An example of statistics in high-resolution X-ray spectroscopy - velocity profiles in the O-star supergiant ζ Ori

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MSSL School in High-Resolution Spectroscopy

2009 March 17

Make every photon count.
Account for every photon.

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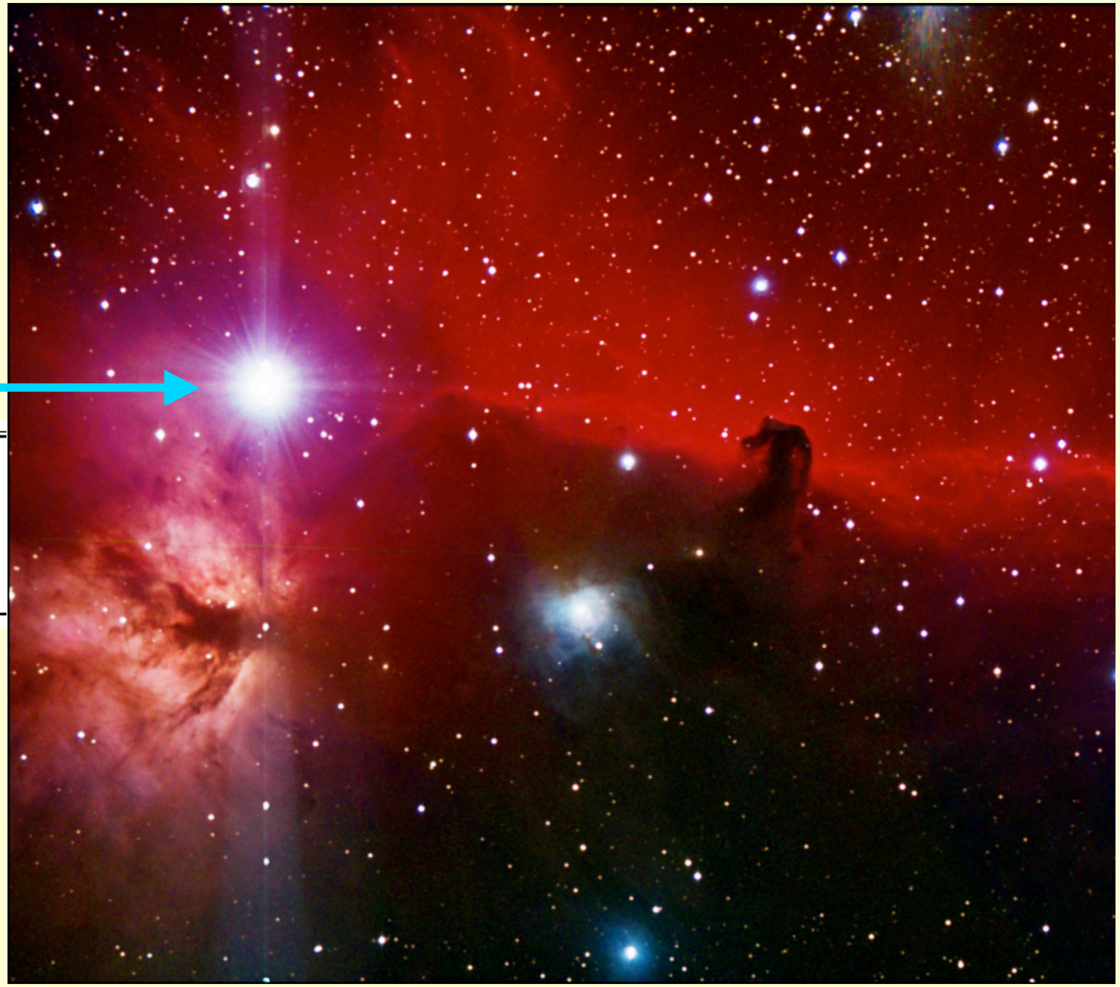
HD37742 O9.7Ib ζ Orionis

Visual magnitude	V	2.03
Effective temperature	$T_{\rm eff}$	30 900 K
Radius	R_*	31 $R_\odot$
Terminal velocity	v_∞	2100 km s^{-1}
Mass-loss rate	$\dot{M}$	1.4×10^{-6} $M_\odot$ yr^{-1}
Distance	d	473 pc
Interstellar column density	$N_{\rm H}$	2.5×10^{20} cm^{-2}



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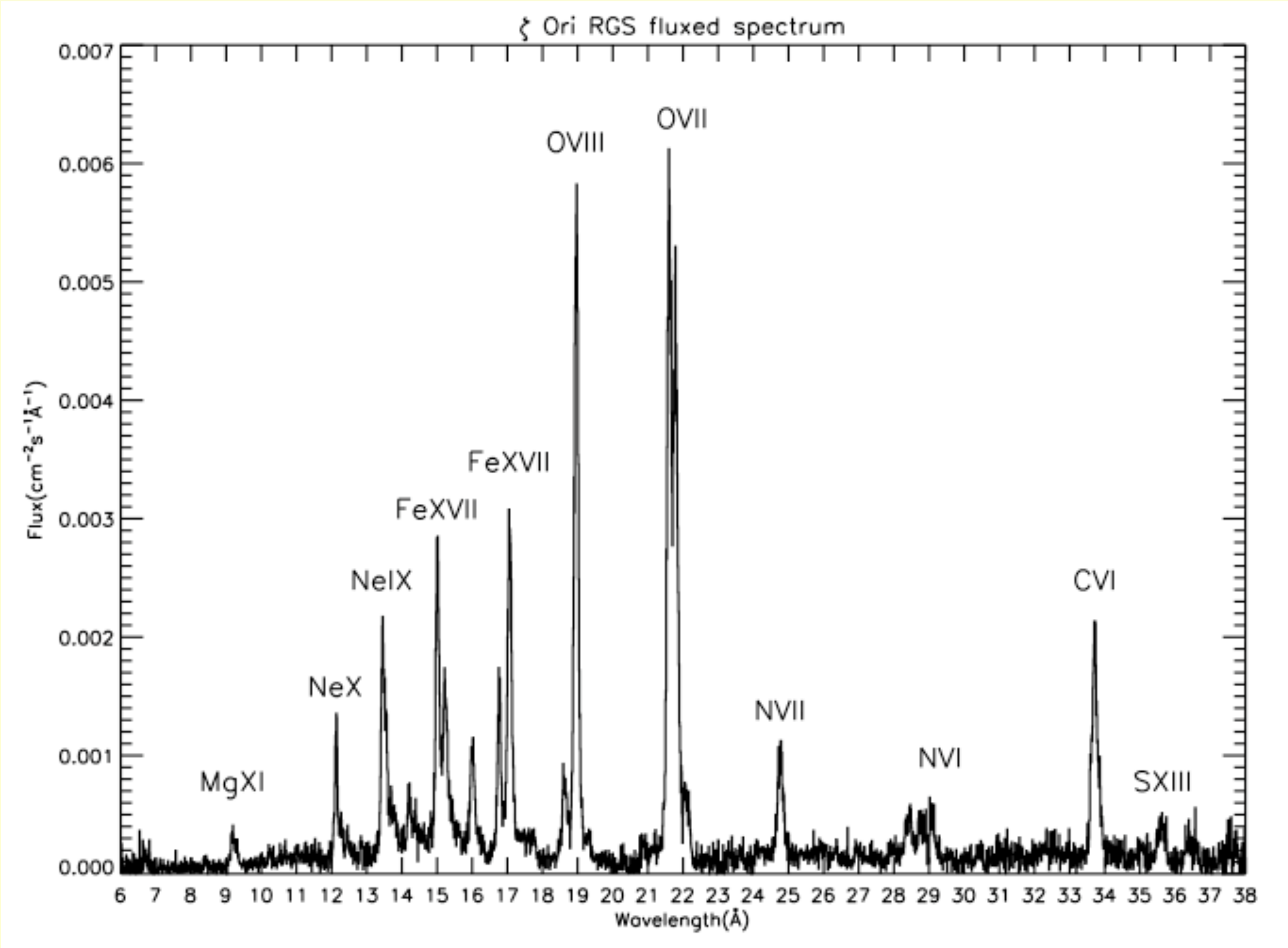
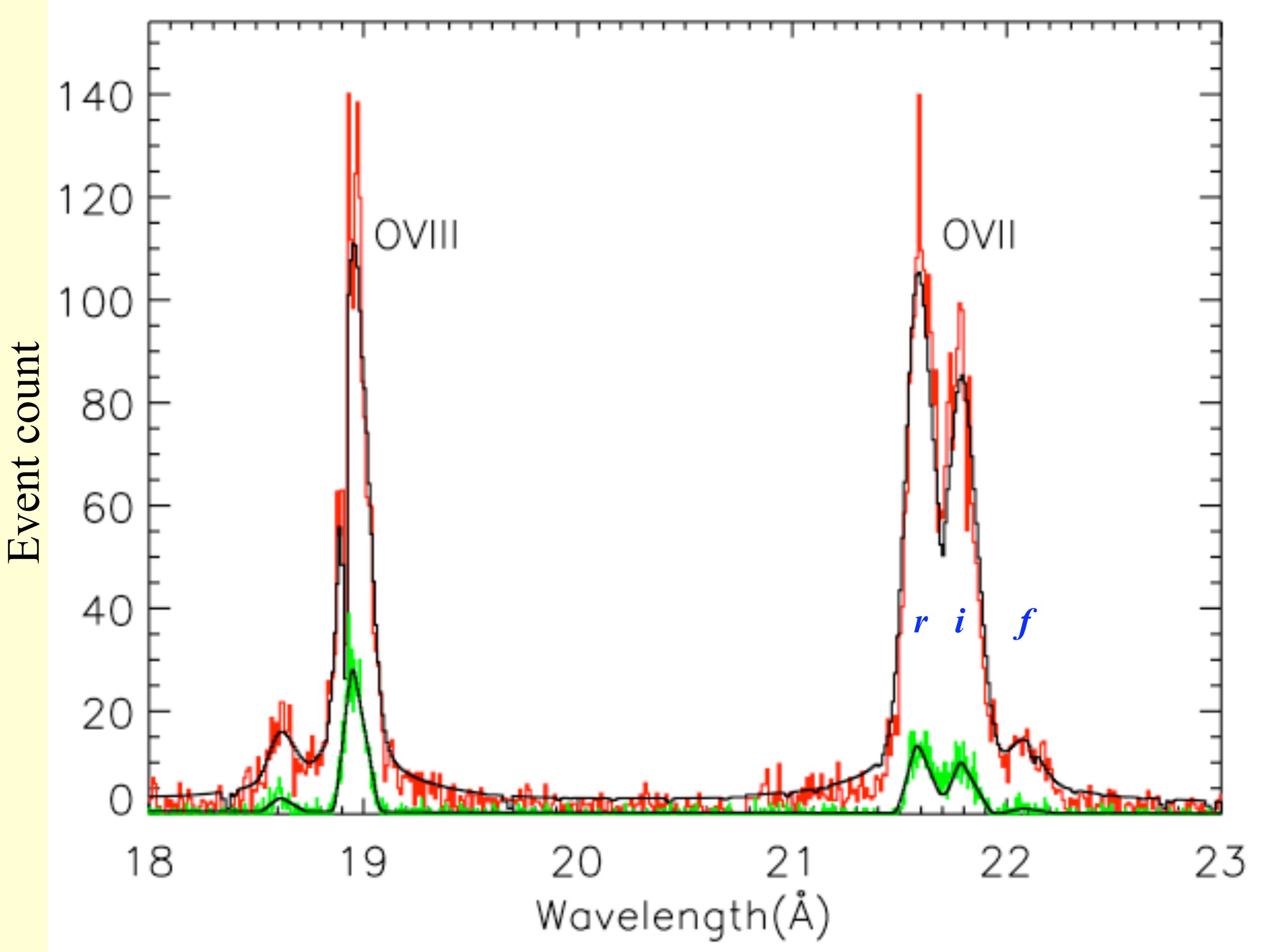

ζ Ori RGS fluxed spectrum
Flux(cm^-2s^-1Å^-1)
Wavelength(Å)
MgXI
NeX
NeIX
FeXVII
FeXVII
OVIII
OVII
NVII
NVI
CVI
SXIII

Part of the high-resolution X-ray spectrum of ζ Ori



XMM RGS

Chandra MEG

Instrument	Order	Counts
RGS1	−1	15 136
RGS2	−1	14 133
RGS1	−2	2771
RGS2	−2	2507
MEG	−1	5556
MEG	+1	3568
HEG	−1	1129
HEG	+1	839

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data ⇔ models

$$\{n_i\}_{i=1,N} \Leftrightarrow \{\mu_i\}_{i=1,N}$$

≥ 0 individual events ⇔ continuously distributed

detector coordinates ⇔ physical parameters

never change ⇔ change limited only by physics

have no errors ⇔ subject to fluctuations

most precious resource ⇔ predictions possible

kept forever in archives ⇔ kept forever in journals and textbooks

statistics

There are two sorts of statistic(s)

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

Likelihood of data on models

$\{n_i\}_{i=1,N}$ data ⟺ statistics ⟺ models $\{\mu_i\}_{i=1,N}$

$$L = \prod_{i=1}^{N} P(n_i \mid \mu_i)$$

Gaussian

$$L = \prod_{i=1}^{N} \frac{1}{\sigma_i \sqrt{2\pi}} \exp\left(-\frac{(n_i - \mu_i)^2}{2\sigma_i^{\,2}}\right) dn_i$$

$$\ln L = -\frac{1}{2} \sum_{i=1}^{N} \frac{(n_i - \mu_i)^2}{\sigma_i^{\,2}} - \sum_{i=1}^{N} \ln \sigma_i + \kappa(\ln dn_i)$$

$$-2 \ln L = \chi^2$$

Poisson

$$L = \prod_{i=1}^{N} \frac{e^{-\mu_i} \mu_i^{n_i}}{n_i!}$$

$$\ln L = \sum_{i=1}^{N} n_i \ln \mu_i - \mu_i - \kappa\left(\ln n_i!\right)$$

$$-2 \ln L = \mathrm{C}$$

Cash 1979, ApJ, 228, 939

$$\mu(\underline{\theta},\underline{\beta},\underline{\Delta},\underline{D})=S(\underline{\theta}(\underline{\Omega}))\otimes R(\underline{\Omega}<\underline{\Delta}>\underline{D})+B(\underline{\beta}(\underline{D}))$$

$\underline{D}$ = set of detector coordinates {X,Y,t,PI,…}

S = source of interest

$\underline{\theta}$ = **set of source parameters**

R = instrumental response

$\underline{\Omega}$ = set of physical coordinates $\{\alpha,\delta,\tau,\upsilon,\ldots\}$

$\underline{\Delta}$ = set of instrumental calibration parameters

B = background

$\underline{\beta}$ = set of background parameters

$$\Rightarrow \quad \ln L(\underline{\theta},\underline{\beta},\underline{\Delta}) \quad \Rightarrow \quad \ln L(\underline{\theta})$$

Uses of the log-likelihood, $\ln L(\underline{\theta})$

- $\ln L$ is what you need to assess all and any data models
  - locate the maximum-likelihood model when $\underline{\theta}=\underline{\theta}^*$
    - minimum χ^2 is a maximum-likelihood Gaussian statistic
    - minimum C is a maximum-likelihood Poisson statistic
  - compute a goodness-of-fit statistic
    - reduced chi-squared $\chi^2/\nu \sim 1$ ideally
    - reduced C $C/\nu \sim 1$ ideally
    - ν = number of degrees of freedom
  - estimate model parameters and uncertainties
    - $\ln L(\underline{\theta})$
      - $\underline{\theta}^* = \{p_1,p_2,p_3,p_4,\ldots,p_M\}$
  - investigate the whole multi-dimensional surface $\ln L(\underline{\theta})$
  - compare two or more models

- calibrating $\ln L$, $2\Delta\ln L \Leftrightarrow \sigma\sqrt{2\Delta\ln L}$
  - $2\Delta\ln L < 1.$ is not interesting
  - $2\Delta\ln L > 10.$ is worth thinking about (*e.g.* 2XMM DET_ML ≥ 8.)
  - $2\Delta\ln L > 100.$ Hmmm…

Goodness-of-fit

- Gaussian model and data are consistent if $\chi^2/\nu \sim 1$
  - ν = "number of degrees of freedom"
    = number of bins – number of free model parameters
    = N - M
  - *cf* $\langle(x-\mu)^2/\sigma^2\rangle=1$
  - same as comparison with best-possible $\nu=0$ model, $\underline{\mu}=\underline{x}$,
    - $\chi^2 = 2(\ln L(\underline{\mu}=\underline{x}) - \ln L(\underline{\theta}))$

- Poisson model and data are consistent if C/ν ~ 1
  - comparison with best-possible $\nu=0$ model, $\underline{\mu}=\underline{n}$
    - $2\sum(n_i \ln n_i - n_i) - 2\sum(n_i \ln\mu_i - \mu_i) = 2\sum n_i \ln(n_i/\mu_i) - (n_i - \mu_i)$
    - XSPEC definition
    - What happens when many $\mu_i \ll 1 \,\&\&\, n_i=0$?

Estimate model parameters and their uncertainties

- Parameter error estimates, $d\underline{\theta}$, around maximum-likelihood solution, $\underline{\theta}^*$
  - $2\ln L(\underline{\theta}^*+d\underline{\theta}) = 2\ln L(\underline{\theta}^*)$ + 1. for 1σ (other choices than 1. sometimes made)

Practical considerations

- S/ν is rarely ~ 1
  - $S = \chi^2 | C$
  - $\ln L(\underline{\theta}, \underline{\beta}, \underline{\Delta})$
  - $\underline{\theta}$ = set of source spectrum parameters
    - physics might need improvement
  - $\underline{\beta}$ = set of background parameters
    - background models can be difficult
  - $\underline{\Delta}$ = set of instrumental calibration parameters
    - 5 or 10% accuracy is a common calibration goal
- solution often dominated by systematic errors
  - `XSPEC`'s `SYS_ERR` is the wrong way to do it
  - no-one knows the right way (although let's listen to those Gaia people…)
- formal probabilities are not to be taken too seriously
  - $S/\nu > 2$ is bad
  - $S/\nu \sim 1$ is good
  - $S/\nu \sim 0$ is also bad
- find out where the model isn't working
  - pay attention to every bin

To rebin or not to rebin a spectrum ?

- Pros
  - Gaussian ≡ Poisson for $n \gg 0$
  - dangers of oversampling
  - saves time
  - everybody does it
  - "improves the statistics"
  - `grppha` and other tools exist
  - on log-log plots $\ln 0 = -\infty$

- Cons
  - rebinning throws away information
  - 0 is a perfectly good measurement
  - images are never rebinned
  - Poisson statistics robust for $n \geq 0$
  - $\mu_1 + \mu_2$ is also a Poisson variable
  - oversampling harmless
  - adding bins does not "improve the statistics"

Leave spectra alone. Don't rebin for $\ln L(\underline{\theta})$. Use Poisson statistics.

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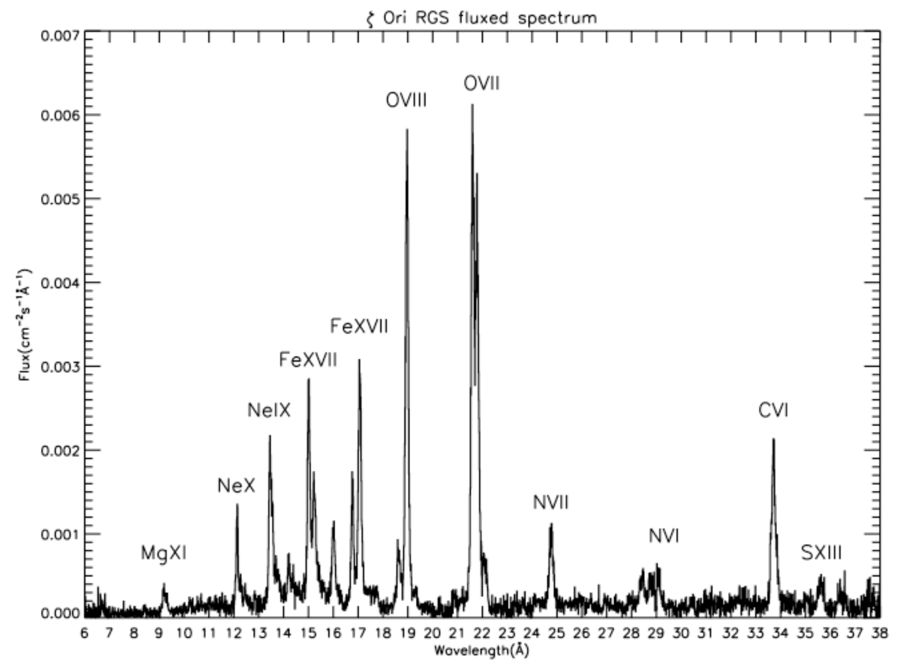
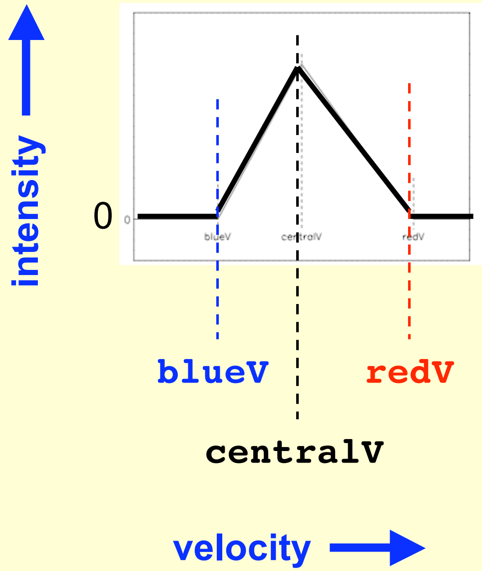
- instead of Gaussian lines use a **`TriLine`** model
- μ=67×**`TriLine`**+continuum





- use the model that best suits your purpose
- …and if there isn't one, make one of your own
  - scripts
    - XSPEC Tcl
    - ISIS Slang
- use **all** the data available

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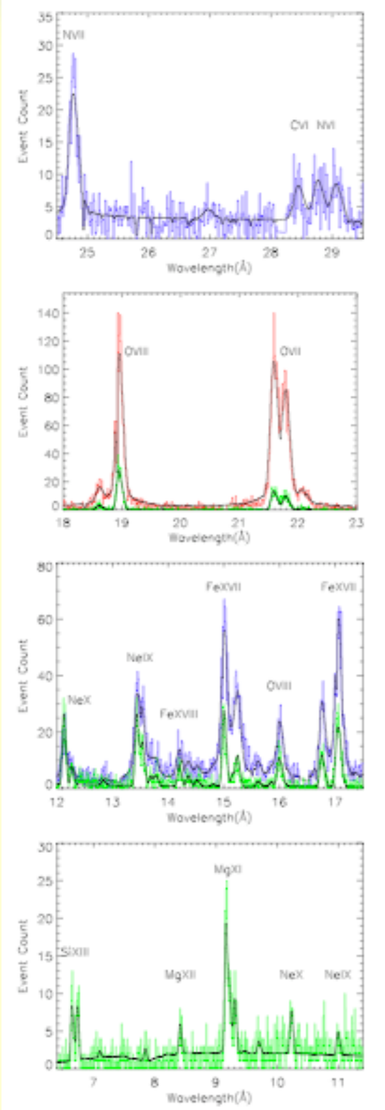
1σ errors for ΔC=1 with `XSPEC> error 1. ...`

Table 3. ζ Orionis best-fit emission-line velocity parameters and underlying continuum for the simultaneous multiple common-profile `TriLine` XSPEC model fit to the *XMM-Newton* RGS 1st and 2nd order spectra of 2002-09-15 and *Chandra* MEG and HEG ±1 order spectra of 2000-04-08.

TriLine velocities		
blueV	-1642 ± 22	km s^{-1}
centralV	-302 ± 29	km s^{-1}
redV	$+1646 \pm 26$	km s^{-1}
bremsstrahlung continuum		
N_H	2.5×10^{20}	cm^{-2}
kT	0.494 ± 0.007	keV
normalisation	$5.66 \pm 0.14 \times 10^{-3}$	
C-statistic = 22 862.4 using 26281 PHA bins		



	blueV	centralV	redV	C-stat	constraint
`TriLine`	-1642 ± 22	-302 ± 29	$+1646 \pm 26$	22 864.4	Best fit of Table 3
`TriLine`	-1641 ± 15	-303 ± 26	$+1641 \pm 15$	22 865.9	|redV| = |blueV|
`TriLine`	-1774 ± 21	0	$+1492 \pm 21$	22 973.1	centralV = 0
`TriLine`	-1684 ± 15	0	$+1684 \pm 15$	23 053.2	centralV = 0, |redV| = |blueV|
	blueW	**centralV**	**redW**	**C-stat**	**constraint**
`SkewLine`	650 ± 25	-318 ± 29	991 ± 27	22 816.7	
`SkewLine`	811 ± 9	-126 ± 10	811 ± 9	22 879.4	redW = blueW
`SkewLine`	880 ± 12	0	738 ± 12	22 947.6	centralV = 0
`SkewLine`	841 ± 10	0	841 ± 10	23 038.4	centralV = 0, redW = blueW

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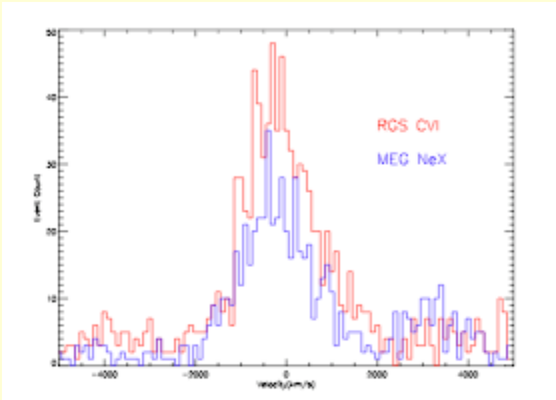
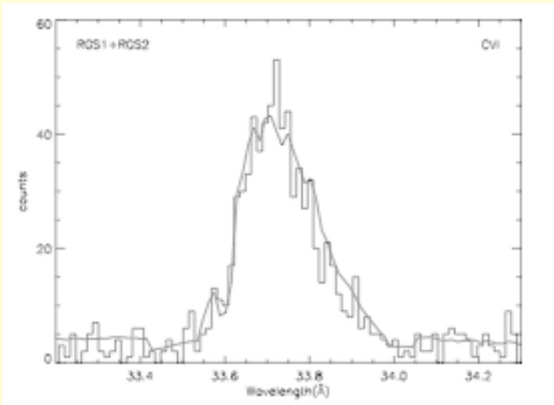
ion	blueV (km s^{-1})	centralV (km s^{-1})	redV (km s^{-1})	C-stat	ΔC
All ions	-1642 ± 22	-302 ± 29	$+1646 \pm 26$	22862.4	
C VI	-1719 ± 135	-270 ± 137	$+1403 \pm 130$	22855.6	6.8
N VII	-1705 ± 55	-111 ± 240	$+1065 \pm 324$	22859.8	2.6
O VII	-1349 ± 72	-509 ± 83	$+1835 \pm 76$	22844.9	17.5
O VIII	-1656 ± 43	-258 ± 59	$+1482 \pm 46$	22838.7	23.7
Fe XVII	-1647 ± 42	-421 ± 62	$+1845 \pm 59$	22848.9	13.5
Ne IX	-1653 ± 77	-211 ± 79	$+1508 \pm 102$	22859.9	2.5
Ne X	-1730 ± 106	-327 ± 126	$+1735 \pm 103$	22861.0	1.4
Mg XI	-1536 ± 153	$+33 \pm 121$	$+1487 \pm 144$	22850.1	12.3
Mg XII	-721 ± 365	-662 ± 227	$+1514 \pm 471$	22855.1	7.3
Si XIII	-1449 ± 124	$+48 \pm 240$	$+1421 \pm 188$	22856.4	6.0





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