Spectro-Perfectionism in SDSS-III

Adam S. Bolton
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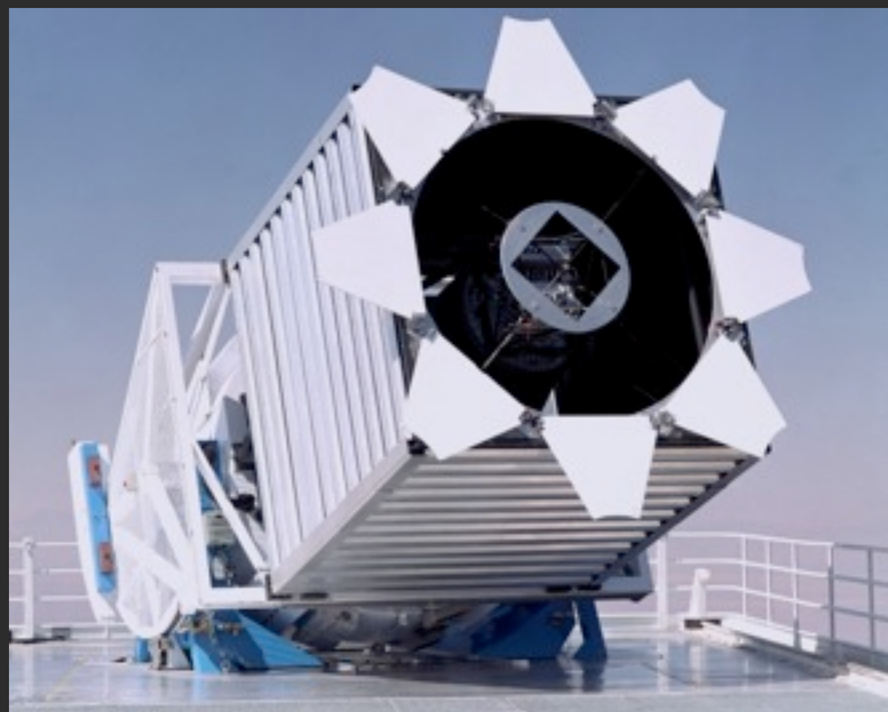
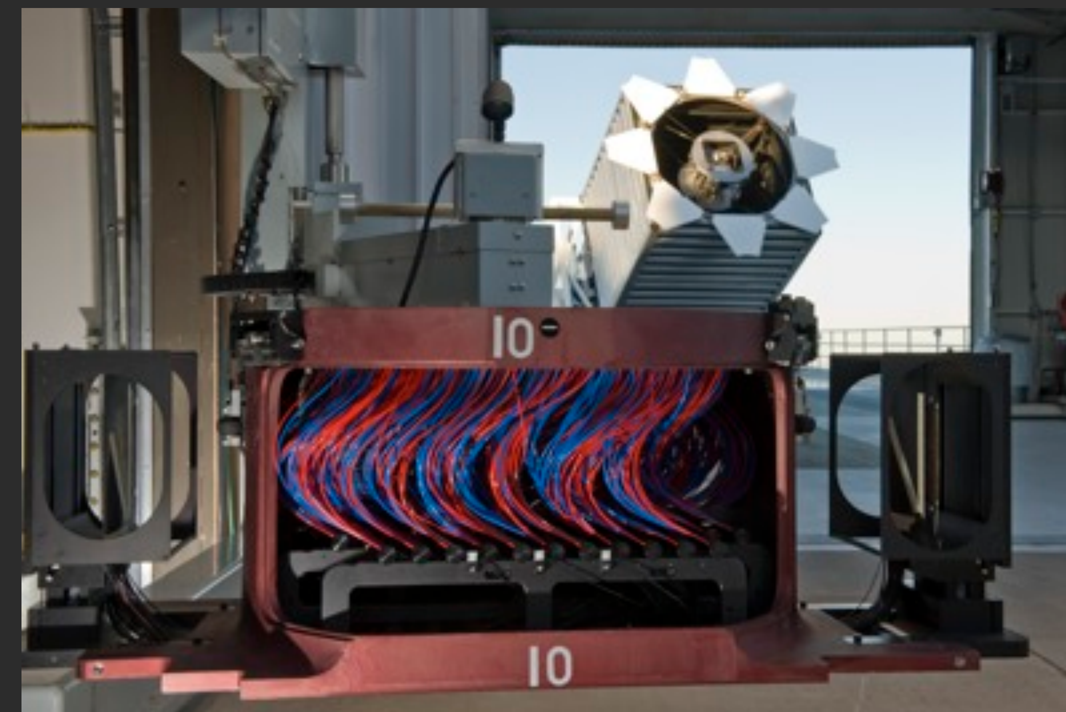
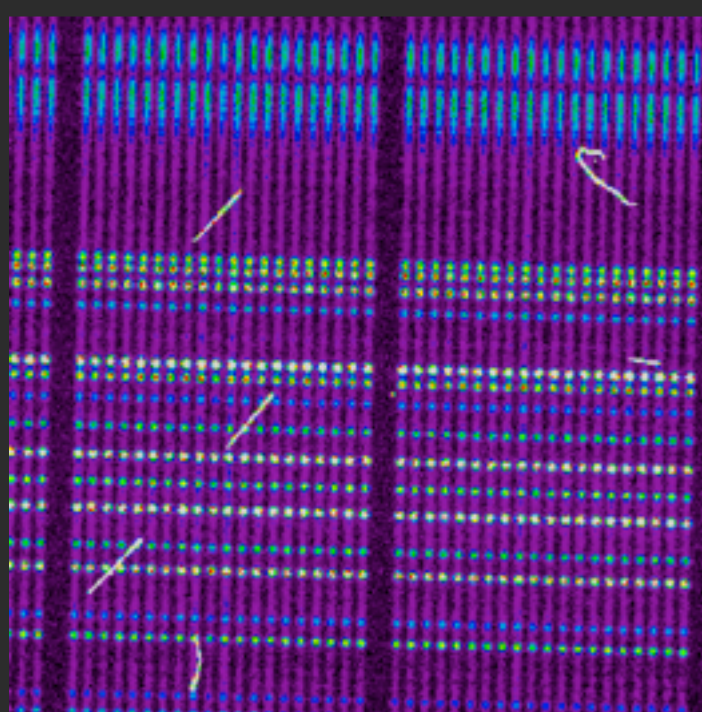
Following the Photons - ROE - 2011-10-10

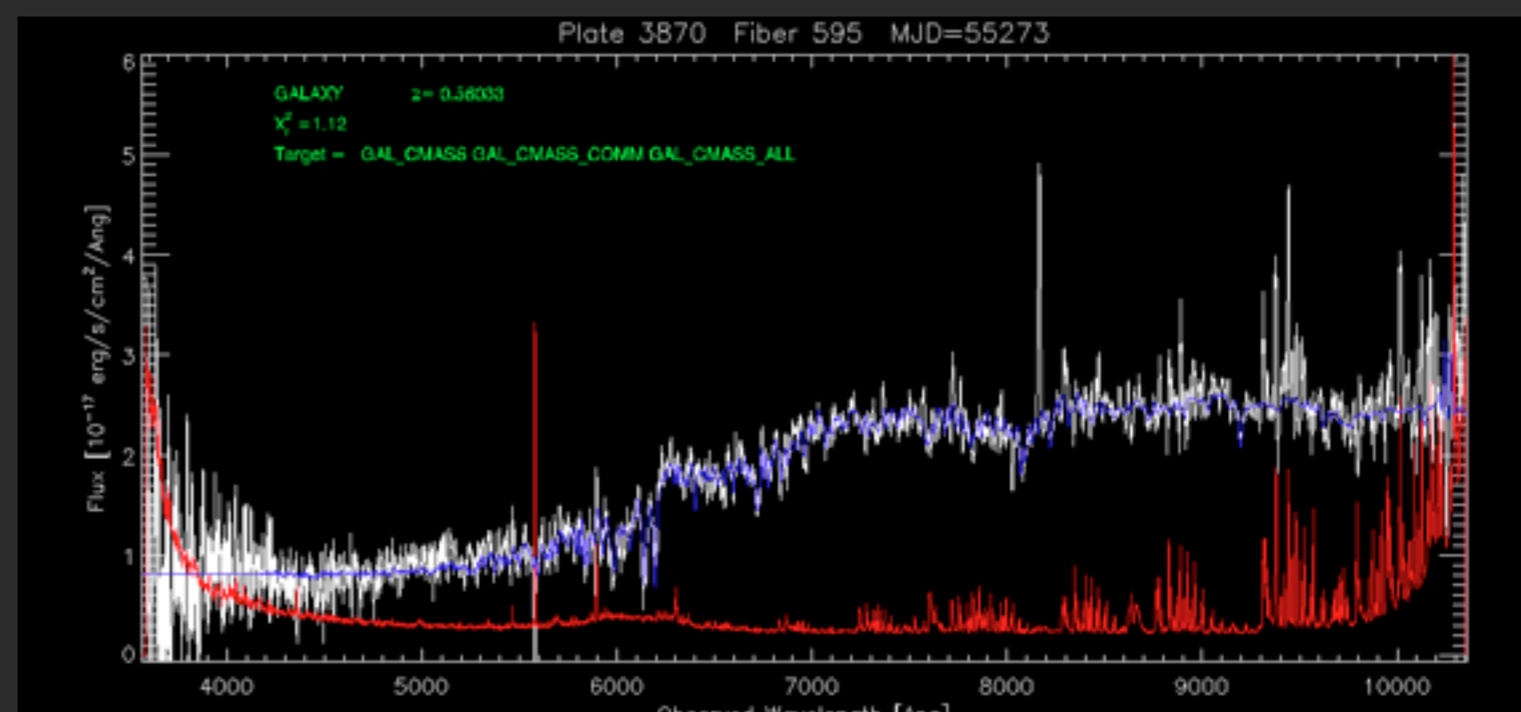
What is SDSS-III?

Eisenstein et al. 2011









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What is SDSS-III?

Eisenstein et al. 2011

BOSS: The Baryon Oscillation Spectroscopic Survey

- One of the four SDSS-III surveys
- 2009-2013 spectroscopic operations
- Redshifts of 1.5 million galaxies to $z = 0.7$
- 160k quasars for Lyman-α forest
- Measurement of baryon acoustic feature vs. z
- Constrain parameters of “dark energy”
- Largest spectro data set for massive galaxy evolution

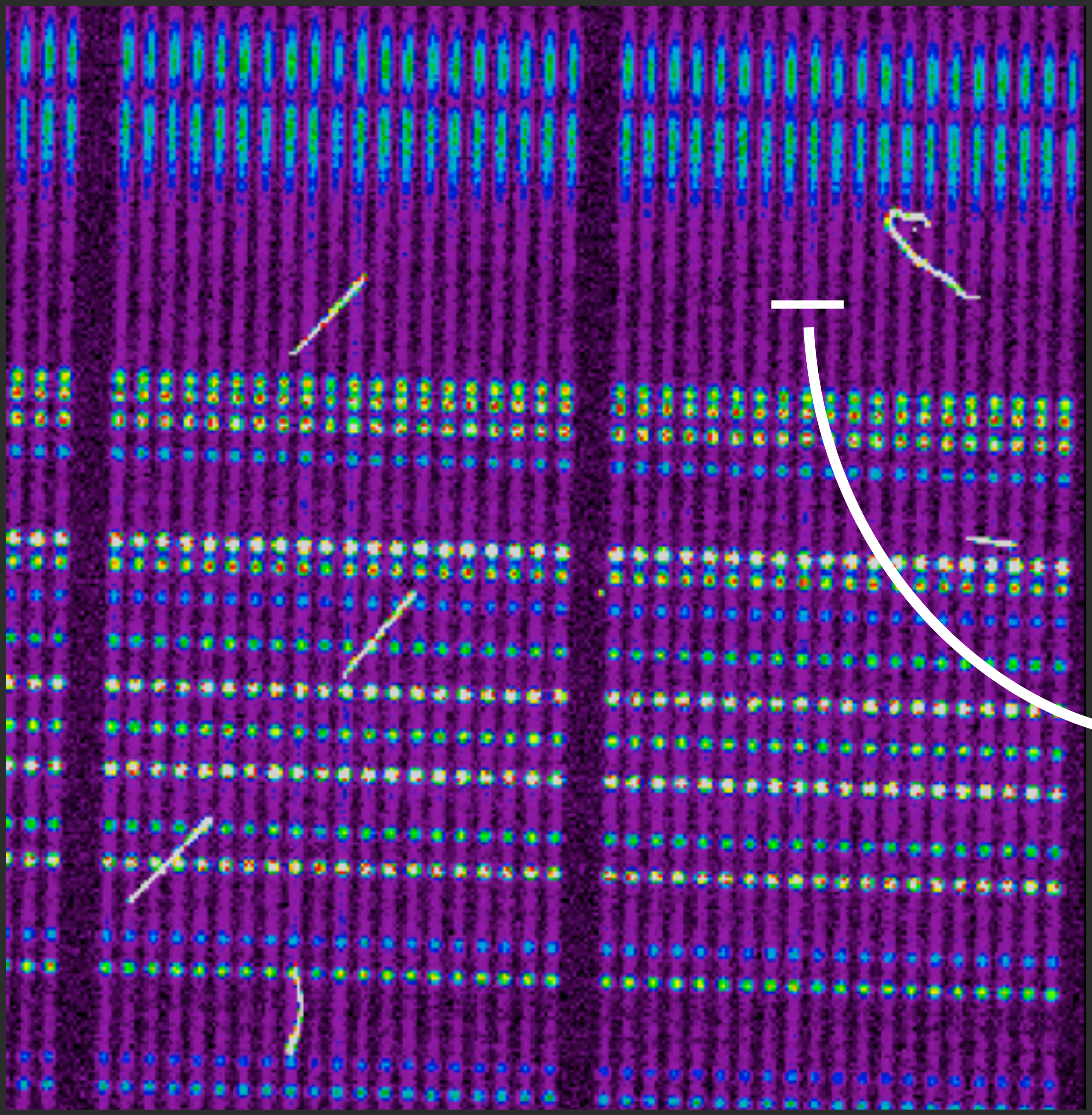
What is...

Spectro-Perfectionism
a.k.a.
2D PSF Extraction
a.k.a.
the Bolton & Schlegel algorithm
?

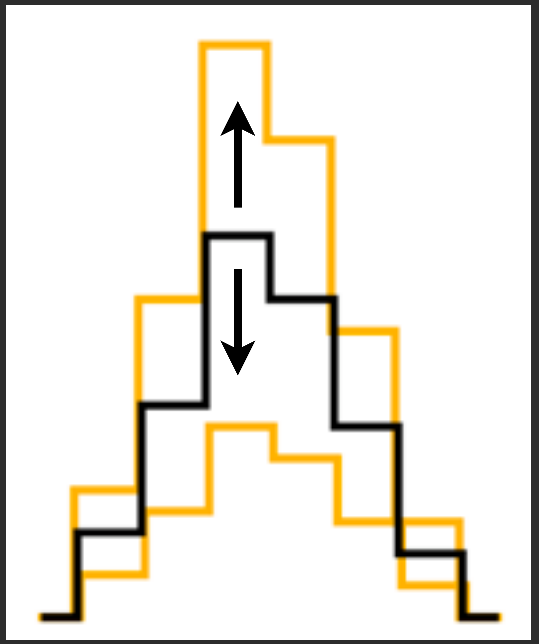
(Bolton & Schlegel 2010, PASP, 122, 248)

Spectroscopic extraction via mathematically correct forward modeling of the raw data via the 2D spectrograph point-spread function (PSF).

Doesn’t “optimal extraction” do this?

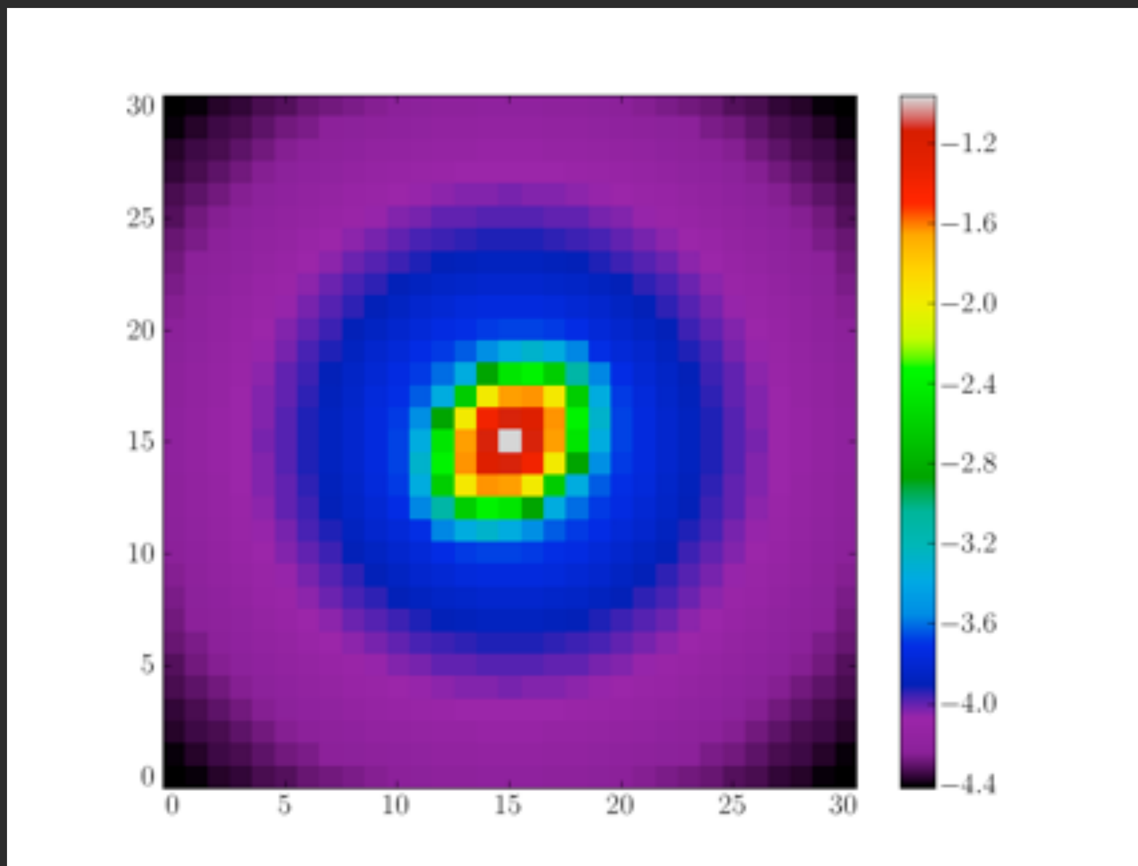


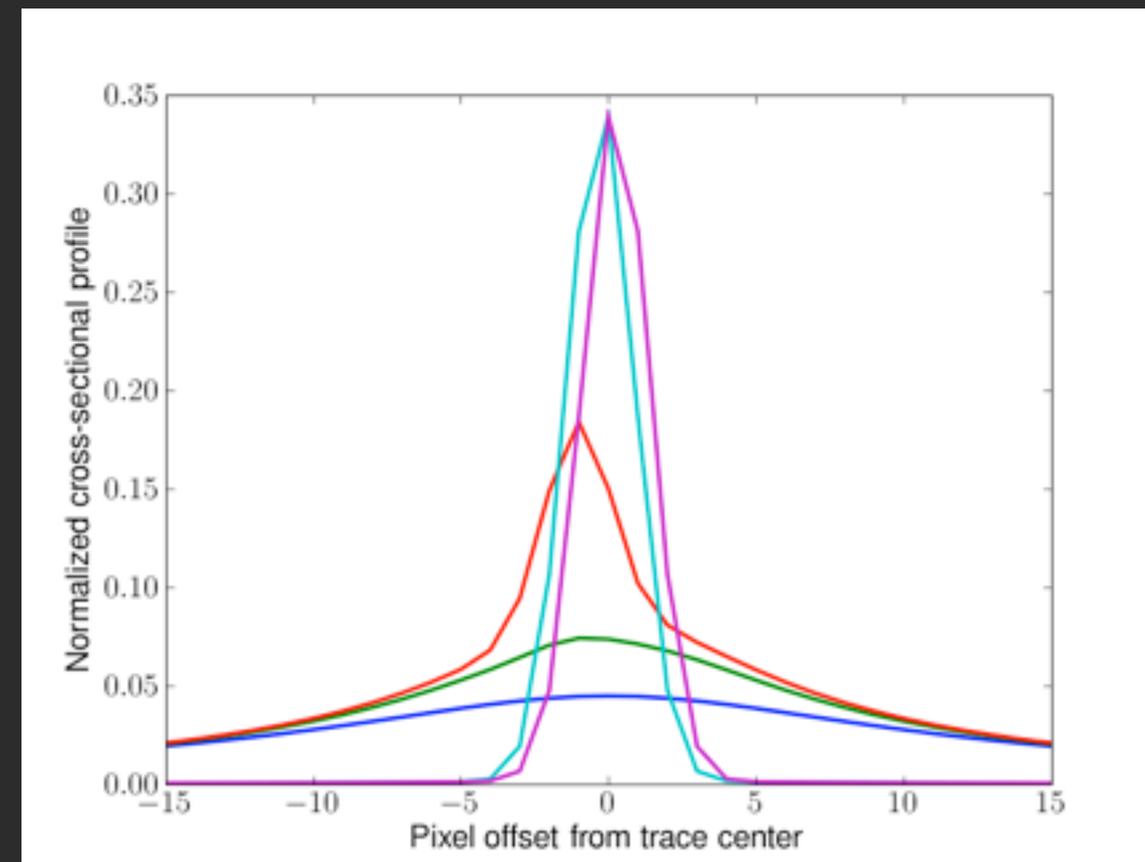
Hewett et al. 1985;
Horne 1986



- Determine cross-sec’n
- Weighted amplitude fit
- Call that your spectrum

How do you extract an emission line?

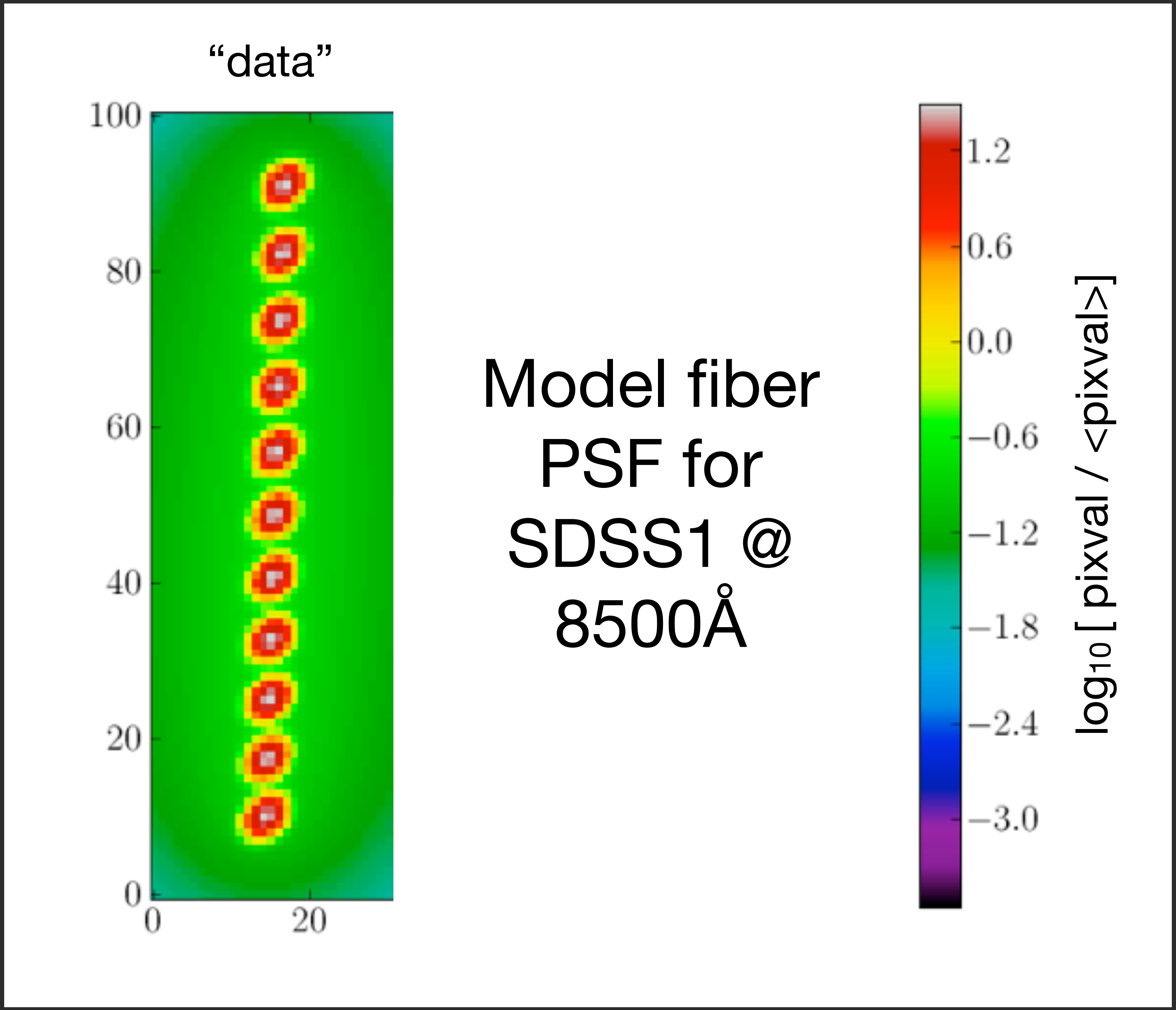




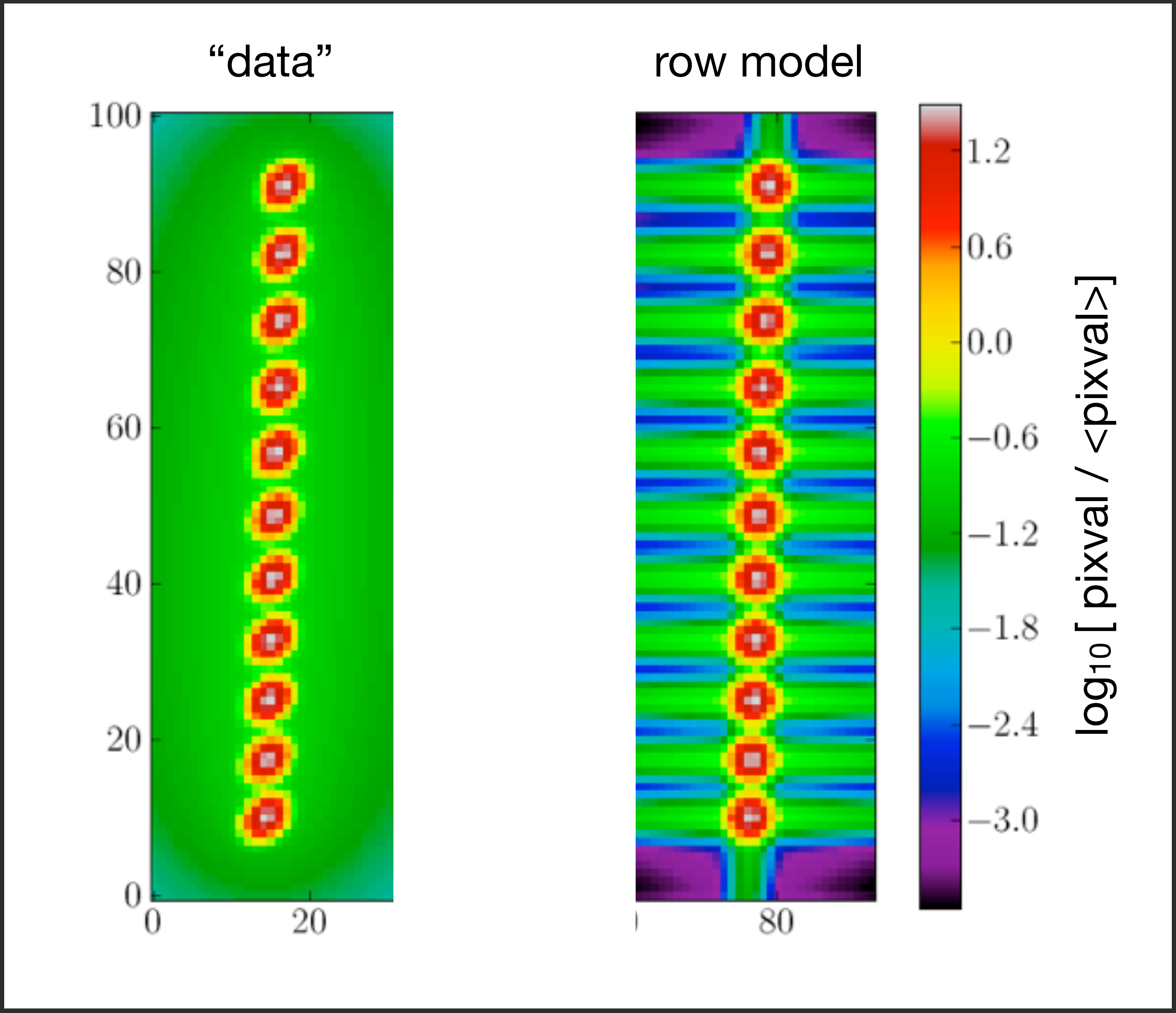
Row-by-row optimal extraction can only be correct when the spectrograph PSF is a *separable* function of x and y.

2D PSF extraction correct for arbitrary PSF shape.

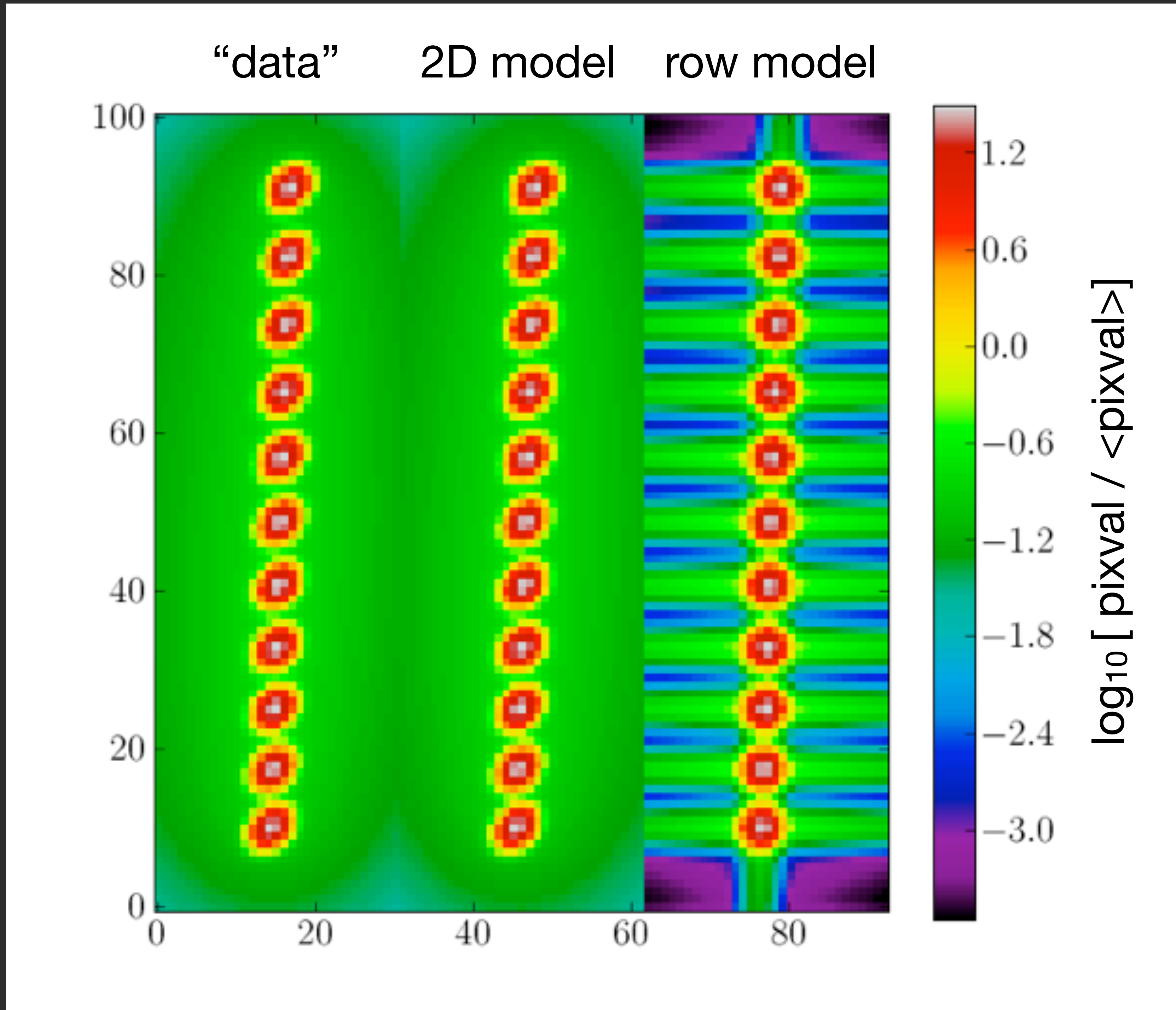
Extraction as image modeling



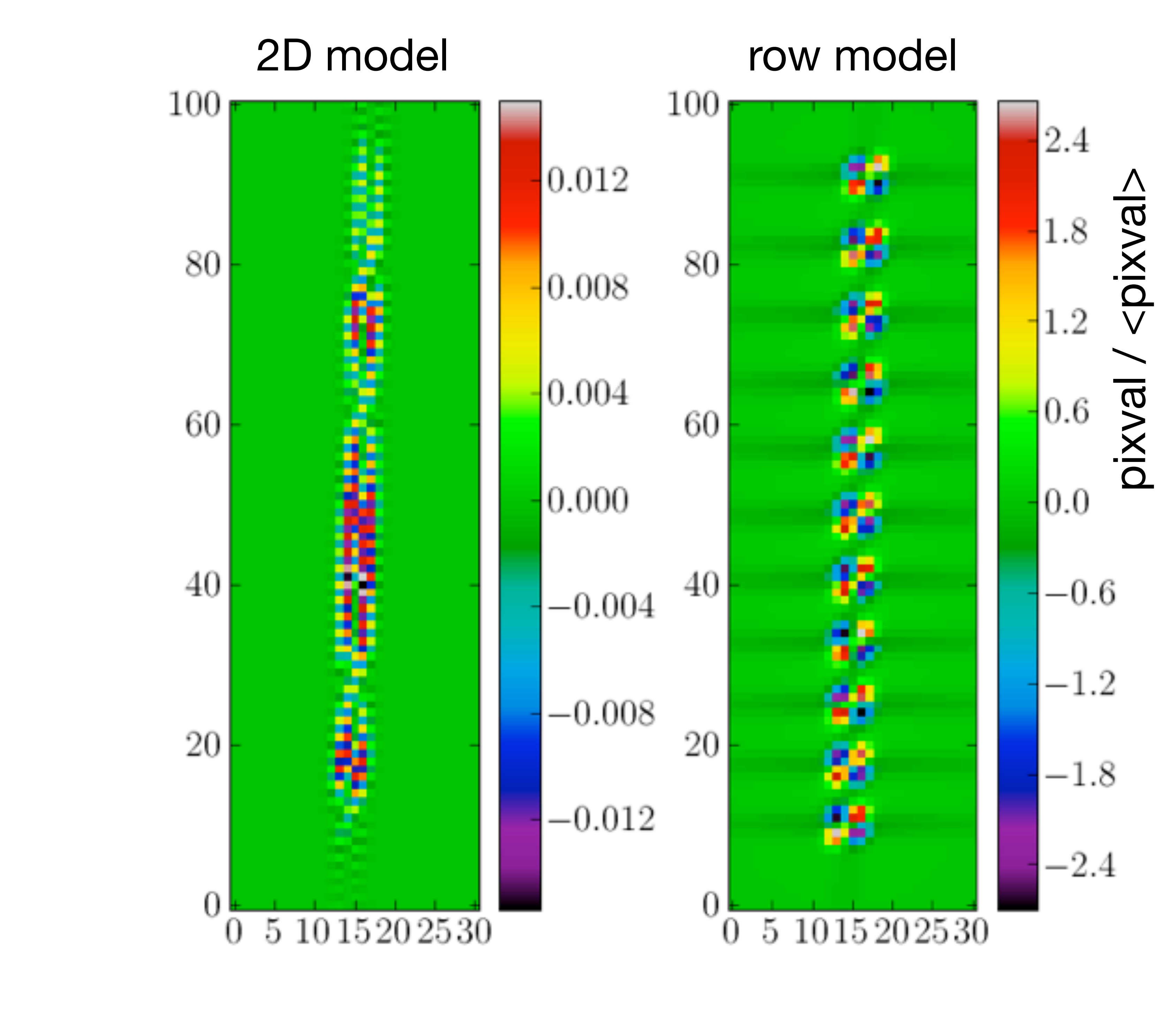
Extraction as image modeling



Extraction as image modeling



2D extraction model residuals



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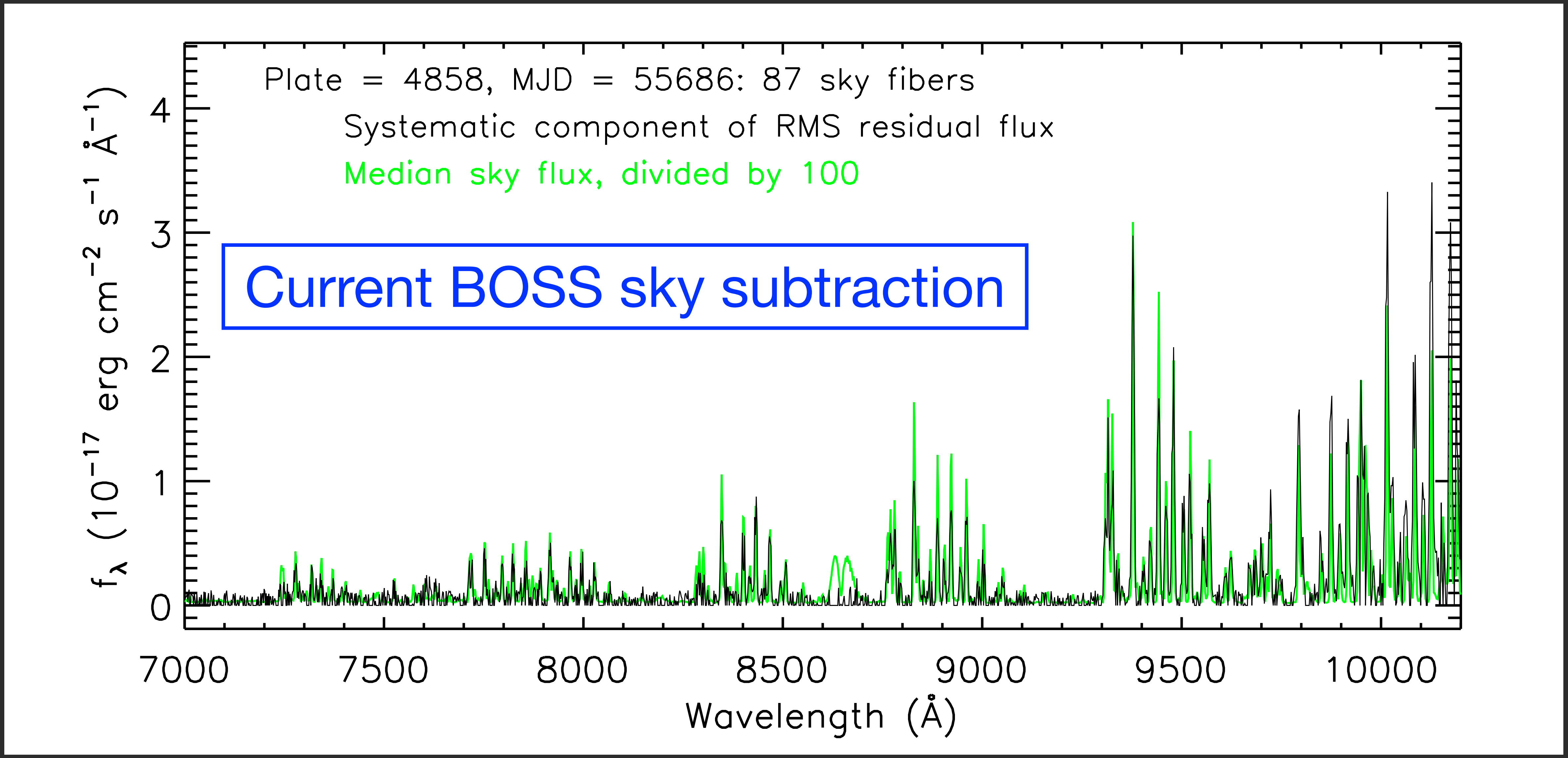
Why does this matter?

1) Poisson-limited sky subtraction

=> Current and future faint-galaxy redshift surveys

(E.g., BOSS, BigBOSS -- esp. [OII] ELG sample, ...)



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Why does this matter?

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=> Current and future faint-galaxy redshift surveys
(E.g., BOSS, BigBOSS -- esp. [OII] ELG sample, ...)

2) Extraction as lossless compression

=> All high-precision spectroscopic science
(Up to and including, e.g., RV planet surveys?)

What is a spectrum, anyway?

Not just

$\boldsymbol{f}$ = extracted spectrum vector

but also

$\boldsymbol{R}$ = band-diagonal line-spread function matrix

and

$\boldsymbol{C}$ = spectrum covariance matrix

Together, these encode the likelihood of a given input spectrum model ***m*** via:

$$\chi^2 (\boldsymbol{m} \mid \text{data}) = (\boldsymbol{f} - \boldsymbol{R}\,\boldsymbol{m})^{\mathrm{T}}\, \boldsymbol{C}^{-1}\, (\boldsymbol{f} - \boldsymbol{R}\,\boldsymbol{m})$$

How do we do this?

Projection of input spectrum to CCD pixel frame of raw data via "calibration matrix" A

(CCD pixel counts) = ***A*** (input spectrum counts) + (noise)

(That is, A_{jk} = predicted counts in pixel "j" from monochromatic input at wavelength "k".

Generalizes and incorporates:

- Trace solution
- Wavelength solution
- 2D spectrograph PSF and its variation (i.e., aberrations)
- Relative and absolute throughput variation
- CCD pixel sensitivity variations
- Etc.

How do we do this?

Projection of input spectrum to CCD pixel frame of raw data via "calibration matrix" A

(CCD pixel counts) = ***A*** (input spectrum counts) + (noise)

(That is, A_{jk} = predicted counts in pixel "j" from monochromatic input at wavelength "k".

Likelihood of any model spectrum ***m*** then encoded by:

$$\chi^2 (\boldsymbol{m} \mid \boldsymbol{p}) = (\boldsymbol{p} - \boldsymbol{A}\,\boldsymbol{m})^T \boldsymbol{N}^{-1} (\boldsymbol{p} - \boldsymbol{A}\,\boldsymbol{m})$$

This is forward-modeling to the raw pixels.

How do we do this?

"De-convolved" minimum-χ^2 spectrum solution would be

$$\boldsymbol{m} = (\boldsymbol{A}^{\mathrm{T}}\boldsymbol{N}^{-1}\boldsymbol{A})^{-1}\,(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{N}^{-1})\,\boldsymbol{p}$$

How do we do this?

"De-convolved" minimum-χ^2 spectrum solution would be

$$\boldsymbol{m} = (\boldsymbol{A}^{\mathrm{T}}\boldsymbol{N}^{-1}\boldsymbol{A})^{-1}\,(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{N}^{-1})\,\boldsymbol{p}$$

Now define resolution R and covariance C via:

$$(\boldsymbol{A}^{\mathrm{T}}\,\boldsymbol{N}^{-1}\,\boldsymbol{A}) = \boxed{\boldsymbol{Q}\,\boldsymbol{Q}} = (\boldsymbol{R}^{\mathrm{T}}\boxed{\boldsymbol{C}^{-1}}\boldsymbol{R})$$

diagonal

Symmetric matrix root

How do we do this?

"De-convolved" minimum-χ^2 spectrum solution would be

$$\mathbf{m} = (\mathbf{A}^T \mathbf{N}^{-1} \mathbf{A})^{-1} (\mathbf{A}^T \mathbf{N}^{-1}) \mathbf{p}$$

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diagonal

Symmetric matrix root

And define extracted spectrum as:

$$\mathbf{f} = \mathbf{R}\, (\mathbf{A}^T \mathbf{N}^{-1} \mathbf{A})^{-1} (\mathbf{A}^T \mathbf{N}^{-1}) \mathbf{p}$$

(Like a "re-convolution" of the de-convolved solution)

How do we do this?

Likelihood of any model spectrum ***m*** encoded by

$$\chi^2 (\boldsymbol{m} \mid \boldsymbol{f}) = (\boldsymbol{f} - \boldsymbol{R}\,\boldsymbol{m})^T \boldsymbol{C}^{-1} (\boldsymbol{f} - \boldsymbol{R}\,\boldsymbol{m})$$

is then mathematically equivalent to

$$\chi^2 (\boldsymbol{m} \mid \boldsymbol{p}) = (\boldsymbol{p} - \boldsymbol{A}\,\boldsymbol{m})^T \boldsymbol{N}^{-1} (\boldsymbol{p} - \boldsymbol{A}\,\boldsymbol{m})$$

(up to a constant offset)

Forward-modeling to a spectrum extracted in this manner is information-equivalent to forward-modeling to the raw CCD pixels.

What is extraction?

Calibration:
Likelihood functional determination

Extraction:
Likelihood functional compression

Measurement:
Likelihood functional projection

Summary of 2D PSF extraction

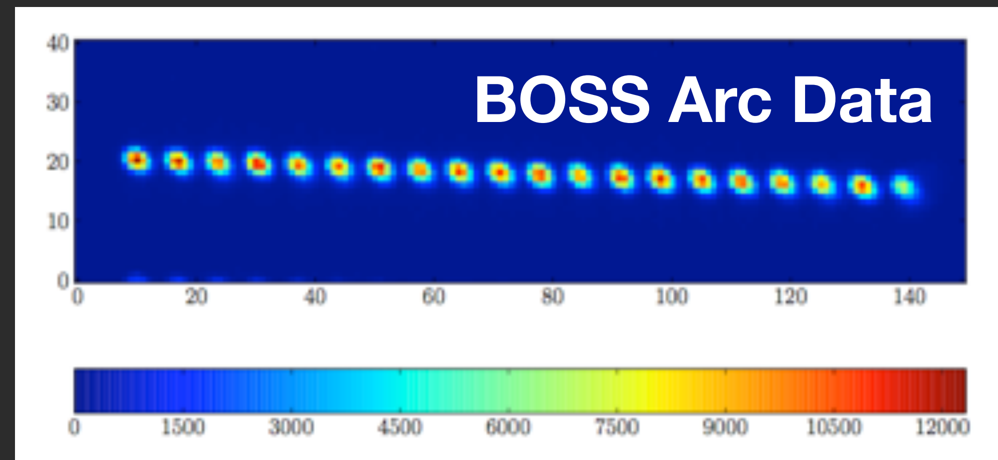
Major Advantages:

- Extraction as lossless compression
- Mathematically correct even for non-separable PSF
- Incorporates explicit model of 2D data
- Poisson-limited sky subtraction
- Data products “look & feel like spectra”

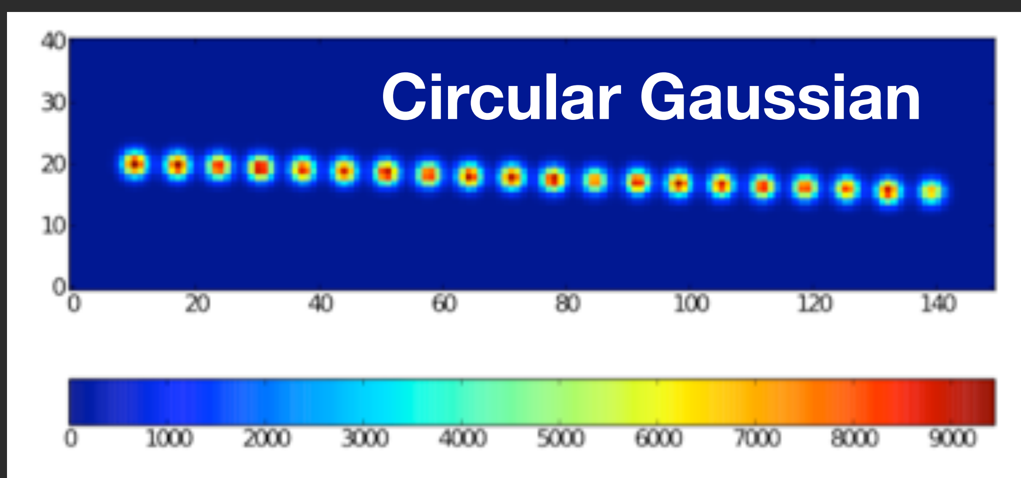
Major Challenges:

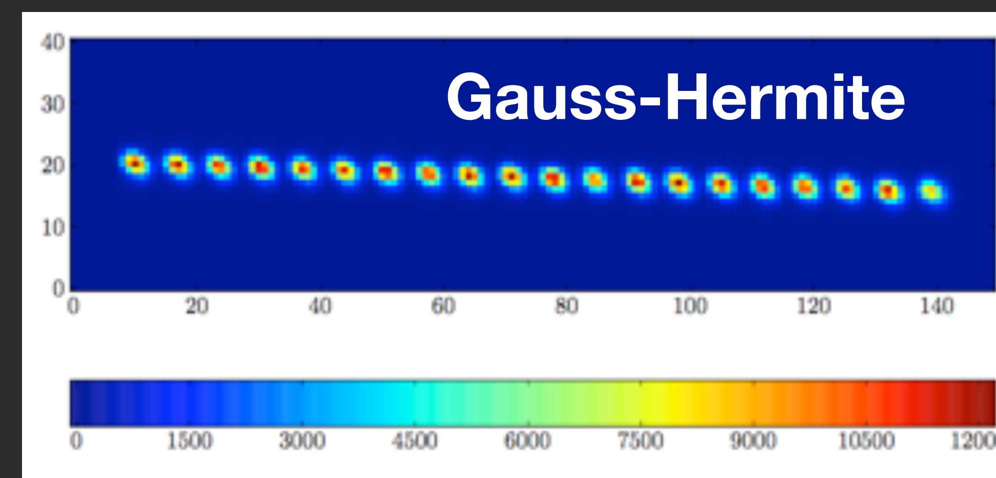
- Extraction coupled across wavelengths
- Requires exquisite calibration
- Some subtlety related to flux normalization

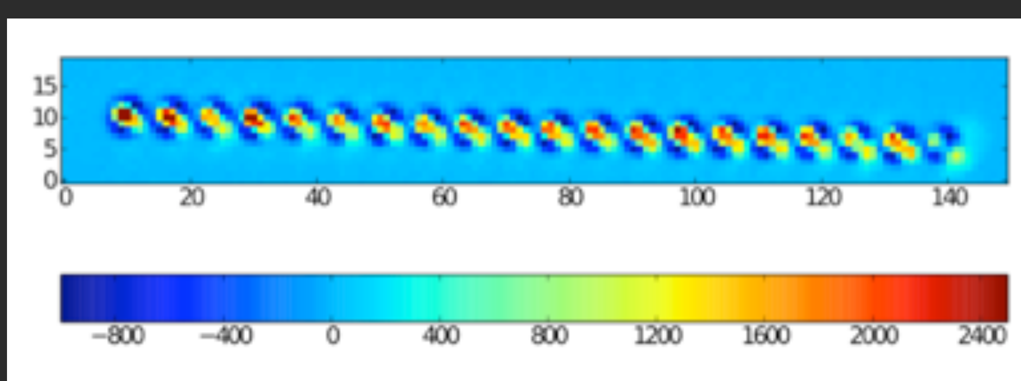
Development & Implementation Status

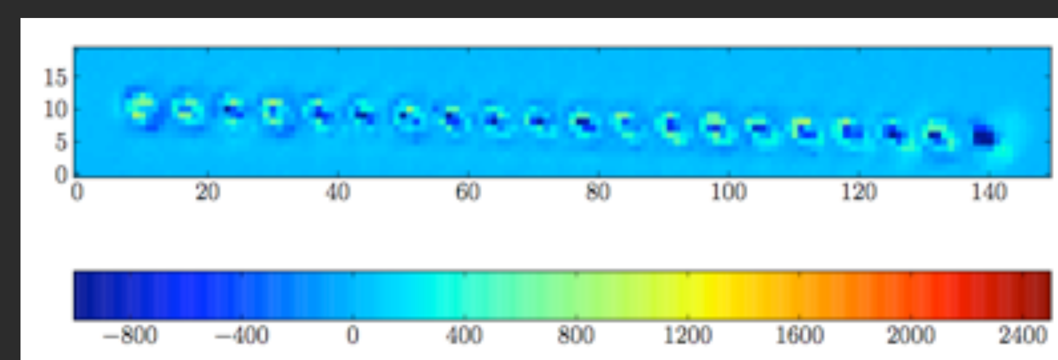


Images from
Parul Pandey
M.S. Thesis
U. of Utah







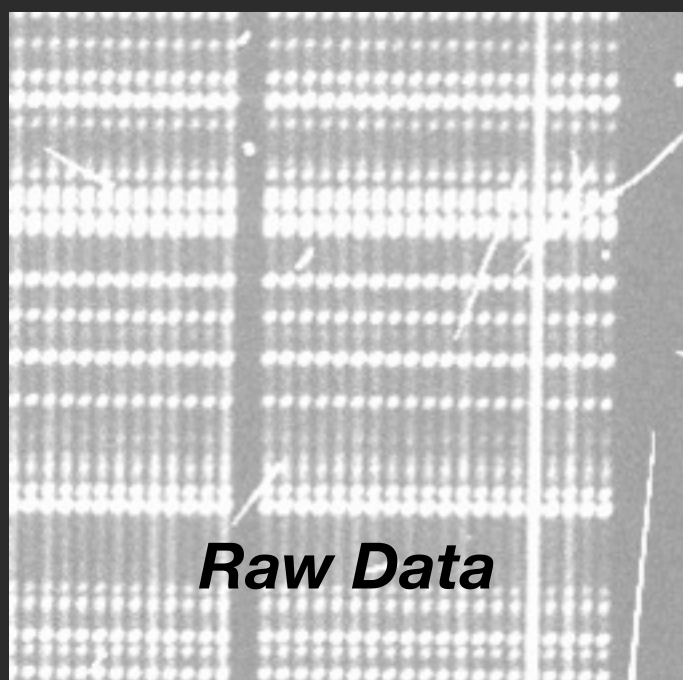


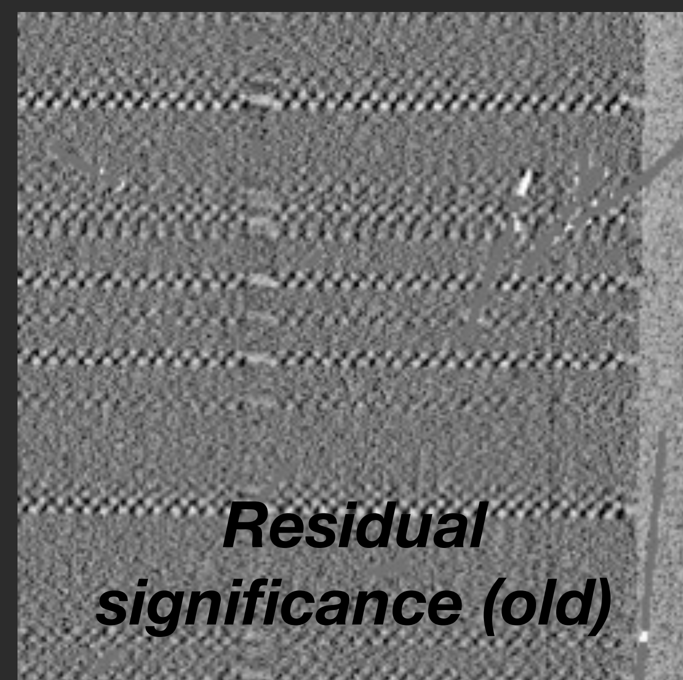
Also: wing component, higher order GH, pixelized PSF

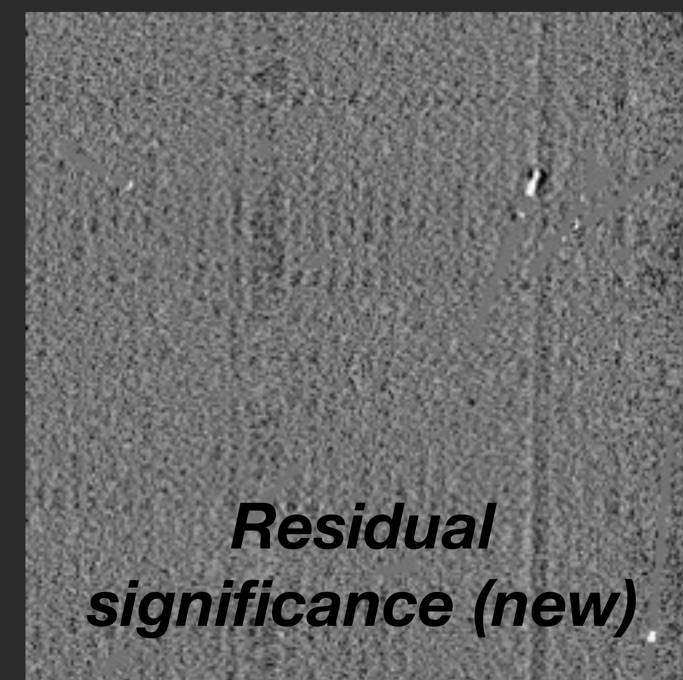
Development & Implementation Status

Demonstrated path for computational tractability:

- Decompose among bundles, exposures, spectrographs, and wavelength ranges







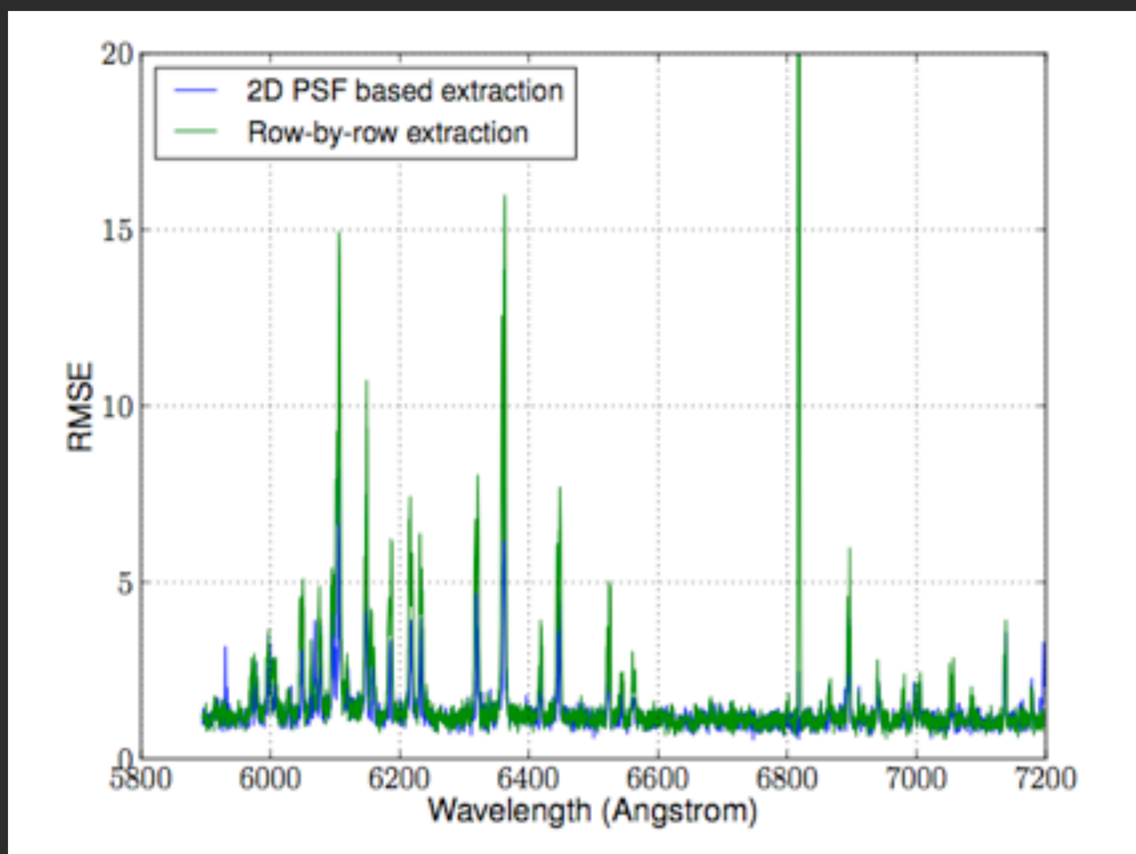
Effort in summer 2011 and ongoing by:

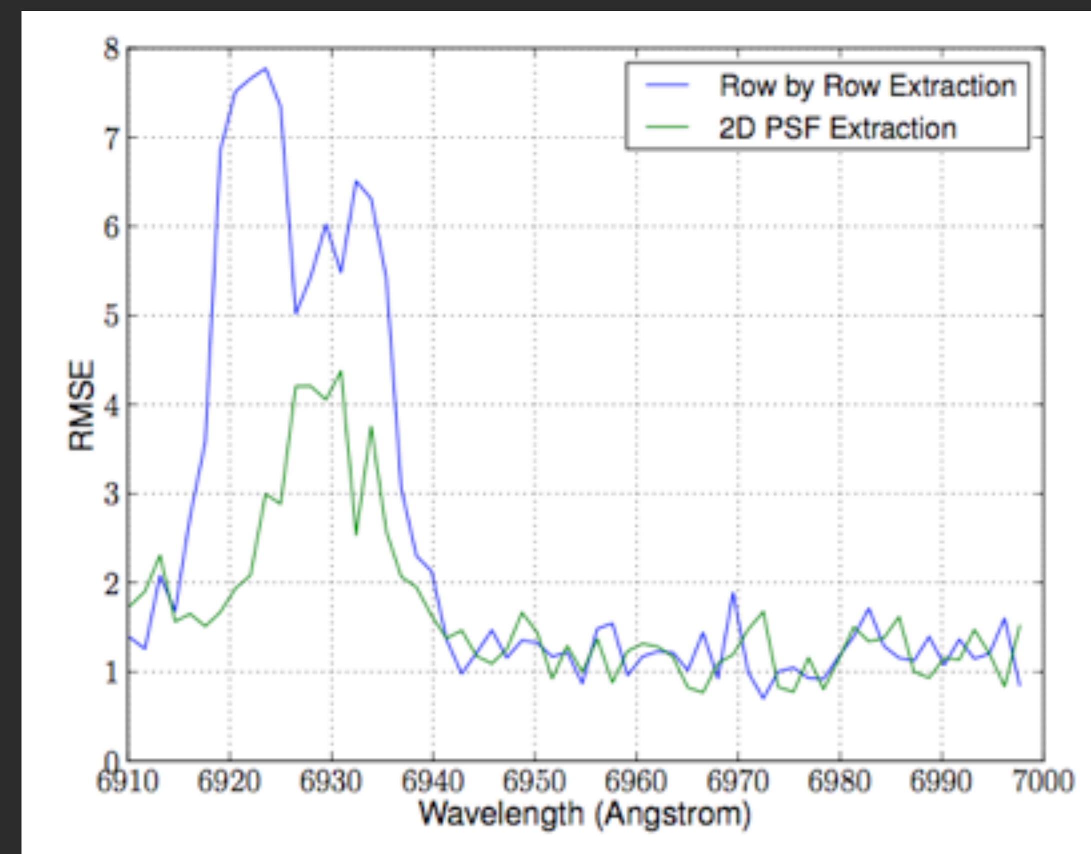
ASB, Joel Brownstein, Parul Pandey (U. of Utah)

Stephen Bailey, Ted Kisner, David Schlegel (LBNL)

Benefits in extracted-spectrum frame

Sky subtraction, as simulated by arc-lamp data





Images from Parul Pandey, M.S. Thesis 2011, U. of Utah

Software Requirements on Hardware

Separability: we absolutely need gaps between bundles of fibers where cross-talk goes to zero

True resolution: metric is not camera spot EE or flux-weighted r^2, but *wavelength autocorrelation of PSF:*

$$[\int p(x,y;\lambda)\ (x,y;\lambda+\Delta\lambda)\ dx\ dy] / [\int p^2(x,y;\lambda)\ dx\ dy]$$

(N.B.: Rayleigh criterion is autocorrelation of 1/4)

Calibration: tunable monochromatic system for mapping out system calibration matrix?

Stability: fractional spectrum bias for assuming wrong PSF q(x,y) instead of right PSF p(x,y) is:

$$b = 1 - [\int p(x,y)\ q(x,y)\ dx\ dy] / [\int p^2(x,y)\ dx\ dy]$$

Software Requirements on Hardware

Ultimately calls for a full integration of data analysis software with instrumental design software

=> Optimize *scientific* metrics in hardware design

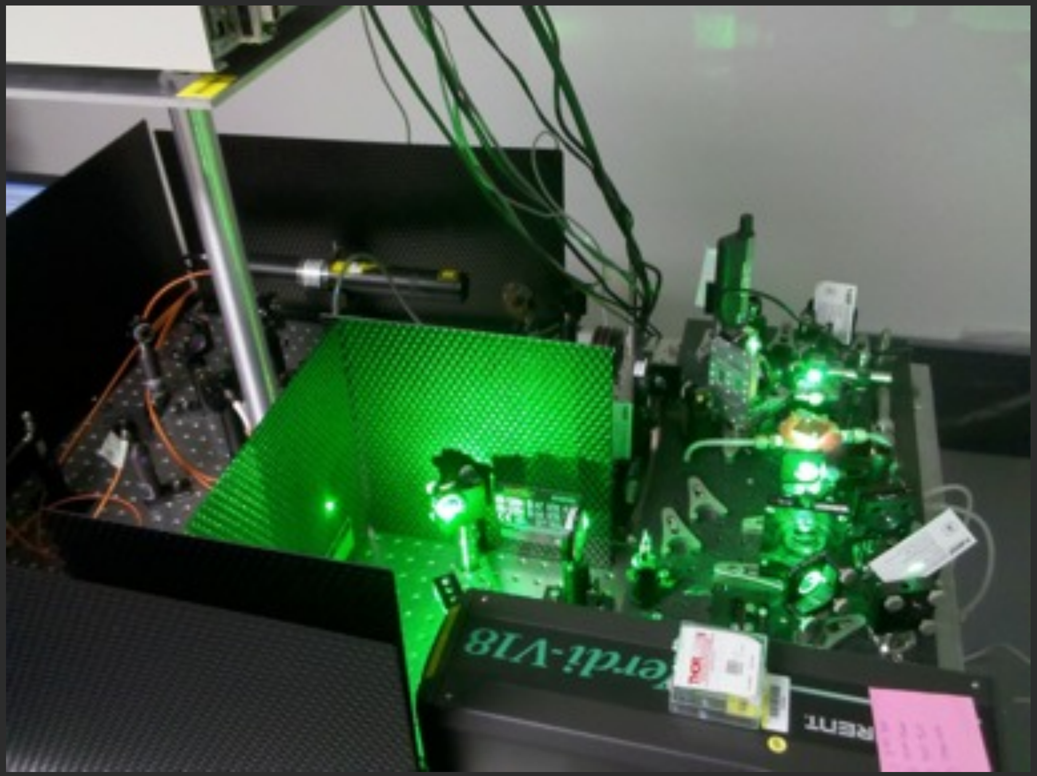
=> Tune instrument directly from science CCD data

=> "Use what you know" during analysis

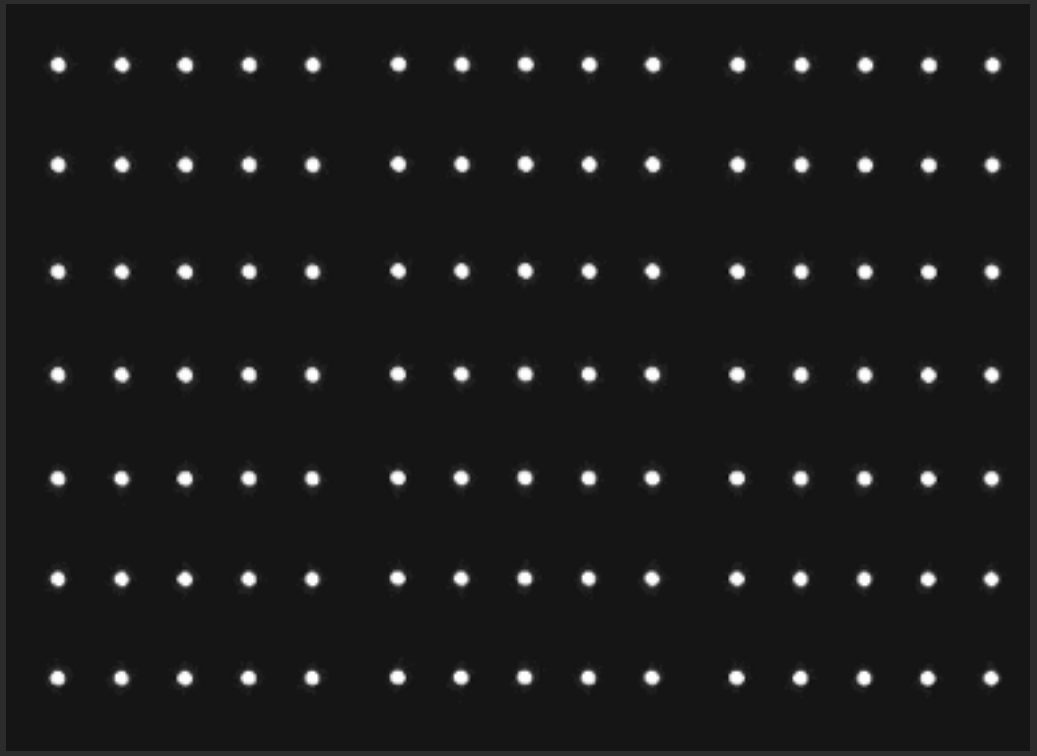
Monochromatic calibration

NIST-BOSS tunable laser experiment (w/ C. Cramer, K. Lykke)

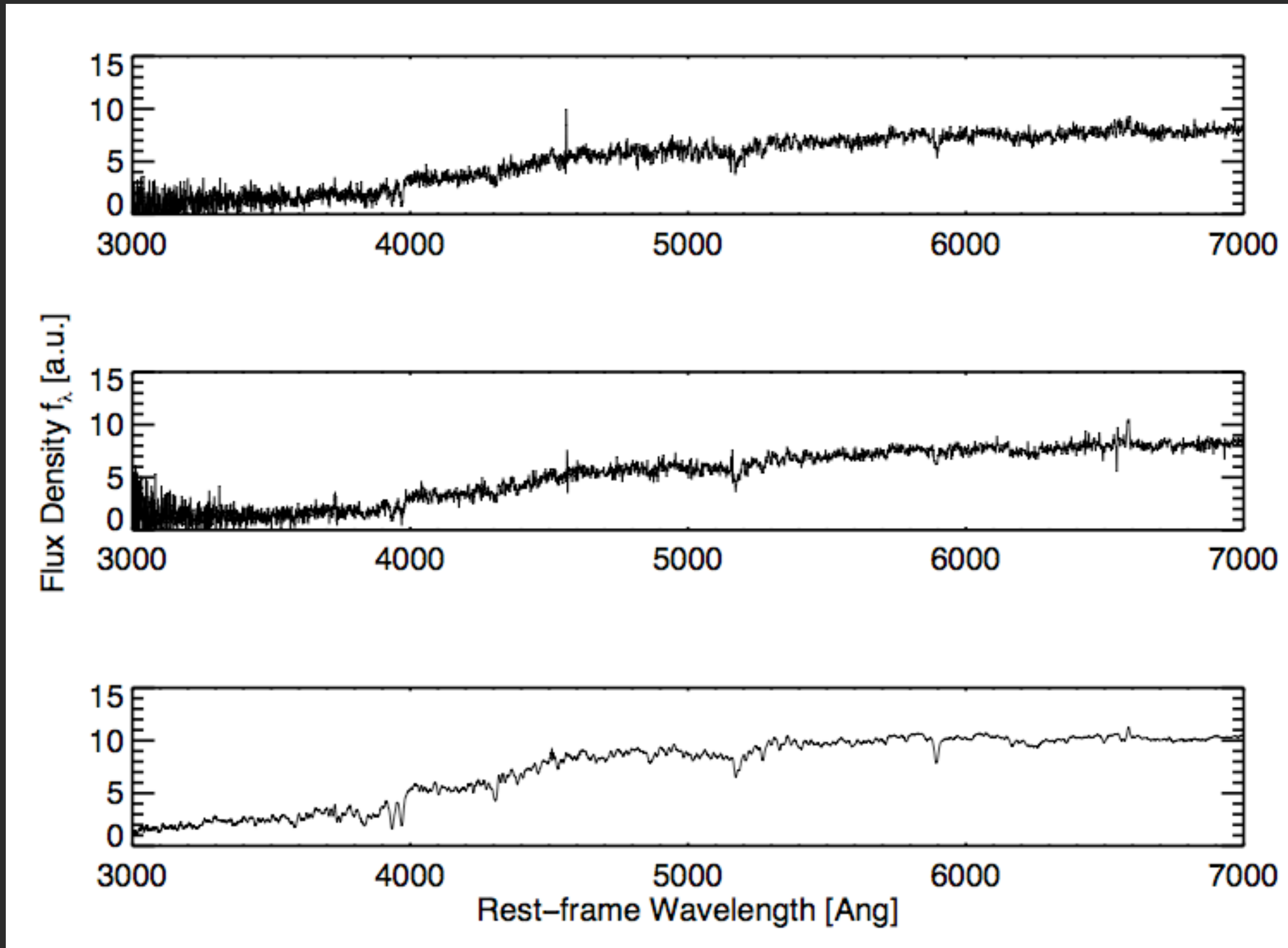
(Also see G. Tarle "Line-O-Matic")



vs.



Application: Bayesian stacking



Shu, ASB, et al., submitted (arXiv 1109.6678)

Application: Bayesian stacking

Model vdisp distribution at fixed z and M as a log-normal distribution (c.f. Bernardi et al. 2003):

$$p(log_{10}\sigma|m,s) = \frac{1}{\sqrt{2\pi}s} e^{-\frac{(log_{10}\sigma - m)^2}{2s^2}} \quad (1)$$

Constrain parameters in (z, M) bins by integrating over all spectra and all vdisp values:

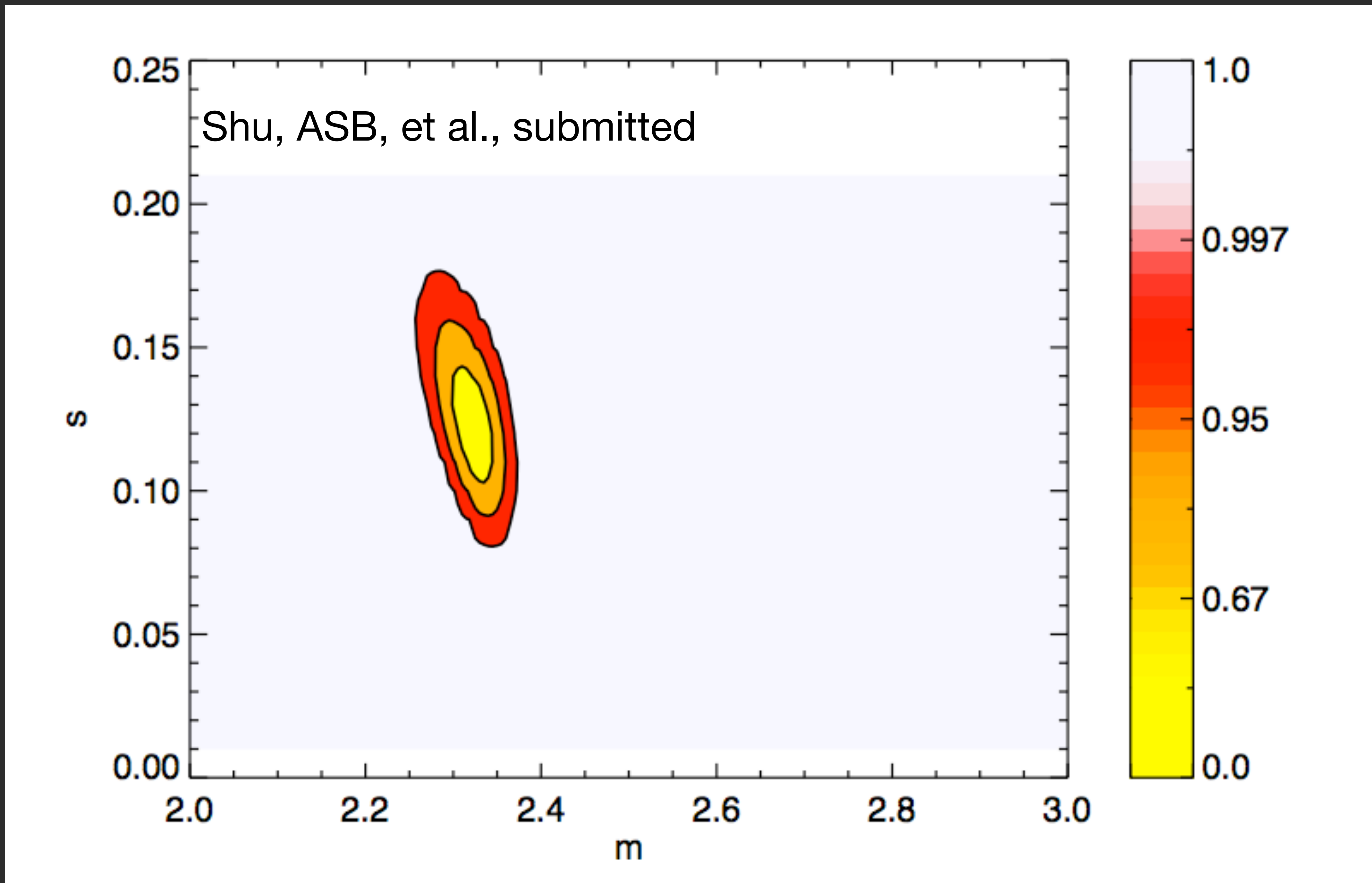
$$\begin{aligned} \mathcal{L}(m,s|\{\vec{d}\}) &= p(\{\vec{d}\}|m,s) \\ &= \prod_i p(d_i|m,s) \quad (2) \\ &= \prod_i \int \mathrm{d}log_{10}\sigma \, p(d_i|log_{10}\sigma)\, p(log_{10}\sigma|m,s) \end{aligned}$$

$$p(m,s|\{\vec{d}\}) = \frac{p(\{\vec{d}\}|m,s)p(m,s)}{p(\{\vec{d}\})} \quad (3)$$

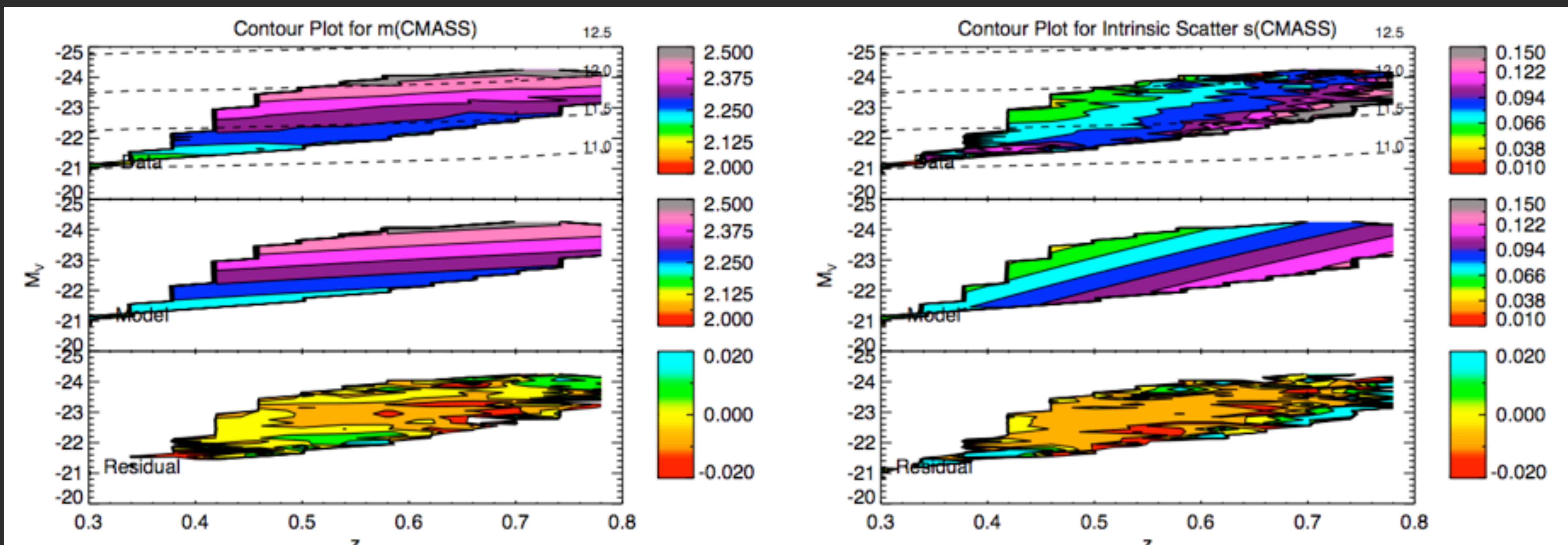
Shu, ASB, et al., submitted (arXiv 1109.6678)

N.B.: if you stack directly, you will measure $\sigma = 10^{[m + s^2 \ln(10)]}$

Posterior probability for a single bin



Distribution results: population evolution



Shu, ASB, et al., submitted

Summary and conclusions

- Full 2D forward modeling of raw data is the way of the future for spectroscopic extraction
- Poisson-limited sky subtraction for ground-based faint-galaxy redshift surveys (BOSS, BigBOSS)
- Lossless compression of spectrum likelihood functional
- We have the algorithmic framework, and are currently putting it into practice
- Major challenges are in calibration, computation, and integration of data analysis with hardware design

Thank You!

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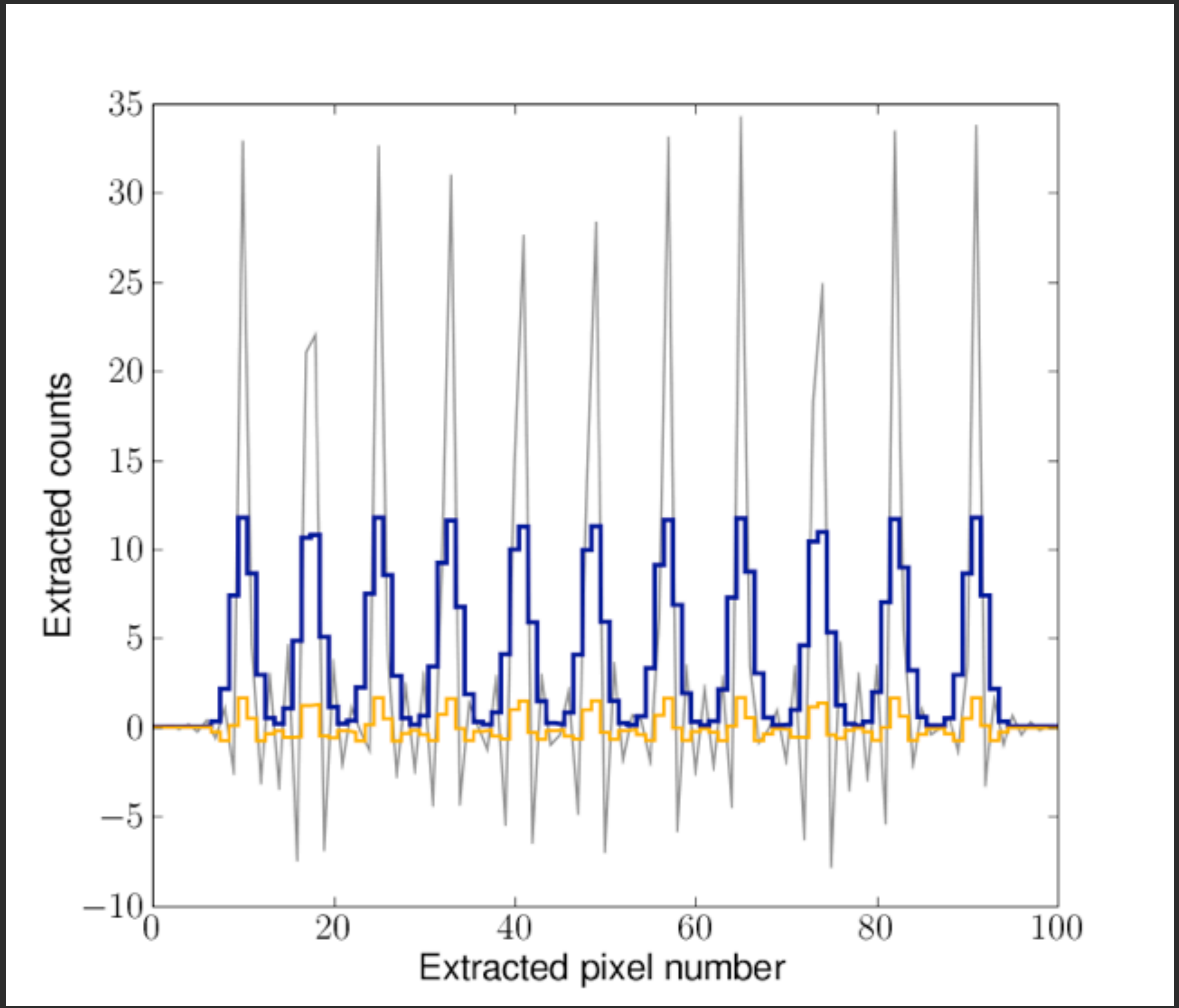
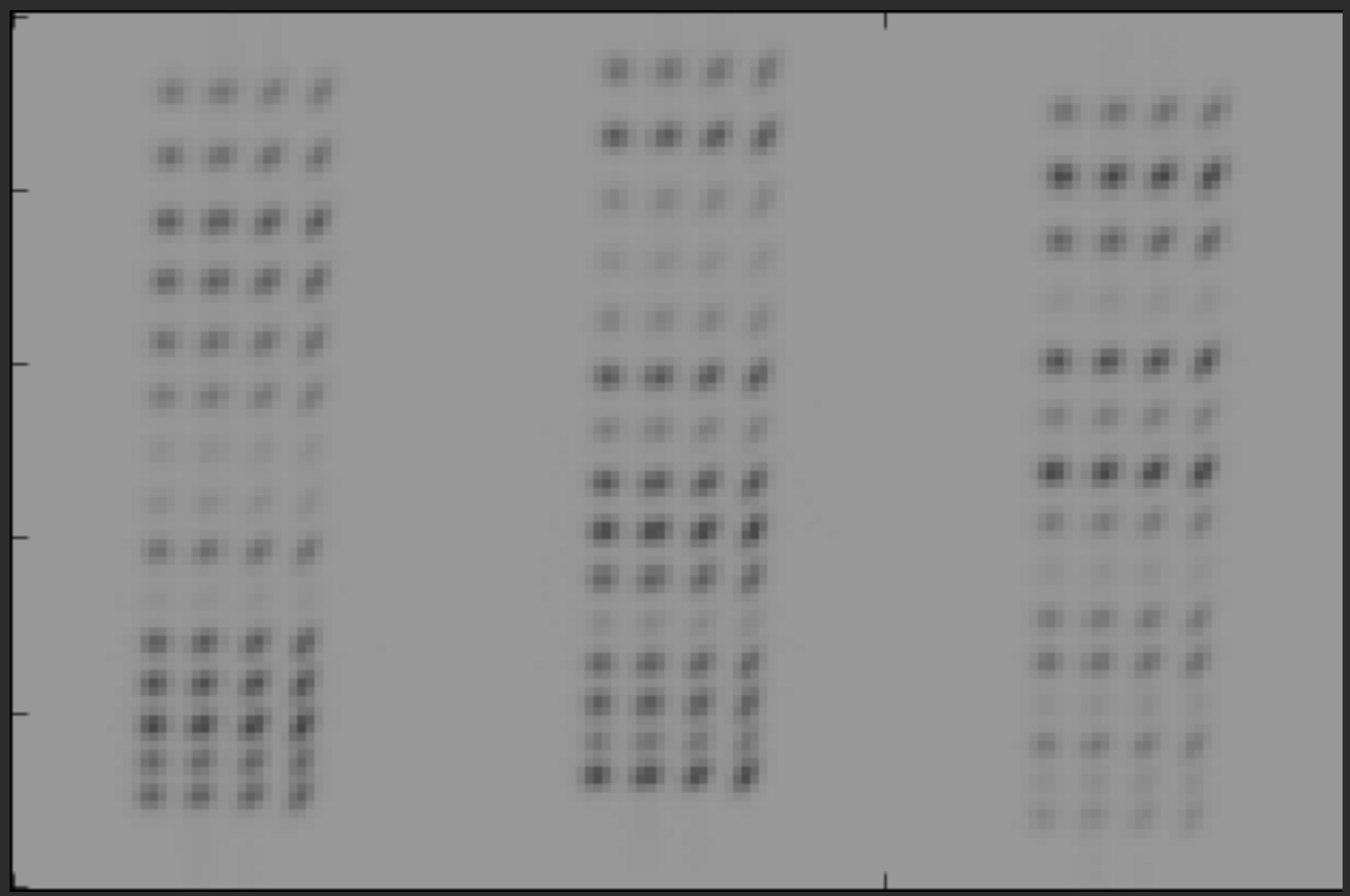
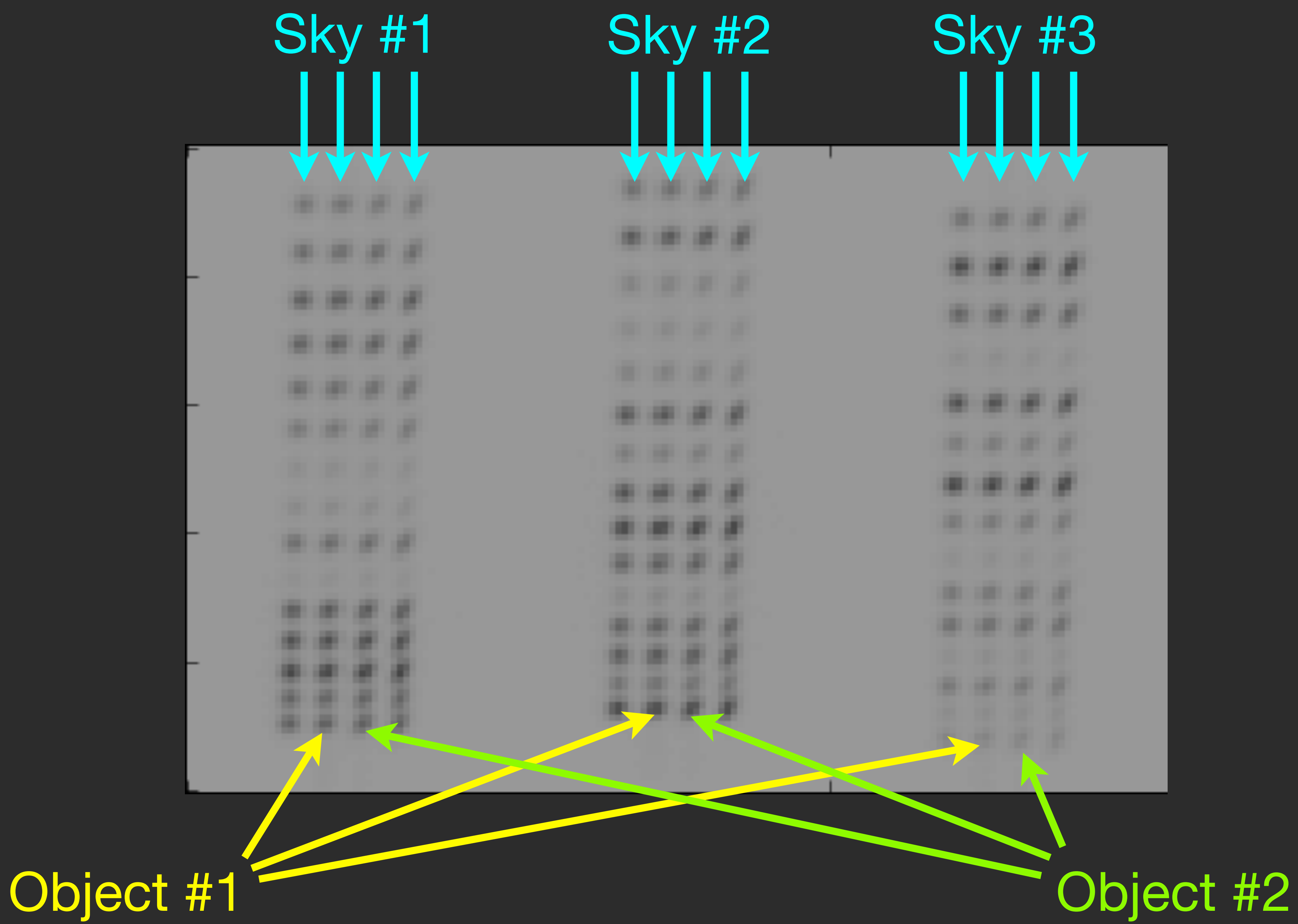
Deconvolution and reconvolution



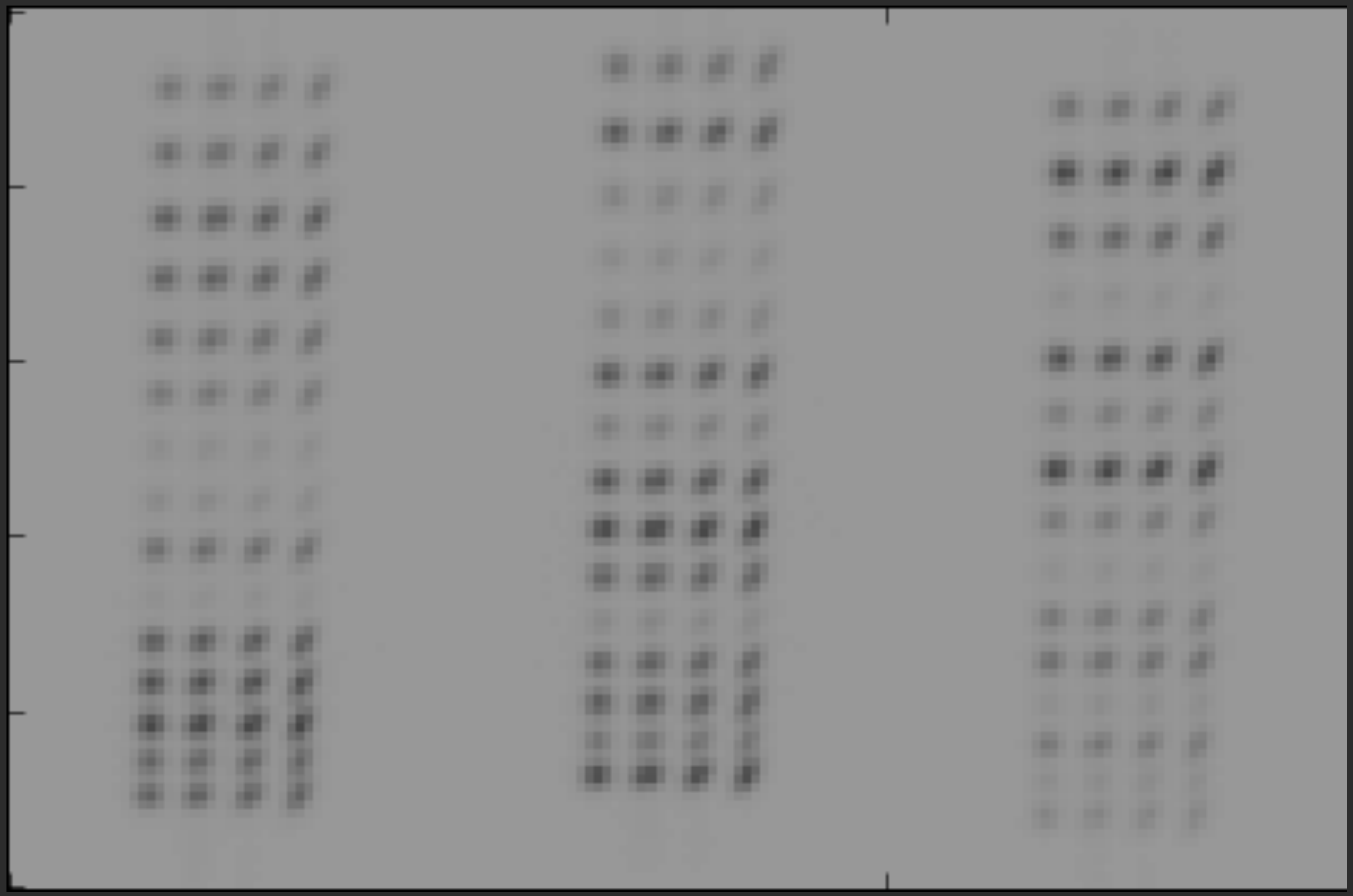
Multi-frame, multi-fiber simulated data



Multi-frame, multi-fiber simulated data



Multi-frame, multi-fiber simulated data

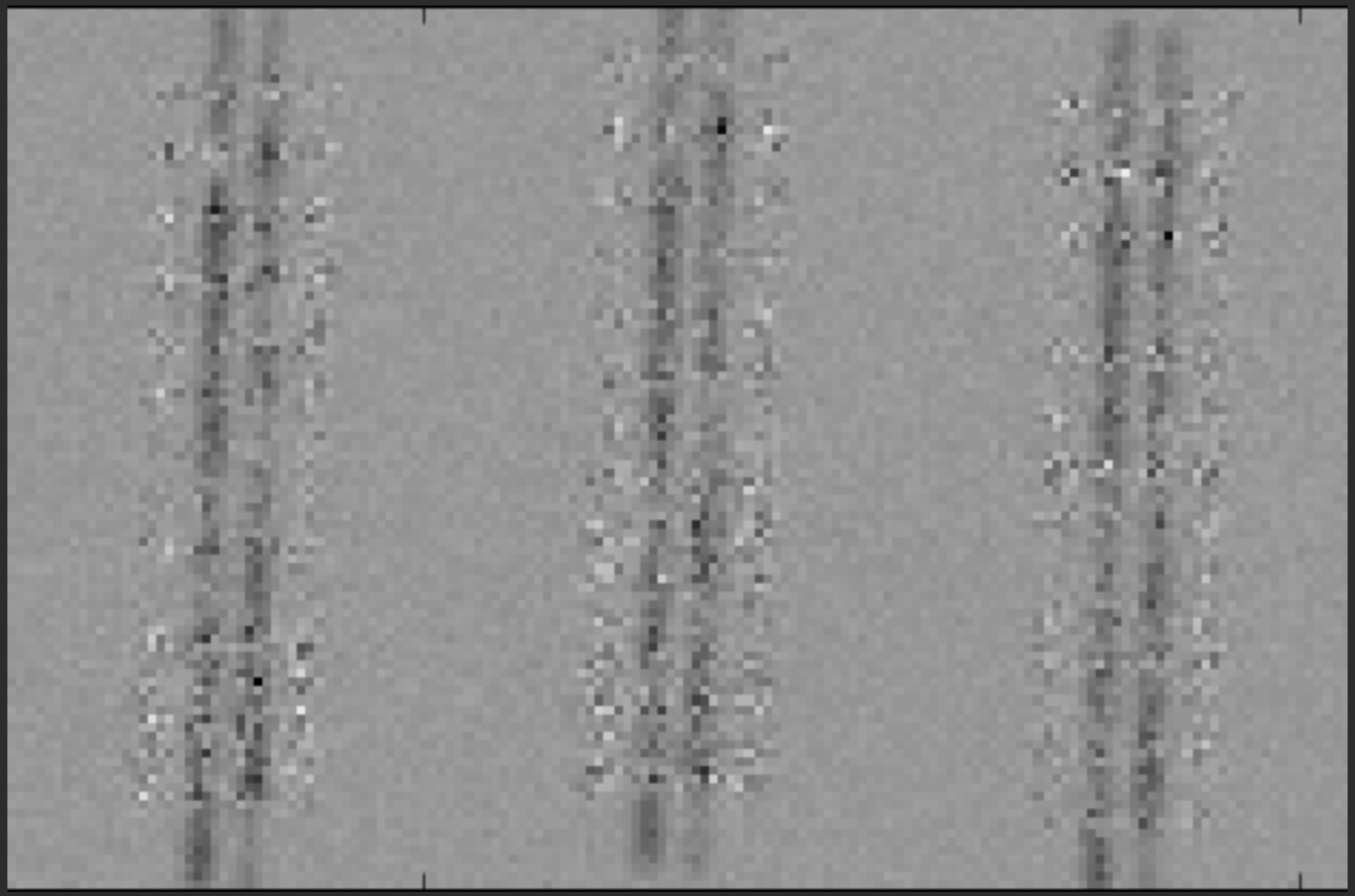


Objflux = Skyflux / 20

ObjSNR ≈ 5 (per extracted sample, sky-noise limited)

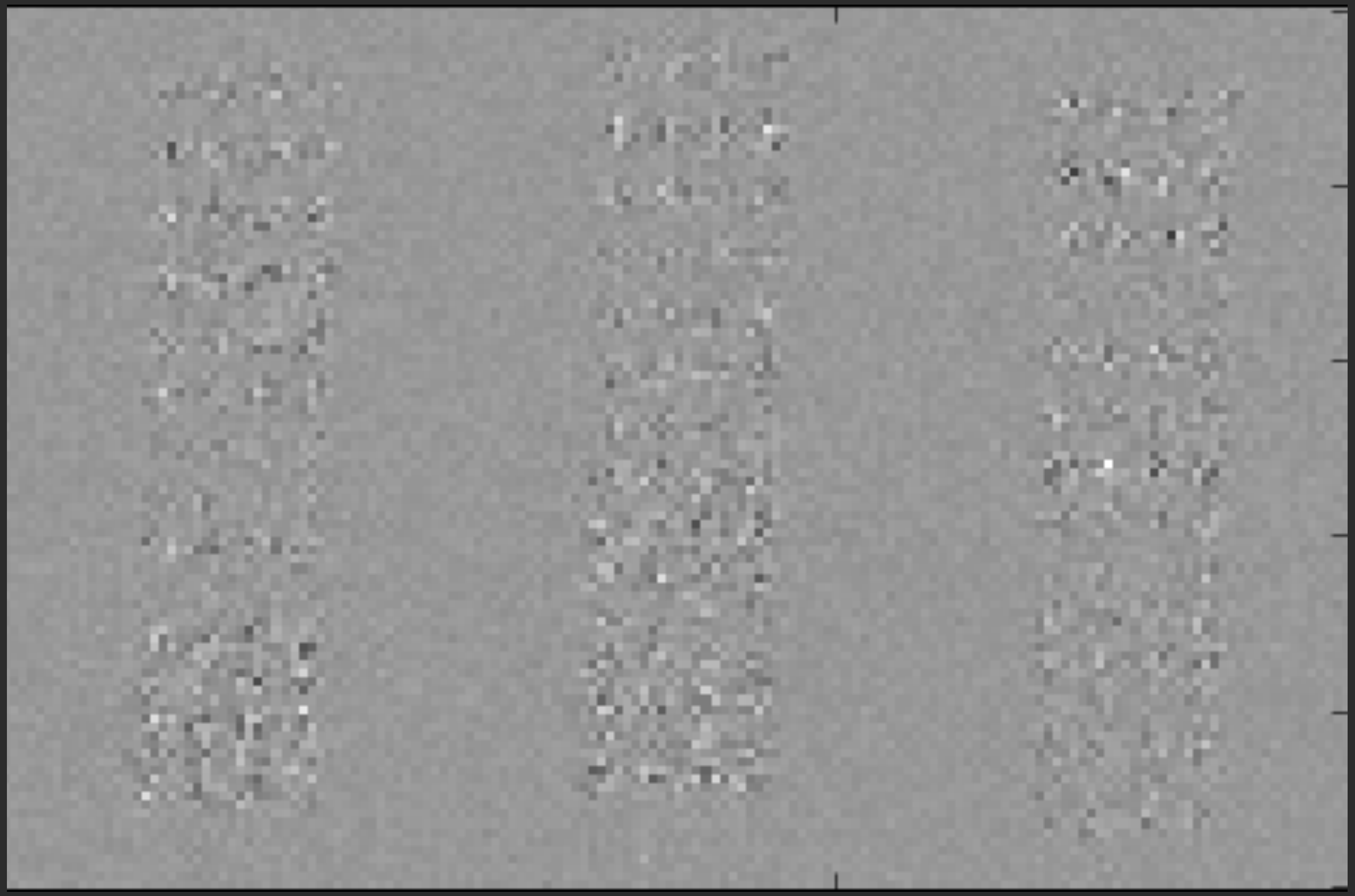
Sky model decomposed & removed

Sky spectrum is modeled "upstream" from optical heterogeneities between fibers



(Grayscale stretch X 40 relative to previous)

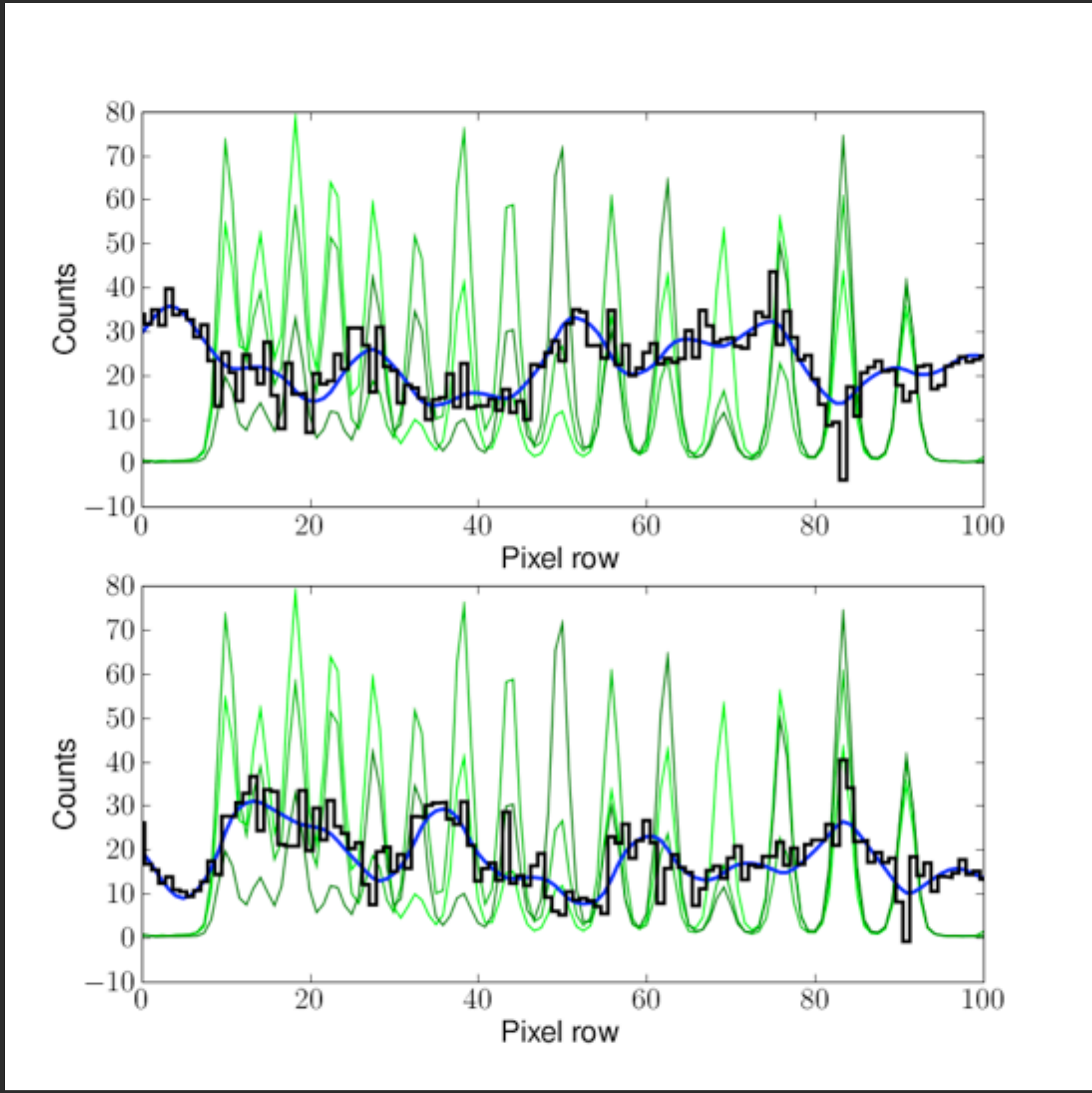
All models removed



Consistent with pure noise

Extracted objects + skies

Sky scaled down by a factor of 20 in plot



RMS error-scaled residuals of unity