Measurement Error and Linear Regression of Astronomical Data

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Classical Regression Model

- Collect n data points, denote i^{th} pair as (η_i, ξ_i), where η is the dependent variable (or 'response'), and ξ is the independent variable (or 'predictor', 'covariate')

- Assume usual additive error model:

$$\eta_i = \alpha + \beta\xi_i + \varepsilon_i$$

$$E(\varepsilon_i) = 0$$

$$Var(\varepsilon_i) = E(\varepsilon_i^2) = \sigma^2$$

- Ordinary Least Squares (OLS) slope estimate is

$$\hat{\beta} = \frac{Cov(\eta,\xi)}{Var(\xi)}$$

- Wait, that's not in Bevington…
- The 'error' term, ε, encompasses real physical variations in source properties, i.e., the intrinsic scatter.

Example: Photoionization Physics in Broad Line AGN

- Test if distance between BLR and continuum source set be photoionization physics
- From definition of ionization parameter, U:

$$R^2 = \frac{L_{ion}}{4\pi c^2 U n_e \overline{E}}$$

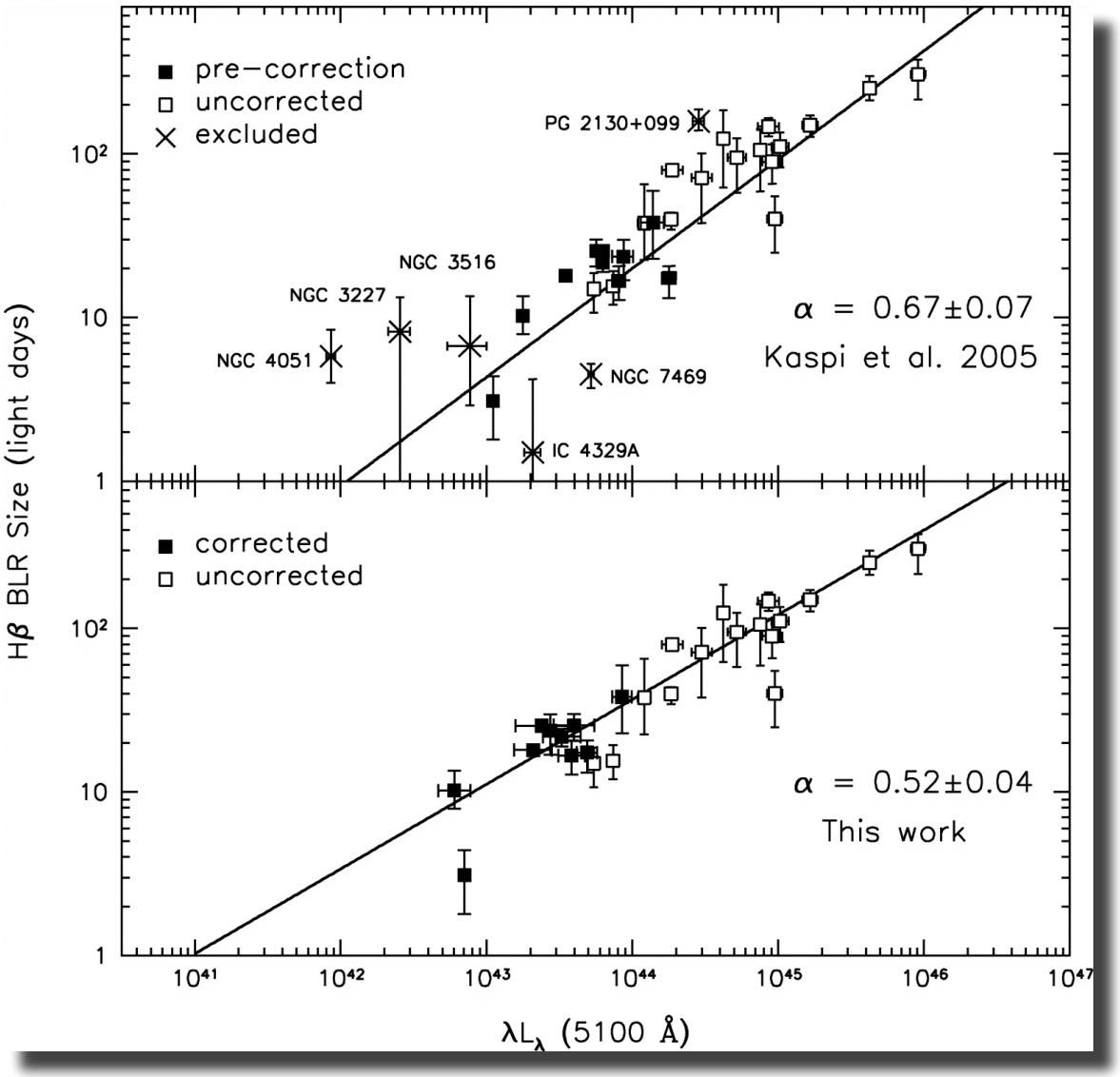
$$\log r = \tfrac{1}{2}\log L_{ion} - \tfrac{1}{2}\log(4\pi c^2) - \tfrac{1}{2}(\log U + \log n_e + \log \overline{E})$$

$$\log r = \alpha + \beta \log L_{ion} + \varepsilon$$

$$\beta = 1/2$$

$$\alpha = -\tfrac{1}{2}[E(\log U + \log n_e + \log \overline{E}) + \log(4\pi c^2)]$$

$$\varepsilon = -\tfrac{1}{2}[(\log U + \log n_e + \log \overline{E}) - E(\log U + \log n_e + \log \overline{E})]$$



Bentz et al., 2006, ApJ, 644, 133

BLR Size vs Luminosity, uncorrected for host galaxy starlight (top) and corrected for starlight (bottom). Some scatter due to measurement errors, but some due to intrinsic variations.

Measurement Errors

- Don't observe (η,ξ), but measured values (y,x) instead.
- Measurement errors add an additional level to the statistical model:

$$\eta_i = \alpha + \beta\xi_i + \varepsilon_i, \quad E(\varepsilon_i) = 0, \quad E(\varepsilon_i^2) = \sigma^2$$

$$x_i = \xi_i + \varepsilon_{x,i}, \quad E(\varepsilon_{x,i}) = 0, \quad E(\varepsilon_{x,i}^2) = \sigma_{x,i}^2$$

$$y_i = \eta_i + \varepsilon_{y,i}, \quad E(\varepsilon_{y,i}) = 0, \quad E(\varepsilon_{y,i}^2) = \sigma_{y,i}^2$$

$$E(\varepsilon_{x,i}\varepsilon_{y,i}) = \sigma_{xy,i}$$

Different Types of Measurement Error

- Produced by measuring instrument
  - CCD Read Noise, Dark Current
- Poisson, Counting Errors
  - Uncertainty in photon count rate creates measurement error on flux.
- Quantities inferred from fitting a parametric model
  - Using a spectral model to ‘measure’ flux density
- Using observable as proxies for unobservables
  - Using stellar velocity dispersion to ‘measure’ black hole mass, using galaxy flux to ‘measure’ star formation rate
  - Measurement error set by intrinsic source variations, won’t decrease with better instruments/bigger telescopes

Measurement errors alter the moments of the joint distribution of the response and covariate, bias the correlation coefficient and slope estimate

$$\hat{b} = \frac{Cov(x,y)}{Var(x)} = \frac{Cov(\xi,\eta) + \sigma_{xy}}{Var(\xi) + \sigma_x^2}$$

$$\hat{r} = \frac{Cov(x,y)}{[Var(x)Var(y)]^{1/2}} = \frac{Cov(\xi,\eta) + \sigma_{xy}}{[Var(\xi) + \sigma_x^2]^{1/2}[Var(\eta) + \sigma_y^2]^{1/2}}$$

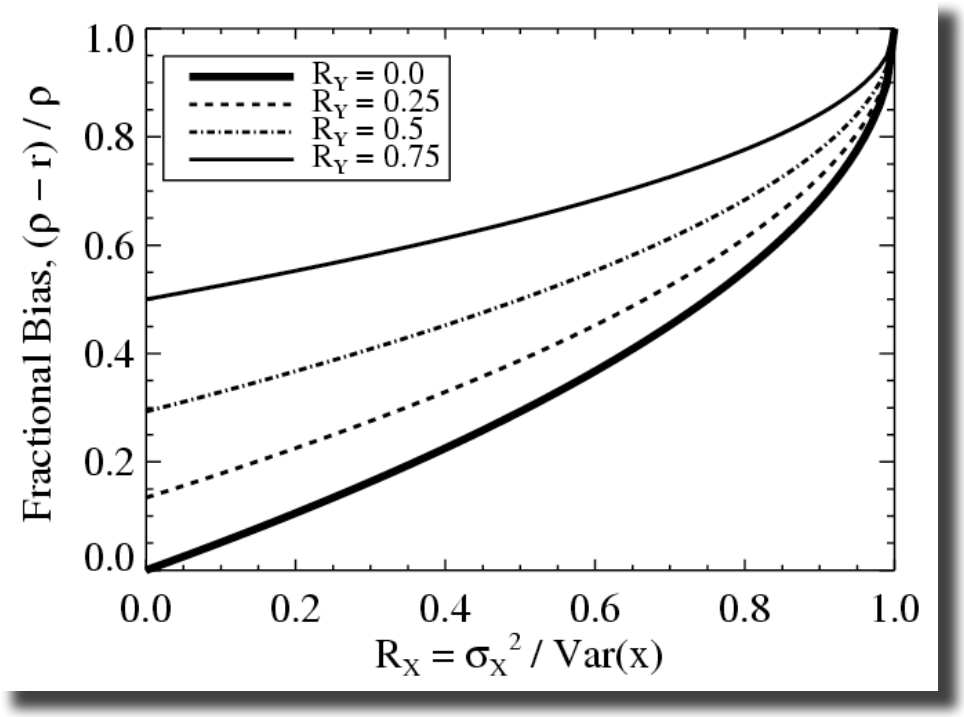
- If measurement errors are uncorrelated, regression slope unaffected by measurement error in the response
- If errors uncorrelated, regression slope and correlation biased toward zero (attenuated).

Degree of Bias Depends on Magnitude of Measurement Error

- Define ratios of measurement error variance to observed variance:

$$R_X = \frac{\sigma_x^2}{Var(x)}, \quad R_Y = \frac{\sigma_y^2}{Var(y)},$$

$$R_{XY} = \frac{\sigma_{xy}}{Cov(x,y)}$$

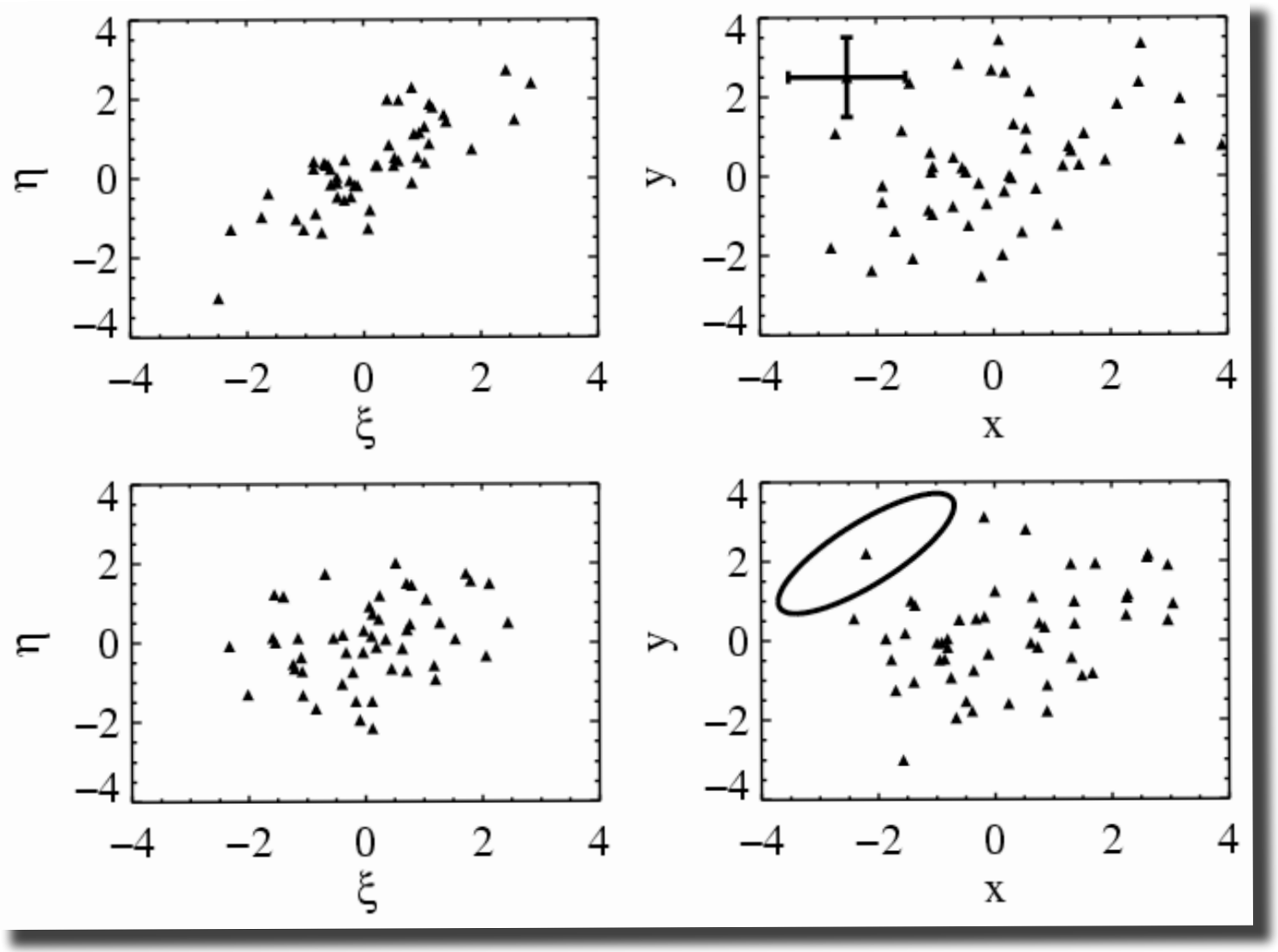


- Bias can then be expressed as:

$$\frac{\hat{b}}{\hat{\beta}} = \frac{1 - R_X}{1 - R_{XY}}, \quad \frac{\hat{r}}{\hat{\rho}} = \frac{(1 - R_X)^{1/2}(1 - R_Y)^{1/2}}{1 - R_{XY}}$$

True Distribution

Measured Distribution



BCES Estimator

- BCES Approach (Akritas & Bershady, ApJ, 1996, 470, 706; see also Fuller 1987, *Measurement Error Models*) is to 'debias' the moments:

$$\hat{\beta}_{BCES} = \frac{Cov(x,y) - \overline{\sigma}_{xy}}{Var(x) - \overline{\sigma}_x^2}, \quad \hat{\alpha}_{BCES} = \overline{y} - \hat{\beta}_{BCES}\overline{x}$$

- Also give estimator for bisector and orthogonal regression slopes
- Asymptotically normal, variance in coefficients can be estimated from the data
- Variance of measurement error can depend on measured value

Advantages vs Disadvantages

- Asymptotically unbiased and normal, variance in coefficients can be estimated from the data
- Variance of measurement error can depend on measured value
- Easy and fast to compute

- Can be unstable, highly variable for small samples and/or large measurement errors
- Can be biased for small samples and/or large measurement errors
- Convergence to asymptotic limit may be slow, depends on size of measurement errors

FITEXY Estimator

- Press et al.(1992, *Numerical Recipes*) define an 'effective χ^2' statistic:

$$\chi^2_{EXY} = \sum_{i=1}^{n} \frac{(y_i - \alpha - \beta x_i)^2}{\sigma^2_{y,i} + \beta^2 \sigma^2_{x,i}}$$

- Choose values of α and β that minimize χ^2_{EXY}
- Modified by Tremaine et al.(2002, ApJ, 574, 740), to account for intrinsic scatter:

$$\chi^2_{EXY} = \sum_{i=1}^{n} \frac{(y_i - \alpha - \beta x_i)^2}{\sigma^2 + \sigma^2_{y,i} + \beta^2 \sigma^2_{x,i}}$$

Advantages vs Disadvantages

- Simulations suggest that FITEXY is less variable than BCES under certain conditions
- Fairly easy to calculate for a given value of σ^2

- Can't be minimized simultaneously with respect to α,β, and σ^2, ad hoc procedure often used
- Statistical properties poorly understood
- Simulations suggest FITEXY can be biased, more variable than BCES
- Not really a 'true' χ^2, can't use $\Delta\chi^2=1$ to find confidence regions
- Only constructed for uncorrelated measurement errors

Structural Approach

- Regard ξ and η as missing data, random variables with some assumed probability distribution
- Derive a complete data likelihood:

$$p(x,y,\xi,\eta \mid \theta,\psi) = p(x,y \mid \xi,\eta)\, p(\eta \mid \xi,\theta)\, p(\xi \mid \psi)$$

- Integrate over the missing data, ξ and η, to obtain the observed (measured) data likelihood function

$$p(x,y \mid \theta,\psi) = \iint p(x,y,\xi,\eta \mid \theta,\psi)\, d\xi\, d\eta$$

Mixture of Normals Model

- Model the distribution of ξ as a mixture of K Gaussians, assume Gaussian intrinsic scatter and Gaussian measurement errors of known variance
- The model is hierarchically expressed as:

$$\xi_i \,|\, \pi, \mu, \tau^2 \sim \sum_{k=1}^{K} \pi_k N(\mu_k, \tau_k^2)$$

$$\eta_i \,|\, \xi_i, \alpha, \beta, \sigma^2 \sim N(\alpha + \beta\xi_i, \sigma^2)$$

$$y_i, x_i \,|\, \eta_i, \xi_i \sim N([\eta_i, \xi_i], \Sigma_i)$$

$$\psi = (\pi, \mu, \tau^2), \quad \theta = (\alpha, \beta, \sigma^2), \quad \Sigma_i = \begin{pmatrix} \sigma_{y,i}^2 & \sigma_{xy,i} \\ \sigma_{xy,i} & \sigma_{x,i}^2 \end{pmatrix}$$

References: Kelly (2007, ApJ in press, arXiv:705.2774),
Carroll et al.(1999, Biometrics, 55, 44)

Integrate complete data likelihood to obtain observed data likelihood:

$$p(x,y \mid \theta,\psi) = \prod_{i=1}^{n} \iint p(x_i,y_i \mid \xi_i,\eta_i)\, p(\eta_i \mid \xi_i,\theta)\, p(\xi_i \mid \psi)\, d\xi_i\, d\eta_i$$

$$= \prod_{i=1}^{n} \sum_{k=1}^{K} \frac{\pi_k}{2\pi \left| V_{k,i} \right|^{1/2}} \exp\left\{ -\tfrac{1}{2} (\mathbf{z}_i - \zeta_k)^T V_{k,i}^{-1} (\mathbf{z}_i - \zeta_k) \right\}$$

$$\mathbf{z}_i = \begin{pmatrix} y_i & x_i \end{pmatrix}^T$$

$$\zeta_k = \begin{pmatrix} \alpha + \beta\mu_k & \mu_k \end{pmatrix}^T$$

$$V_{k,i} = \begin{pmatrix} \beta^2\tau_k^2 + \sigma^2 + \sigma_{y,i}^2 & \beta\tau_k^2 + \sigma_{xy,i} \\ \beta\tau_k^2 + \sigma_{xy,i} & \tau_k^2 + \sigma_{x,i}^2 \end{pmatrix}$$

Can be used to calculate a maximum-likelihood estimate (MLE), perform Bayesian inference. See Kelly (2007) for generalization to multiple covariates.

What if we assume that ξ has a uniform distribution?

- The likelihood for uniform p(ξ) can be obtained in the limit $\tau \longrightarrow \infty$:

$$p(x,y \mid \theta) \propto \prod_{i=1}^{n} \left(\sigma^2 + \sigma_{y,i}^2 + \beta^2 \sigma_{x,i}^2\right)^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}\frac{(y_i - \alpha - \beta x_i)^2}{\sigma^2 + \sigma_{y,i}^2 + \beta^2 \sigma_{x,i}^2}\right\}$$

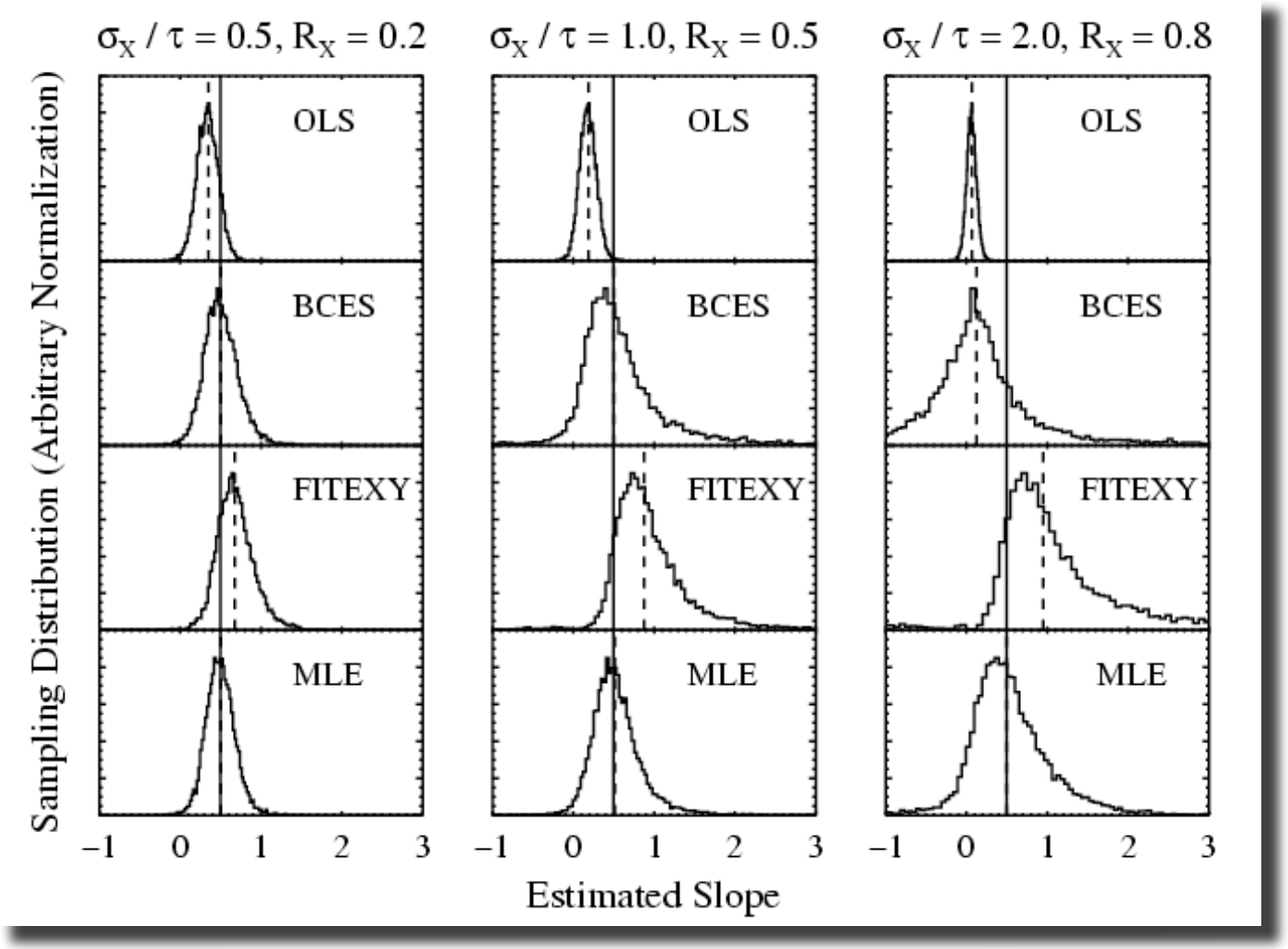
- Argument of exponential is χ^2_{EXY} statistic!
- But minimizing χ^2_{EXY} is not the same as maximizing the likelihood…
- For homoskedastic measurement errors, maximizing this likelihood leads to the ordinary least-squares estimate, so still biased.

Advantages vs Disadvantages

- Simulations suggest MLE for normal mixture approximately unbiased, even for small samples and large measurement error
- Lower variance than BCES and FITEXY
- MLE for σ^2 rarely, if ever, equal to zero
- Bayesian inference can be performed, valid for any sample size
- Can be extended to handle non-detections, truncation, multiple covariates
- Simultaneously estimates distribution of covariates, may be useful for some studies

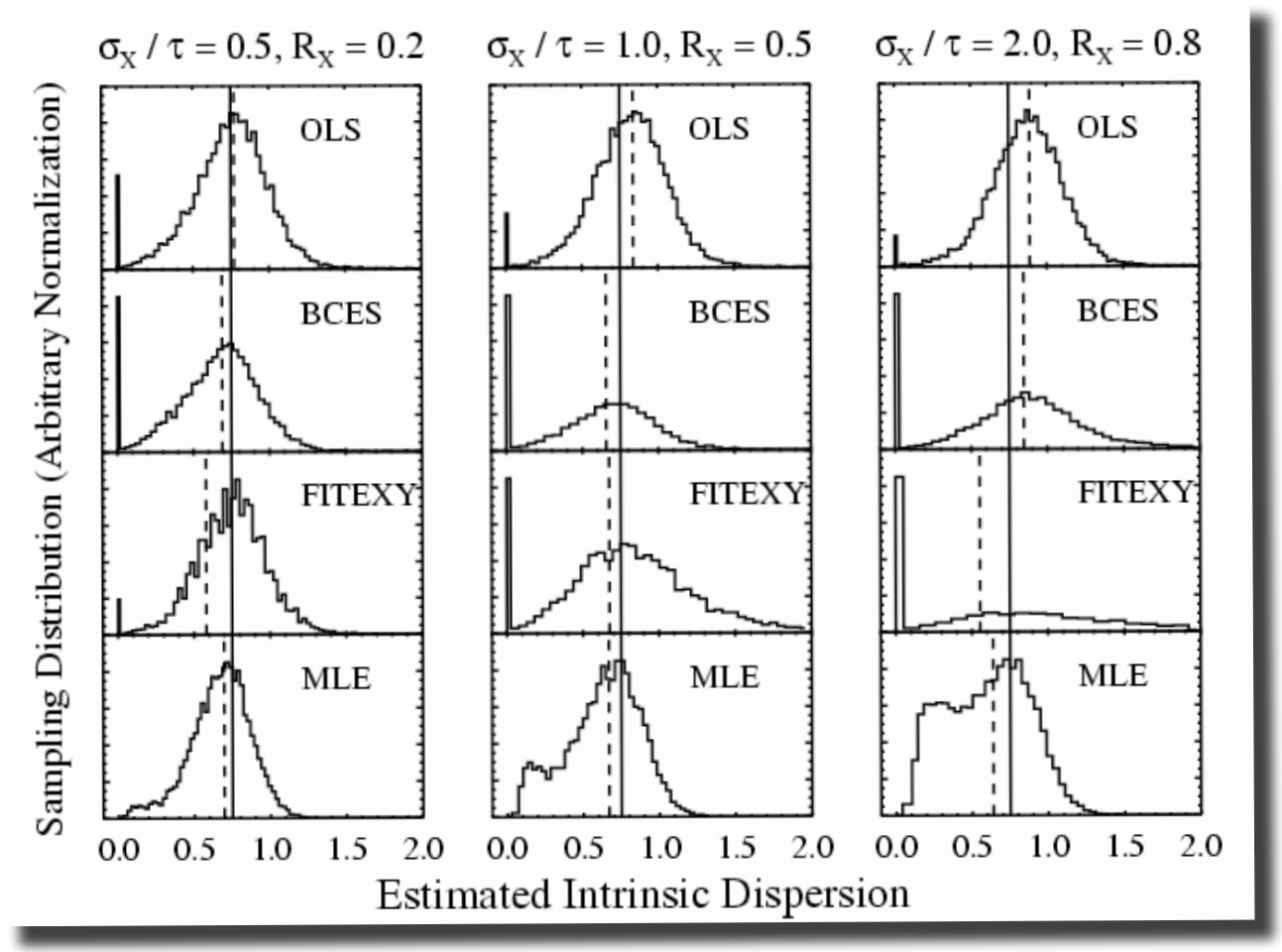
- Computationally intensive, more complicated than BCES and FITEXY
- Assumes measurement error variance known, does not depend on measurement
- Needs a parametric form for the intrinsic distribution of covariates (but mixture model flexible and fairly robust).

Simulation Study: Slope



Dashed lines mark the median value of the estimator, solid lines mark the true value of the slope. Each simulated data set had 50 data points, and y-measurement errors of $\sigma_y \sim \sigma$.

Simulation Study: Intrinsic Dispersion



Dashed lines mark the median value of the estimator, solid lines mark the true value of σ. Each simulated data set had 50 data points, and y-measurement errors of $\sigma_y \sim \sigma$.

Effects of Sample Selection

- Suppose we select a sample of n sources, out of a total of N possible sources
- Introduce indicator variable, I, denoting whether a source is included. $I_i = 1$ if the i^{th} source is included, otherwise $I_i = 0$.
- Selection function for i^{th} source is $p(I_i=1|y_i,x_i)$
- Selection function gives the probability that the i^{th} source is included in the sample, given the values of x_i and y_i.

See Little & Rubin (2002, *Statistical Analysis with Missing Data*) or Gelman et al.(2004, *Bayesian Data Analysis*) for further reading.

- Complete data likelihood is

$$p(x,y,\xi,\eta,I \mid \theta,\psi,N) \propto \binom{N}{n} \prod_{i \in A_{obs}} p(x_i,y_i,\xi_i,\eta_i,I_i \mid \theta,\psi) \prod_{j \in A_{mis}} p(x_j,y_j,\xi_j,\eta_j,I_j \mid \theta,\psi)$$

- Here, A_{obs} denotes the set of n included sources, and A_{mis} denotes the set of N-n sources not included
- Binomial coefficient gives number of possible ways to select a subset of n sources from a sample of N sources
- Integrating over the missing data, the observed data likelihood now becomes

$$p(x_{obs},y_{obs},I \mid \theta,\psi,N) \propto \binom{N}{n} \prod_{i \in A_{obs}} p(x_i,y_i \mid \theta,\psi)$$

$$\times \prod_{j \in A_{mis}} \iint p(I_j = 0 \mid x_j,y_j)\, p(x_j,y_j \mid \theta,\psi)\, dx_j\, dy_j$$

Selection only dependent on covariates

- If the sample selection only depends on the covariates, then p(I|x,y) = p(I|x).
- Observed data likelihood is then

$$p(x_{obs}, y_{obs}, I \mid \theta, \psi, N) \propto \binom{N}{n} \prod_{i \in A_{obs}} p(x_i, y_i \mid \theta, \psi)$$

$$\times \prod_{j \in A_{mis}} \iint p(I_j = 0 \mid x_j)\, p(y_j \mid x_j, \theta, \psi)\, p(x_j \mid \psi)\, dx_j\, dy_j$$

$$\propto \binom{N}{n} \prod_{i \in A_{obs}} p(x_i, y_i \mid I_i = 1, \theta, \psi_{obs}) \prod_{j \in A_{mis}} \int p(x_j \mid I_j = 0, \psi_{mis})\, p(I_j = 0 \mid \psi_{mis})\, dx_j$$

- Therefore, if selection is only on the covariates, then inference on the regression parameters is unaffected by selection effects.

Selection depends on dependent variable: truncation

- Take Bayesian approach, posterior is

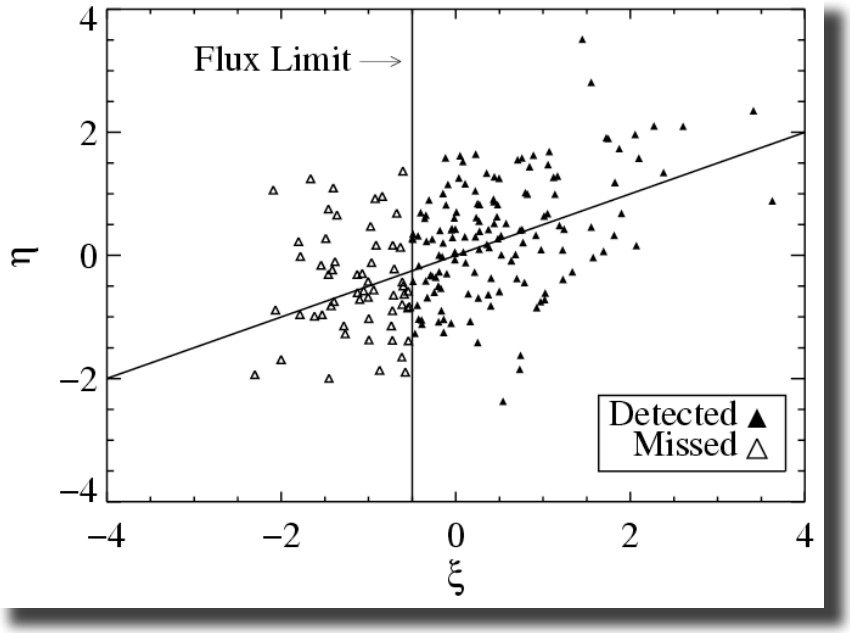
$$p(\theta,\psi,N \mid x_{obs},y_{obs},I) \propto p(\theta,\psi,N)\,p(x_{obs},y_{obs},I \mid \theta,\psi,N)$$

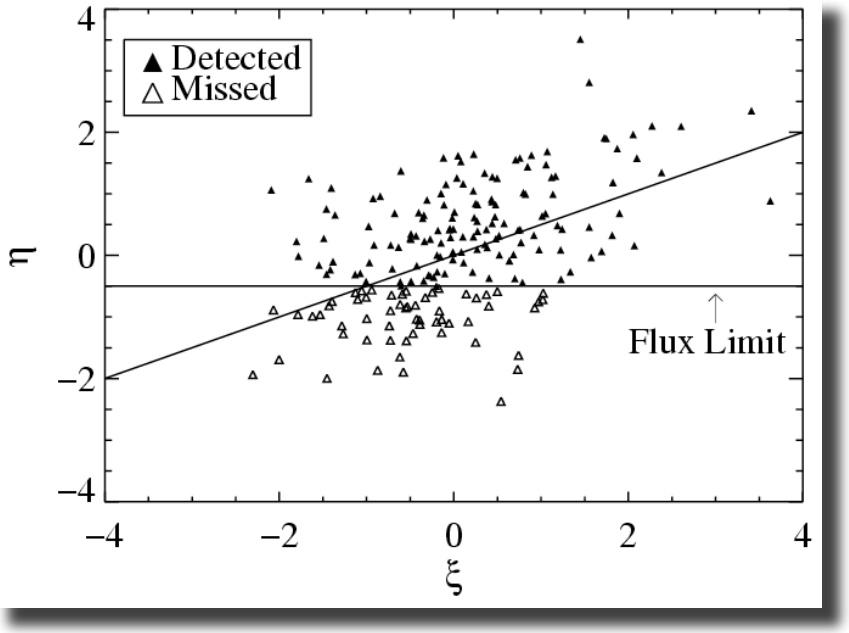
- Assume uniform prior on log$N$, p(θ,ψ,N) $\propto N^{-1}$p(θ,ψ)
- Since we don't care about N, sum posterior over $n < N < \infty$:

$$p(\theta,\psi \mid x_{obs},y_{obs},I) \propto \left[p(I=1 \mid \theta,\psi)\right]^{-n} \prod_{i \in A_{obs}} p(x_i,y_i \mid \theta,\psi)$$

$$p(I=1 \mid \theta,\psi) = \iint p(I=1 \mid x,y)\,p(x,y \mid \theta,\psi)\,dx\,dy$$

Covariate Selection vs Response Selection





Covariate Selection: No effect on distribution of y at a given x

Response Selection: Changes distribution of y at a given x

Non-detections: 'Censored' Data

- Introduce additional indicator variable, D, denoting whether a data point is detected or not: D=1 if detected.
- Assuming selection function independent of response, observed data likelihood becomes

$$p(x,y,D \mid \theta,\psi) \propto \prod_{i \in A_{\mathrm{det}}} p(x_i, y_i \mid \theta,\psi)$$

$$\times \prod_{j \in A_{cens}} p(x_j \mid \psi) \int p(D_j = 0 \mid y_j, x_j)\, p(y_j \mid x_j, \theta,\psi)\, dy_j$$

- A_{det} denotes set of detected sources, A_{cens} denotes set of censored sources.
- Equations for $p(x|\psi)$ and $p(y|x,\theta,\psi)$ under the mixture of normals models are given in Kelly (2007).

Bayesian Inference

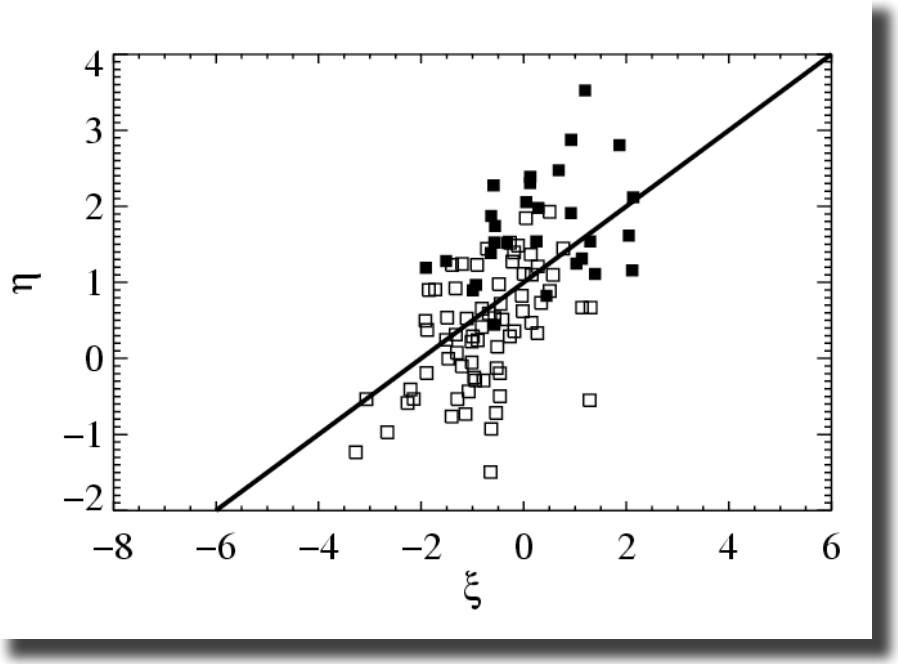
- Calculate posterior probability density for mixture of normals structural model
- Posterior valid for any sample size, doesn't rely on large sample approximations (e.g., asymptotic distribution of MLE).
- Assume prior advocated by Carroll et al.(1999)
- Use markov chain monte carlo (MCMC) to obtain draws from posterior

Gibbs Sampler

- Method for obtaining draws from posterior, easy to program
- Start with initial guesses for all unknowns
- Proceed in three steps:
  - Simulate new values of missing data, including non-detections, given the observed data and current values of the parameters
  - Simulate new values of the parameters, given the current values of the prior parameters and the missing data
  - Simulate new values of the prior parameters, given the current parameter values.
- Save random draws at each iterations, repeat until convergence.
- Treat values from latter part of Gibbs sampler as random draw form the posterior

Details given in Kelly (2007). Computer routines available at IDL Astronomy User's Library, http://idlastro.gsfc.nasa.gov/homepage.html

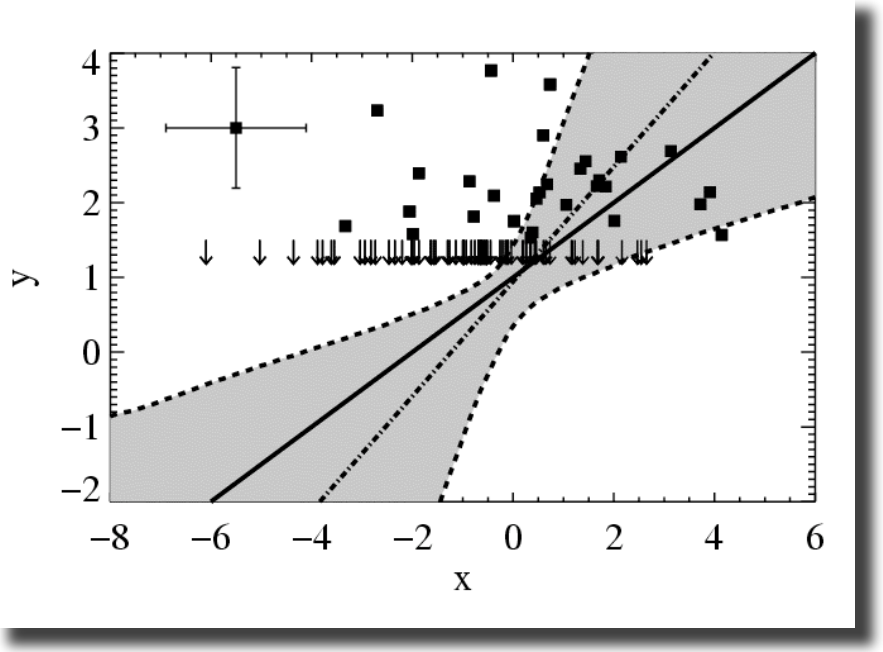
Example: Simulated Data Set with Non-detections



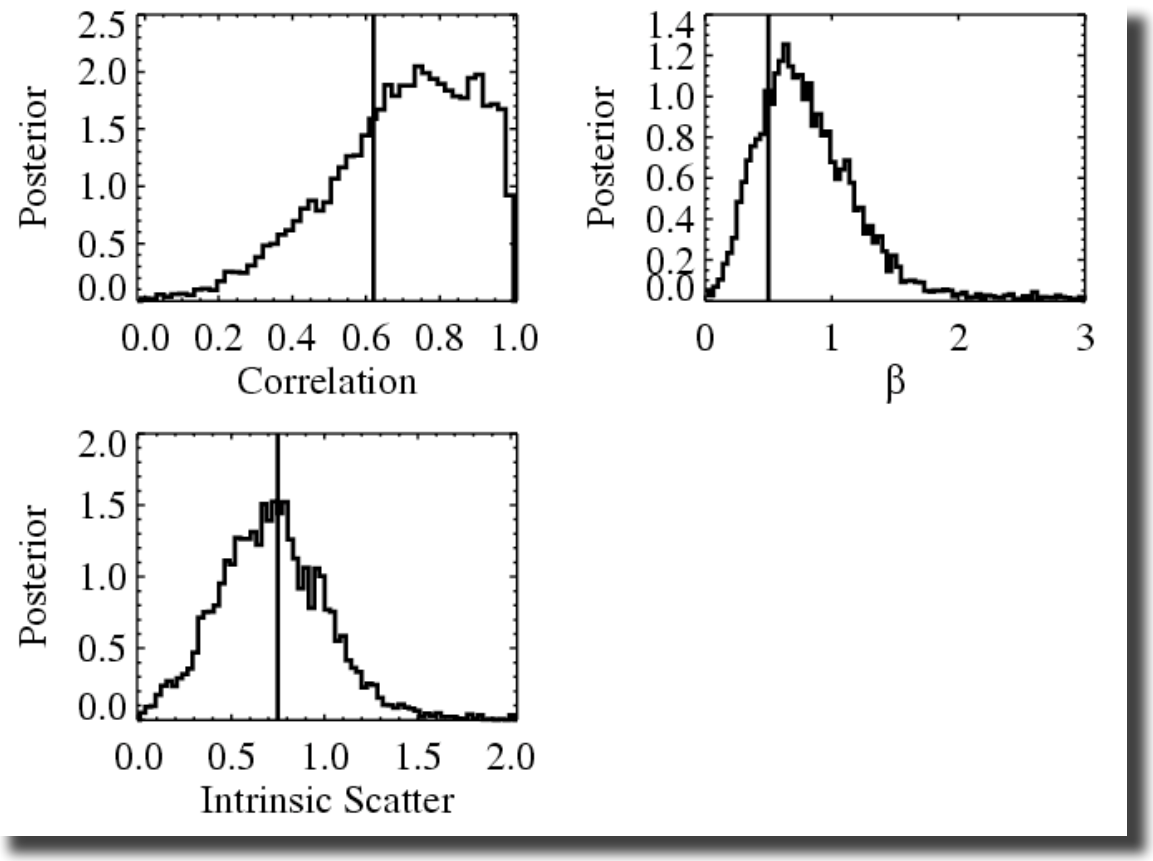
Filled Squares: Detected data points

Hollow Squares: Undetected data points

Solid line is true regression line, Dashed-dotted is posterior Median, shaded region contains Approximately 95% of posterior probability



Posterior from MCMC for simulated data with non-detections

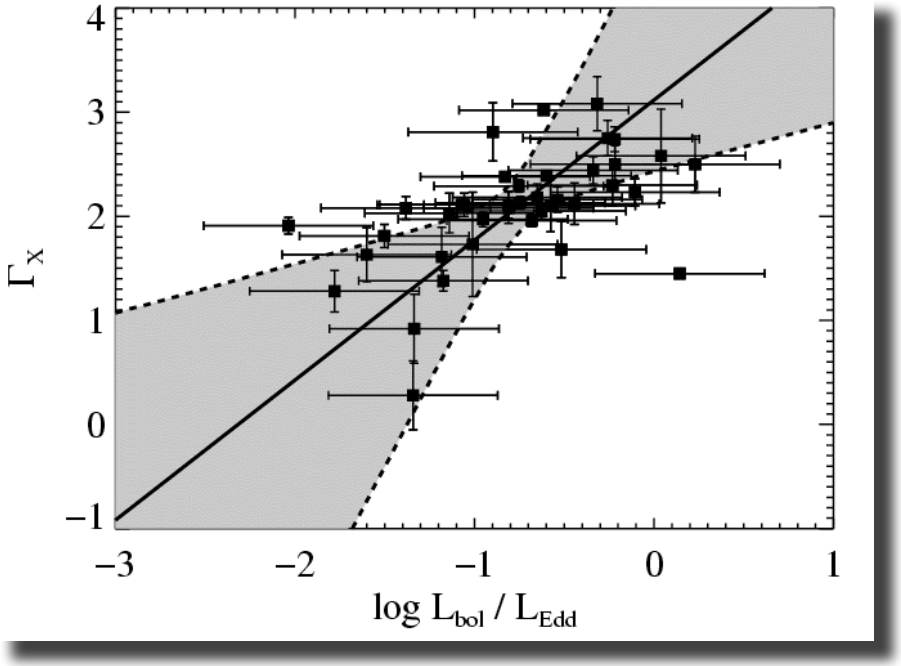


Solid vertical line marks true value. For comparison, a naïve MLE that ignores meas. error found

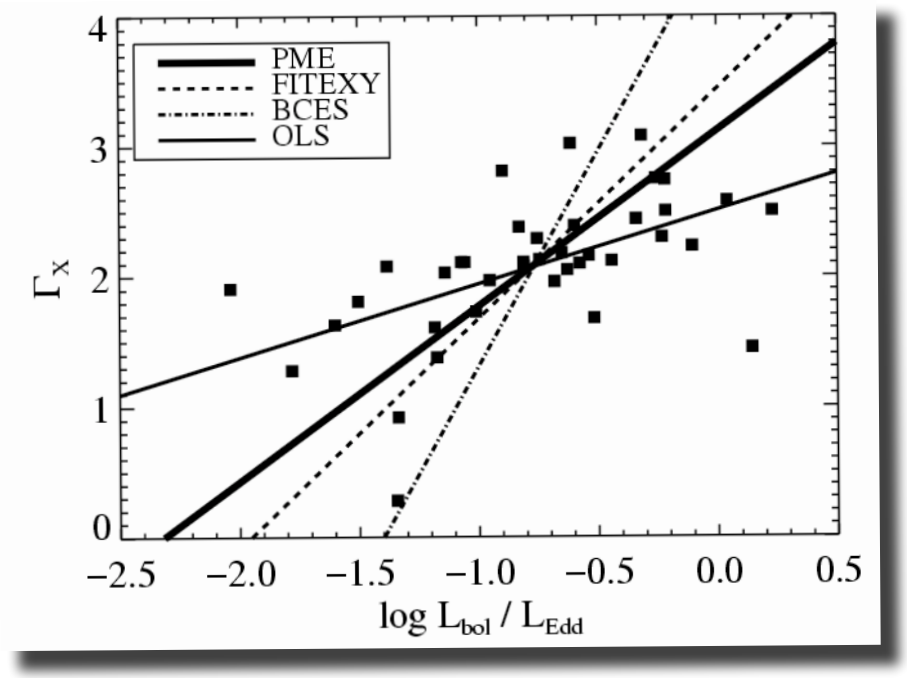
$$\beta_{MLE} = 0.229 \pm 0.077$$

This is biased toward zero at a level of 3.5σ

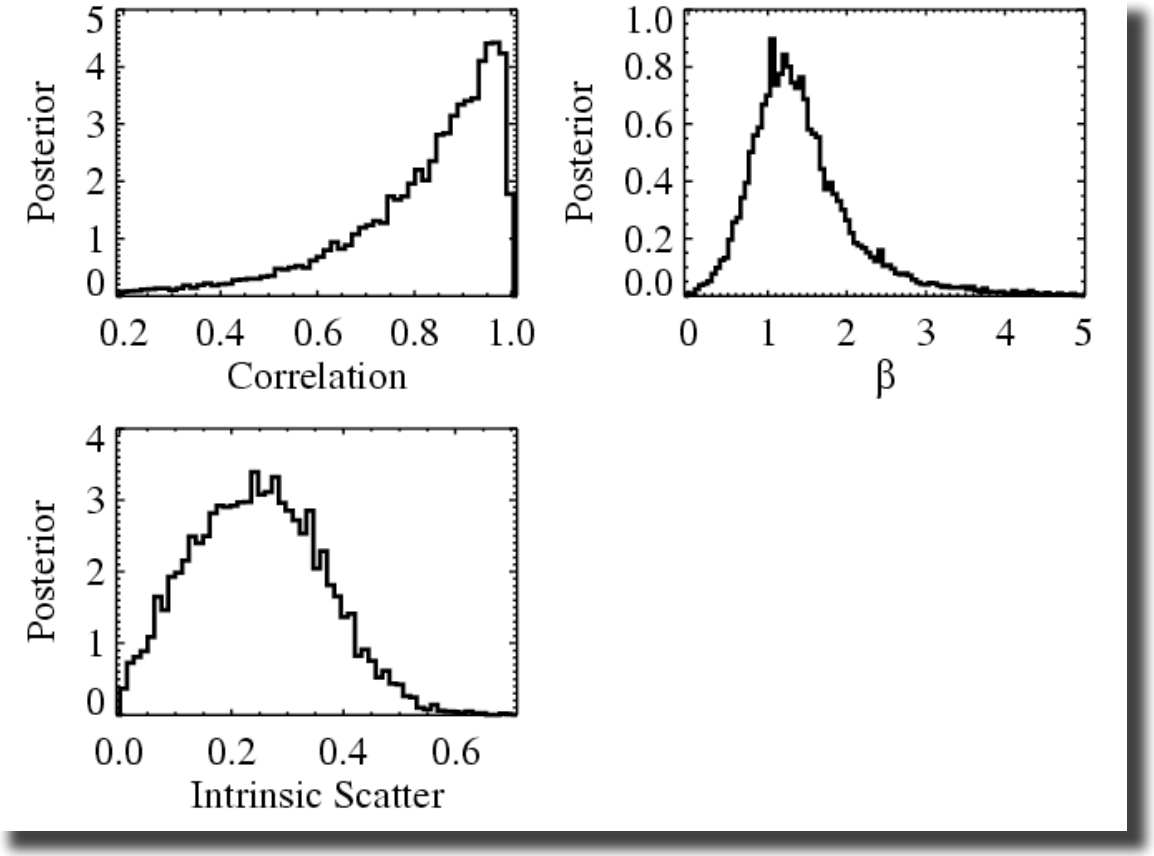
Example: Dependence of Quasar X-ray Spectral Slope on Eddington Ratio



Solid line is posterior median,
Shaded region contains 95%
Of posterior probability.



Posterior for Quasar Spectral Slope vs Eddington Ratio



For Comparison:

$$\hat{\beta}_{OLS} = 0.56 \pm 0.14$$

$$\hat{\beta}_{BCES} = 3.29 \pm 3.34$$

$$\hat{\beta}_{EXY} = 1.76 \pm 0.49$$

$$\hat{\sigma}_{OLS} = 0.41$$

$$\hat{\sigma}_{BCES} = 0.32$$

$$\hat{\sigma}_{EXY} = 0.0$$

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