.93	2.70	2.55	2.43	2.35	2.28	2.22	2.18	2.10	2.03	1.94	1.90	1.85	1.81	1.75	1.70	1.64
30	4.17	3.32	2.92	2.69	2.53	2.42	2.33	2.27	2.21	2.16	2.09	2.01	1.93	1.89	1.84	1.79	1.74	1.68	1.62
40	4.08	[illegible]	2.84	2.61	2.45	2.34	2.25	2.18	2.12	2.08	2.00	1.92	1.84	1.79	1.74	1.69	1.64	1.58	1.51
60	4.00	3.15	2.76	2.53	2.37	2.25	2.17	2.10	2.04	1.99	1.92	1.84	1.75	1.70	1.65	1.59	1.53	1.47	1.39
120	3.92	3.07	2.68	2.45	2.29	2.18	2.09	2.02	1.96	1.91	1.83	1.75	1.66	1.61	1.55	1.50	1.43	1.35	1.25
∞	3.84	3.00	2.60	2.37	2.21	2.10	2.01	1.94	1.88	1.83	1.75	1.67	1.57	1.52	1.46	1.39	1.32	1.22	1.00

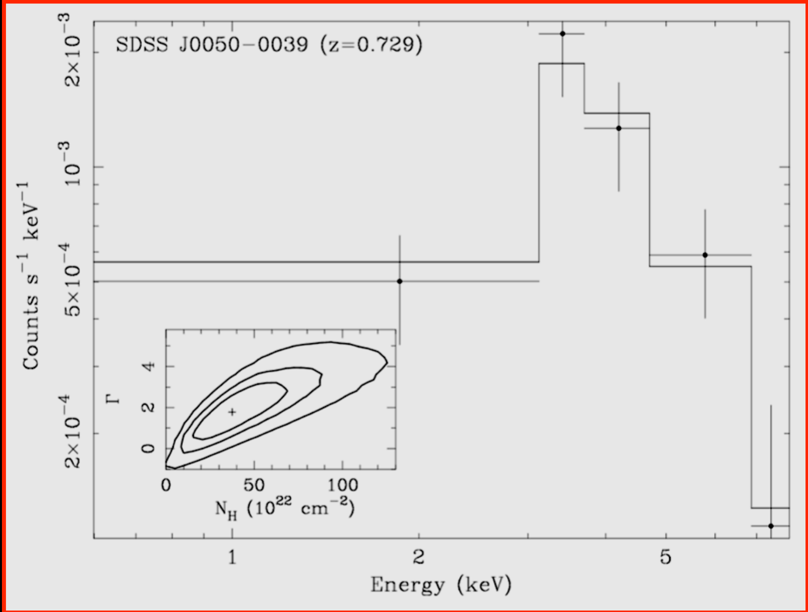
$P(F) = 0.025$

P(F)=0.025

f_2 \ f_1	1	2	3	4	5	6	7	8	9	10	12	15	20	24	30	40	60	120	∞
1	647.79	799.50	864.16	899.58	921.85	937.11	948.22	956.66	963.28	968.63	976.71	984.87	993.10	997.25	1001.4	1005.6	1009.8	1014.0	1018.3
2	38.51	39.00	39.16	39.25	39.30	39.33	39.36	39.37	39.39	39.40	39.42	39.43	39.45	39.46	39.46	39.47	39.48	39.49	39.50
3	17.44	16.04	15.44	15.10	14.88	14.74	14.62	14.54	14.47	14.42	14.34	14.25	14.17	14.12	14.08	14.04	13.99	13.95	13.90
4	12.22	10.65	9.98	9.60	9.36	9.20	9.07	8.98	8.90	8.84	8.75	8.66	8.56	8.51	8.46	8.41	8.36	8.31	8.26
5	10.01	8.43	7.76	7.39	7.15	6.98	6.85	6.76	6.68	6.62	6.52	6.43	6.33	6.28	6.23	6.18	6.12	6.07	6.02
6	8.81	7.26	6.60	6.23	5.99	5.82	5.70	5.60	5.52	5.46	5.37	5.27	5.17	5.12	5.07	5.01	4.96	4.90	4.85
7	8.07	6.54	5.89	5.52	5.29	5.12	4.99	4.90	4.82	4.76	4.67	4.57	4.47	4.42	4.36	4.31	4.25	4.20	4.14
8	7.57	6.06	5.42	5.05	4.82	4.65	4.53	4.43	4.36	4.30	4.20	4.10	4.00	3.95	3.89	3.84	3.78	3.73	3.67
9	7.21	5.71	5.08	4.72	4.48	4.32	4.20	4.10	4.03	3.96	3.87	3.77	3.67	3.61	3.56	3.51	3.45	3.39	3.33
10	6.94	5.46	4.83	4.47	4.24	4.07	3.95	3.85	3.78	3.72	3.62	3.52	3.42	3.37	3.31	3.26	3.20	3.14	3.08
11	6.72	5.26	4.63	4.28	4.04	3.88	3.76	3.66	3.59	3.53	3.43	3.33	3.23	3.17	3.12	3.06	3.00	2.94	2.88
12	6.55	5.10	4.47	4.12	3.89	3.73	3.61	3.51	3.44	3.37	3.28	3.18	3.07	3.02	2.96	2.91	2.85	2.79	2.72
13	6.41	4.97	4.35	4.00	3.77	3.60	3.48	3.39	3.31	3.25	3.15	3.05	2.95	2.89	2.84	2.78	2.72	2.66	2.60
14	6.30	4.86	4.24	3.89	3.66	3.50	3.38	3.29	3.21	3.15	3.05	2.95	2.84	2.79	2.73	2.67	2.61	2.55	2.49
15	6.20	4.76	4.15	3.80	3.58	3.41	3.29	3.20	3.12	3.06	2.96	2.86	2.76	2.70	2.64	2.58	2.52	2.46	2.40
16	6.12	4.69	4.08	3.73	3.50	3.34	3.22	3.12	3.05	2.99	2.89	2.79	2.68	2.63	2.57	2.51	2.45	2.38	2.32
17	6.04	4.62	4.01	3.66	3.44	3.28	3.16	3.06	2.98	2.92	2.82	2.72	2.62	2.56	2.50	2.44	2.38	2.32	2.25
18	5.98	4.56	3.95	3.61	3.38	3.22	3.10	3.01	2.93	2.87	2.77	2.67	2.56	2.50	2.44	2.38	2.32	2.26	2.19
19	5.92	4.51	3.90	3.56	3.33	3.17	3.05	2.96	2.88	2.82	2.72	2.62	2.51	2.45	2.39	2.33	2.27	2.20	2.13
20	5.87	4.46	3.86	3.51	3.29	3.13	3.01	2.91	2.84	2.77	2.68	2.57	2.46	2.41	2.35	2.29	2.22	2.16	2.09
21	5.83	4.42	3.82	3.48	3.25	3.09	2.97	2.87	2.80	2.73	2.64	2.53	2.42	2.37	2.31	2.25	2.18	2.11	2.04
22	5.79	4.38	3.78	3.44	3.22	3.05	2.93	2.84	2.76	2.70	2.60	2.50	2.39	2.33	2.27	2.21	2.14	2.08	2.00
23	5.75	4.35	3.75	3.41	3.18	3.02	2.90	2.81	2.73	2.67	2.57	2.47	2.36	2.30	2.24	2.18	2.11	2.04	1.97
24	5.72	4.32	3.72	3.38	3.15	2.99	2.87	2.78	2.70	2.64	2.54	2.44	2.33	2.27	2.21	2.15	2.08	2.01	1.94
25	5.69	4.29	3.69	3.35	3.13	2.97	2.85	2.75	2.68	2.61	2.51	2.41	2.30	2.24	2.18	2.12	2.05	1.98	1.91
26	5.66	4.27	3.67	3.33	3.10	2.94	2.82	2.73	2.65	2.59	2.49	2.39	2.28	2.22	2.16	2.09	2.03	1.95	1.88
27	5.63	4.24	3.65	3.31	3.08	2.92	2.80	2.71	2.63	2.57	2.47	2.36	2.25	2.19	2.13	2.07	2.00	1.93	1.85
28	5.61	4.22	3.63	3.29	3.06	2.90	2.78	2.69	2.61	2.55	2.45	2.34	2.23	2.17	2.11	2.05	1.98	1.91	1.83
29	5.59	4.20	3.61	3.27	3.04	2.88	2.76	2.67	2.59	2.53	2.43	2.32	2.21	2.15	2.09	2.03	1.96	1.89	1.81
30	5.57	4.18	3.59	3.25	3.03	2.87	2.75	2.65	2.57	2.51	2.41	2.31	2.20	2.14	2.07	2.01	1.94	1.87	1.79
40	5.42	4.05	3.46	3.13	2.90	2.74	2.62	2.53	2.45	2.39	2.29	2.18	2.07	2.01	1.94	1.88	1.80	1.72	1.64
60	[illegible]	3.93	[illegible]	3.01	2.79	2.63	2.51	2.41	2.33	2.27	2.17	2.06	1.94	1.88	1.82	1.74	1.67	1.58	1.48
120	[illegible]	3.80	[illegible]	2.89	2.67	2.52	2.39	2.30	2.22	2.16	2.05	1.94	1.82	1.76	1.69	1.61	1.53	1.43	1.31
∞	5.02	3.69	3.12	2.79	2.57	2.41	2.29	2.19	2.11	2.05	1.94	1.83	1.71	1.64	1.57	1.48	1.39	1.27	1.00

See notes at the beginning of the table.

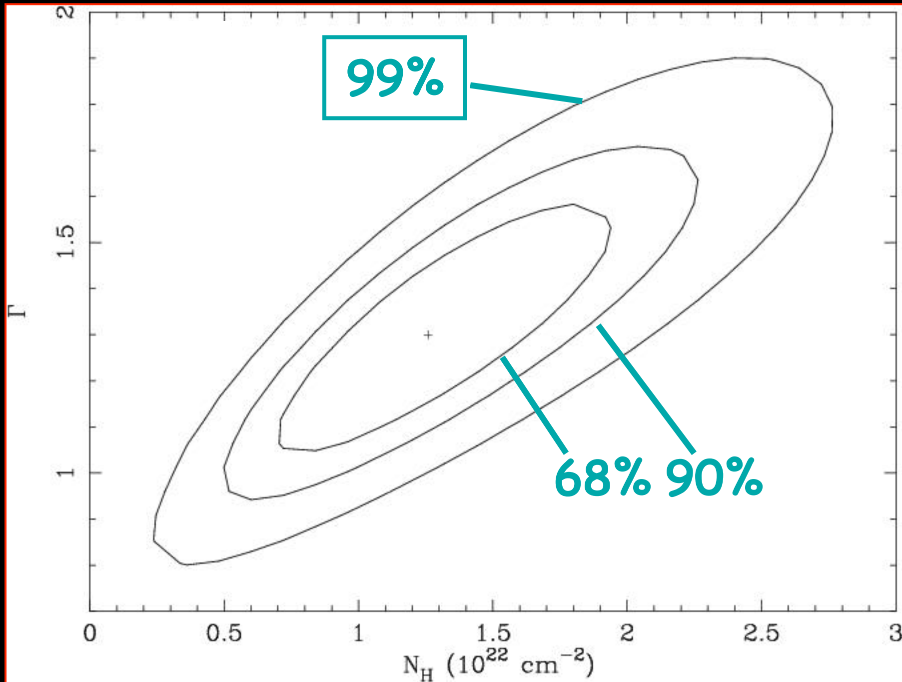
Errors within XSPEC: the contour plots



contour plots: show the statistical uncertainties related to two parameters

CONFIDENCE INTERVALS		
Confidence	sigma	(Delta)chi^2
68.3%	1.0	1.00
90.0%	1.6	2.71
95.5%	2.0	4.00
99.0%	2.6	6.63
99.7%	3.0	9.00

see Avni (1976)



Confidence	sigma	delta_chi-square
68.3%	1.0	1.00
90.0%	1.6	2.71
95.5%	2.0	4.00
99.0%	2.6	6.63
99.7%	3.0	9.00

Ex.1: Error at 90% confidence level for one parameter of interest:
xspec> error #param 2.71

Ex. 2: Error at 90% confidence level for two parameters of interest:
xspec> error #param 4.61

Ex. 3: Error at 99% confidence level for one parameter of interest:
xspec> error #param 6.63

Table entry for p is the critical value $(\chi^2)^*$ with probability p lying to its right.

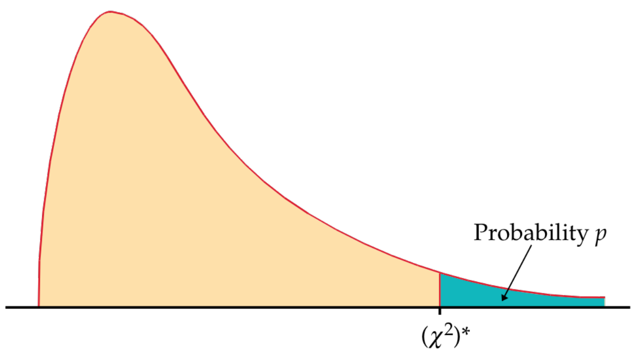


TABLE F

χ^2 distribution critical values

	Tail probability p											
df	.25	.20	.15	.10	.05	.025	.02	.01	.005	.0025	.001	.0005
1	1.32	1.64	2.07	2.71	3.84	5.02	5.41	6.63	7.88	9.14	10.83	12.12
2	2.77	3.22	3.79	4.61	5.99	7.38	7.82	9.21	10.60	11.98	13.82	15.20
3	4.11	4.64	5.32	6.25	7.81	9.35	9.84	11.34	12.84	14.32	16.27	17.73
4	5.39	5.99	6.74	7.78	9.49	11.14	11.67	13.28	14.86	16.42	18.47	20.00
5	6.63	7.29	8.12	9.24	11.07	12.83	13.39	15.09	16.75	18.39	20.51	22.11

Parameter of interest →

Low-counting statistic regime

The fit statistic routinely used is referred to as the χ^2 statistic

$$S = \sum_i \big(\underbrace{S_i - B_i t_s / t_b}_{O_K} - \underbrace{m_i t_s}_{E_K}\big)^2 / \big(\underbrace{(\sigma_S)_i^2 + (\sigma_B)_i^2}_{\sigma_K}\big)$$

where S_i = src counts in the I={1,…,N} data bins with exposure t_S, B_i = background counts with exposure t_B and m_i = model predicted count rate; $(\sigma_S)^2$ and $(\sigma_B)^2$ = variance on the src and background counts, typically estimated by S_i and B_i

BUT

the χ^2 statistic fails in low-counting regime

(few counts in each data bin)

Possible solution: to rebin the data so that each bin contains a large enough number of counts

BUT

⇒ Loss of information and dependence upon the rebinning method adopted

Viable solution: to modify S so that it performs better in low-count regime

⇒ Estimate the variance for a given data bin by the average counts from surrounding bins (Churazov et al. 1996)

BUT

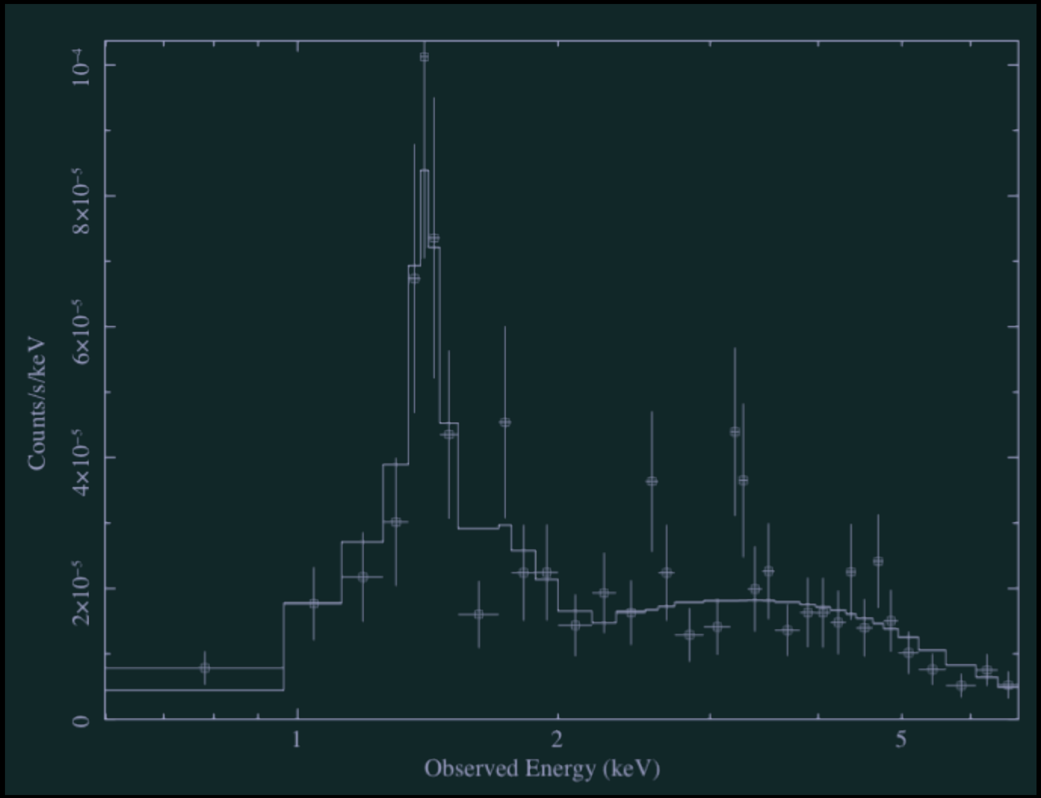
need for Monte-Carlo simulations to support the result

The Cash statistic

Construct a maximum-likelihood estimator based on the Poisson distribution of the detected counts

(Cash 1979; Wachter et al. 1979) in presence of background counts ⇒ implemented into XSPEC

Finding the maximum likelihood means finding the best fit of parameters that maximize the Poisson likelihood



Spectrum fitted using the **C-stat** and then rebinned just for presentation purposes

- χ^2 statistics ⇔ Gaussian statistics
- C-statistics ⇔ Poisson statistics

How does statistics enter into X-ray spectral fitting?

(adapted from K. Arnaud presentation;
see also "Handbook of X-ray Astronomy", edited by
K. Arnaud, R. Smith, A. Siemiginowska)

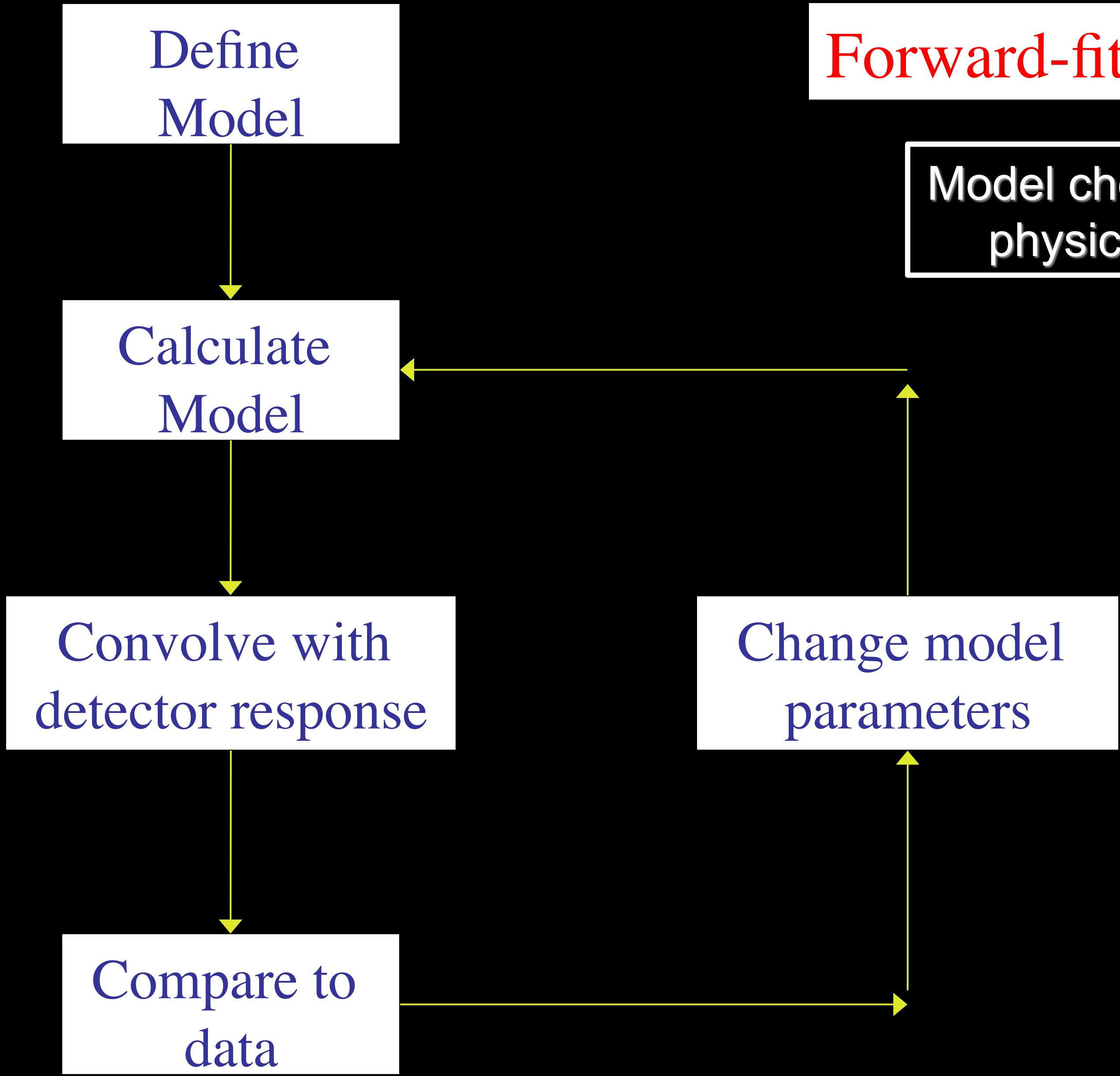
Forward-fitting

The standard method of analyzing X-ray spectra is "forward-fitting". This comprises the following steps…

- Calculate a model spectrum.
- Multiply the result by an instrumental response matrix.
- Compare the result with the actual observed data by calculating some statistic.
- Modify the model spectrum and repeat till the best value of the statistic is obtained.

Forward-fitting algorithm

Model choice based on the physics of the source



This only works if the model spectrum can be expressed in a reasonably small number of parameters (although I have seen people fit spectra using models with over 100 parameters).

The aim of the forward-fitting is then to obtain the best-fit and confidence ranges of these parameters.

Spectral fitting programs

- XSPEC - part of HEAsoft. General spectral fitting program with many models available.

- Sherpa - part of CIAO. Multi-dimensional fitting program which includes the XSPEC model library and can be used for spectral fitting.

- SPEX - from SRON in the Netherlands. Spectral fitting program specialising in collisional plasmas and high resolution spectroscopy.

- ISIS - from the MIT Chandra HETG group. Mainly intended for the analysis of grating data. Incorporated in Sherpa as GUIDE.

Models

All models are wrong, but some are useful - George Box

X-ray spectroscopic models are usually built up from individual components. These can be thought of as two basic types -additive (an emission component e.g. blackbody, line,…) or multiplicative (something which modifies the spectrum e.g. absorption).

$$\text{Model} = M_1 * M_2 * (A_1 + A_2 + M_3 * A_3) + A_4$$

Additive Models

Basic additive (emission) models include :

- blackbody
- thermal bremsstrahlung
- power-law
- collisional plasma
- Gaussian or Lorentzian lines

There are many more models available covering specialised topics such as accretion disks, comptonized plasmas, non-equilibrium ionization plasmas, multi-temperature collisional plasmas…

Multiplicative (and other) Models

and multiplicative models include :

- photoelectric absorption due to our Galaxy
- photoelectric absorption due to ionized material
- high energy exponential roll-off.
- edge with $1/E^3$ roll-off.

XSPEC also has a couple of other types of model components (convolution, mixing) which are used like a multiplicative model but perform more complicated operations on the current model.

Finding the best-fit (I)

Finding the best-fit means minimizing the statistic value. There are many algorithms available to do this in a computationally efficient fashion (see Numerical Recipes).

Most methods used to find the best-fit are local i.e. they use some information around the current parameters to guess a new set of parameters. All these methods are liable to get stuck in a local minimum. Watch out for this !

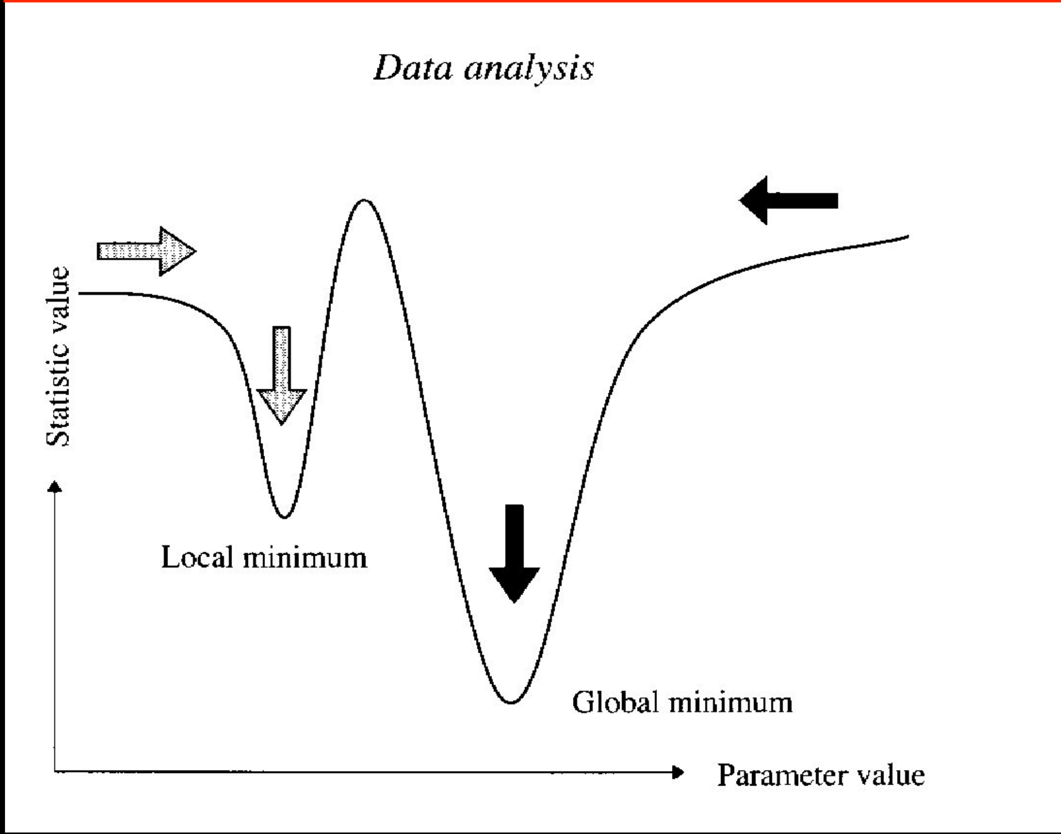
The more complicated your model and the more highly correlated the parameters then the more likely that the algorithm will not find the absolute best-fit.

Finding the best-fit (II)

Sometimes you can spot that you are stuck in a local minimum by using the XSPEC **error** or **steppar** commands. These both step through parameter values, error in the vicinity of the current best-fit and steppar over a user-defined grid, and thus can stumble across a better fit. Crude but sometimes effective.

You can do this in a semi-automated fashion by using a local minimization algorithm and following this with the error command with the ability to restart if a new minimum is found during the search.

Global vs. local minimum



If the fit process is started at the "right place", then it will converge to the true minimum

The more complicated the model and the more highly correlated the parameters, then the more likely that the algorithm will hardly find the true minimum

Dealing with background

o Unless you are looking at a bright point source with *Chandra*, you will probably have a background component to the spectrum in addition to the source in which you are interested.

o You can include background in the model but this is complicated and is not usually used.

o The usual method is to extract a spectrum from another part of the image or another observation. Spectral fitting programs then use both the source and background spectra.

o If the background spectrum is extracted from a different sized region than the source, then the background spectrum is scaled by the spectral fitting program (using the BACKSCAL keyword in the FITS file).

Spectra with few counts

o Be careful if you have few photons/bin. χ^2 is biased in this case with fluctuations below the model having more weight than those above, causing the fit model to lie below the true model.

o A common solution is to bin up your spectrum so all the bins have > some number of photons. Don't do this - it loses information and introduces a bias that is difficult to quantify.

o Solutions are to use a different weighting scheme (e.g., *weight churazov* option in XSPEC) or a maximum likelihood statistic (the "C-statistic" - *stat cstat* in XSPEC).

o The problem with these options is that while they give best fit parameters they do not provide a goodness-of-fit measure.

Final advices and admonitions

- Remember that the purpose of spectral fitting is to attain understanding, not fill up tables of numbers
- Physics behind X-ray spectral modeling is fundamental; then statistics needed to support the results
- Don't misuse the F-test, and use confidence contours
- Try to test whether you really have found the best-fit

and always remember …

"There are three sorts of lies: lies, damned lies and statistics"