Embedding Astronomical Computer Models into Principled Statistical Analyses

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Outline

1. Computer Models in Astronomy and Statistics
2. Stellar Evolution
   - Model for Stellar Evolution
   - Computer Models for White Dwarf Evolution
   - Statistical Computation and Numerical Results
3. Calibration of X-ray Detectors
   - Computer Models for Instrument Calibration
   - Statistical Methods
   - The Fully Bayesian Solution
   - Empirical Illustration

Outline

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Computer Models

- Complex scientific phenomena can often only be modeled via simultaneous mathematical equations.
- E.g., Pharmacokinetics, Meteorology, Climatology, Seismology, Transportation, Immunology, Astronomy, etc.
- These *computer models* involve
  - unknown input parameters and
  - prediction or simulation of observations.

—*Deterministic and Stochastic Computer Models.*
—*Similar to Statistical Likelihood Functions.*

- Require sophisticated and time consuming computation.
- Goal: Use data to learn about parameters and models.

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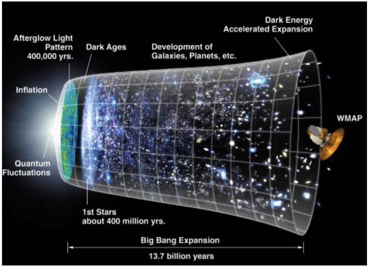
Computer Models in Astronomy

Computer Models are used to

- model stellar evolution,
- describe properties of planetary and stellar atmospheres,
- simulate chemical reactions in interstellar clouds,



- calculate the emergence of clusters and superclusters of galaxies in the early Universe,
- determine the yield of the elements during the Big Bang

Goal: Embed such computer models into a Bayesian statistical analysis.

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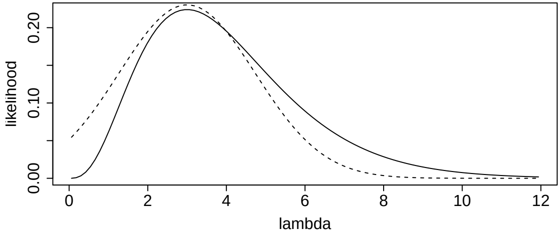
Bayesian Statistical Analyses: Likelihood

Likelihood Functions: The distribution of the data given the model parameters. E.g., $Y \sim \text{Poisson}(\lambda_S)$:

$$\text{likelihood}(\lambda_S) = e^{-\lambda_S} \lambda_S^Y / Y!$$

Maximum Likelihood Estimation: Suppose $Y = 3$



The likelihood and its normal approximation.

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Can estimate λ_S and its error bars.

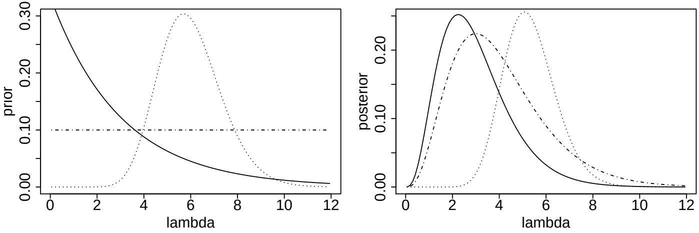
Bayesian Analyses: Prior and Posterior Dist'ns

Prior Distribution: Knowledge obtained *prior* to current data.

Bayes Theorem and Posteror Distribution:

$$\text{posterior}(\lambda) \propto \text{likelihood}(\lambda)\text{prior}(\lambda)$$

Combine past and current information:



Bayesian analyses rely on probability theory

Multi-Level Models

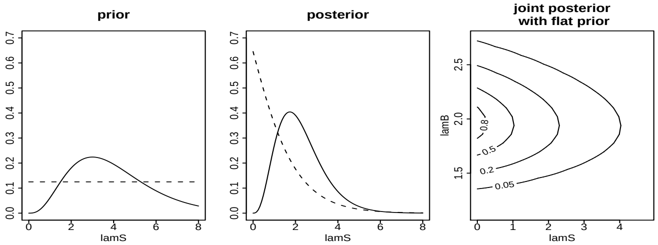
A Poisson Multi-Level Model:

Level 1: $Y|Y_B, \lambda_S \stackrel{\text{dist}}{\sim} \text{Poisson}(\lambda_S) + Y_B$,

Level 2: $Y_B|\lambda_B \stackrel{\text{dist}}{\sim} \text{Pois}(\lambda_B)$ and $X|\lambda_B \stackrel{\text{dist}}{\sim} \text{Pois}(\lambda_B \cdot 24)$,

Level 3: specify a prior distribution for λ_B, λ_S.

Each level of the model specifies a dist'n given unobserved quantities whose dist'ns are given in lower levels.



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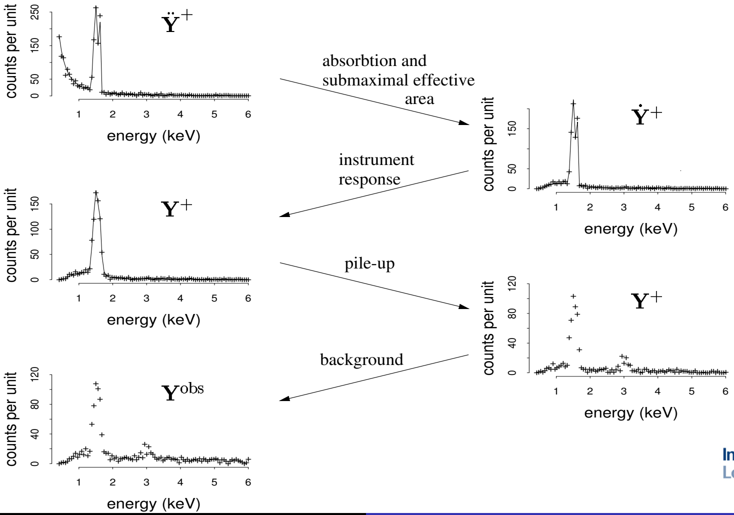
Multi-Level Models: X-ray Spectral Analysis



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Embedding Computer Models in a Bayesian Analyses

We aim to use computer models as components of statistical models for parameter fitting.

Build multi-level models

- Combine computer models with other model components via multi-level or hierarchical models,
- Combine multiple computer models via parametric models,
- Enable standard techniques for model fitting, checking, comparison, and improvement.

Computation becomes the real issue!

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Stellar Formation

Stars form when the dense parts of a molecular cloud collapse into a ball of plasma.

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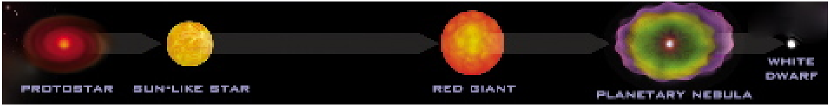
Evolution of a Sun-like Star



- Fusion of Hydrogen into Helium in the core can last millions or billions of years, depending on the initial stellar mass.
- When H is depleted, He may fuse into heavier elements.
- At the same time the star goes through dramatic physical changes, growing and cooling into a *red giant* star.
- The star undergoes mass loss forming a *planetary nebula*.
- Eventually only the core is left, a *white dwarf star*.
- White dwarf is a stellar ember and cools slowly via conduction, convection, and/or radiation.

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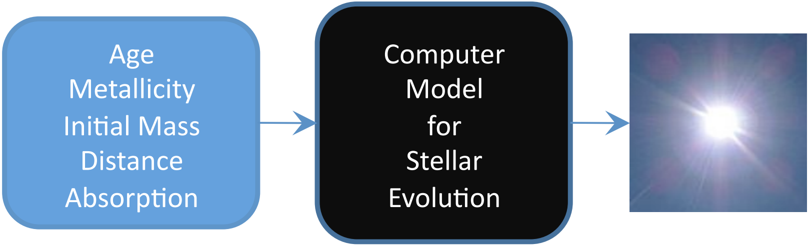
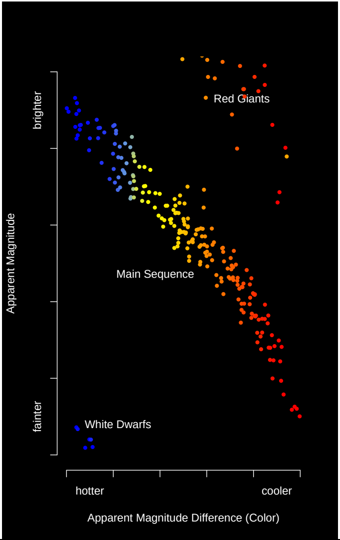
Compter Model for Sun-Like Stellar Evolution



- Computer model predicts how the emergent and apparent spectra evolve as a function of input parameters.
- We observe photometric magnitudes, the apparent luminosity in each of several wide wavelength bands.

The Data: Color Magnitude Diagrams



Color-Magnitude Diagram

- Plot Magnitude Difference vs. Magnitude.
- Identifies stars at different stages of their lives.
- Evolution of a CMD.
- Facilitates physical intuition as to likely values of parameters.
- "Chi-by-eye" fitting.

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Computer Models for MS/RG Evolution

Computer Models Predict Magnitudes From Stellar Parameters

- Must iteratively solve set of coupled differential equations.
- This creates a static physical model of a star, which is how a star of a particular mass and *radial abundance profile* would appear in terms of its luminosity and color.
- Stars are evolved by updating the mass and abundance profile to account for the newly produced elements.
- Finally interstellar absorption and distance can be used to convert absolute magnitudes into apparent magnitudes.

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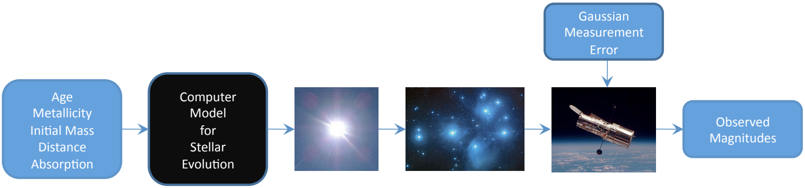
Embedding Computer Model intp Statistical Model



- Typically more parameters than measurements per star.
- We study stellar clusters with (nearly) common age, metallicity, distance, and absorption.
- Magnitudes observed with Gaussian measurement errors.

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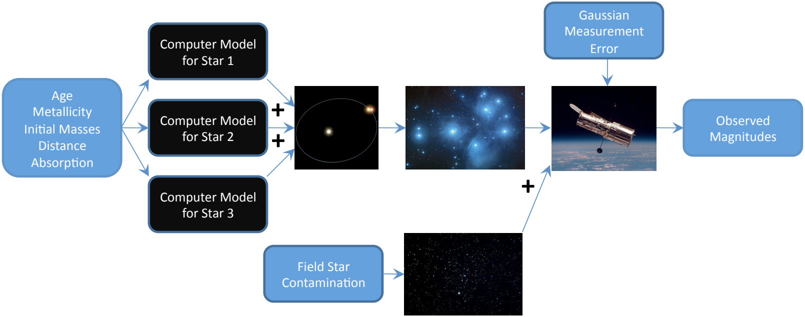
Multi-Star Systems and Field Star Contamination



- Between 1/3 and 1/2 of “stars” are unresolved binaries.
  - *Sum luminosities from multiple computer model runs.*
- Cluster data is contaminated with field stars.
  - *Finite mixture model.*

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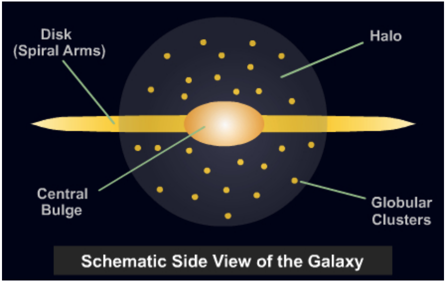
Study of WDs: Age of Galactic Structures

- Age of galactic *halo* or *disk* can only be estimated with older stars.
- Stellar clusters are pulled apart as they interact gravitationally with other stars and clusters.



- Older stars tend to be “in the field” — not in clusters.
- The colors of a single white dwarf are much more informative as to its age than are the colors of a MS star.

We would like to model white dwarf colors.

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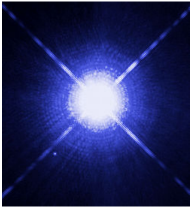
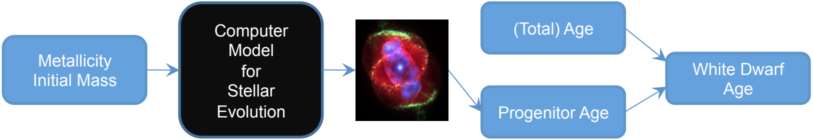
White Dwarfs Physics



- White dwarf spectra are not predicted from MS/RG models
- Different physical processes require different models:
  1. Computer Model for White Dwarf Cooling
  2. Computer Model for White Dwarf Atmosphere
  3. Initial Final Mass Relationship (IFMR)

Computing the Progenitor Age

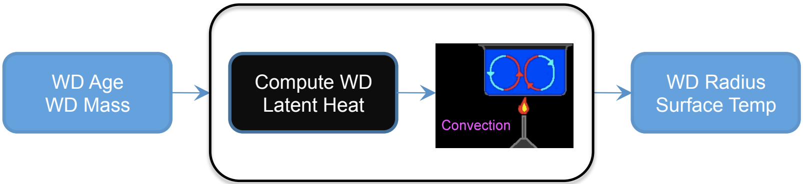


Begin with the MS / RG model:

- Rather than running the MS/RG model for a fixed *age*, we run it until the giant evolves into a white dwarf.
- This gives us the progenitor age of the MS / RG star.
- Subtract from total cluster age to get *White Dwarf Age*.

The White Dwarf Cooling Model

Computer Model for White Dwarf Cooling



A White Dwarf is a Cooling Ember

- Heat passes to the surface via some combination of *conduction, convection, and/or radiation*.
- Depends on the local temperature.
- Numerically modeling these processes yields the *surface temperature and radius*.

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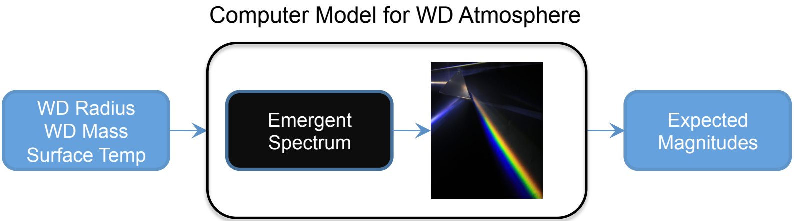
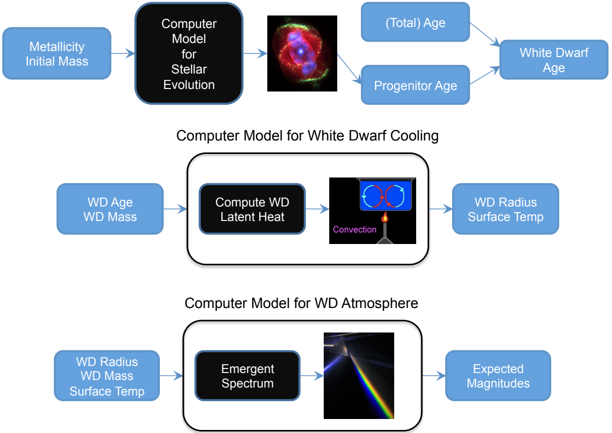
The White Dwarf Atmosphere Model



- Predicts the distribution of the wavelength of emitted electromagnetic radiation.
- We account for the filters used in photometric magnitudes.
- We account for absorption and distance.

The Missing Link: White Dwarf Mass



We must model the white dwarf mass.

A Simple Model for the WD Mass

The Initial Final Mass Relationship (IFMR):

- Predict the White Dwarf mass a function of the Initial Mass.
- With narrow range of mass, relation is approximately linear:

$$\text{White Dwarf Mass} = \alpha + \beta \text{ Initial Mass}$$

  - More massive stars evolve into white dwarfs sooner.
  - Progenitors of visible cluster white dwarfs had similar mass.
- Goals:
  - Account for IFMR uncertainty in a coherent model.
  - Fit IFMR over a wide range of masses using several clusters, each with (different) linear models.

Parametric Bridge between Computer Models.

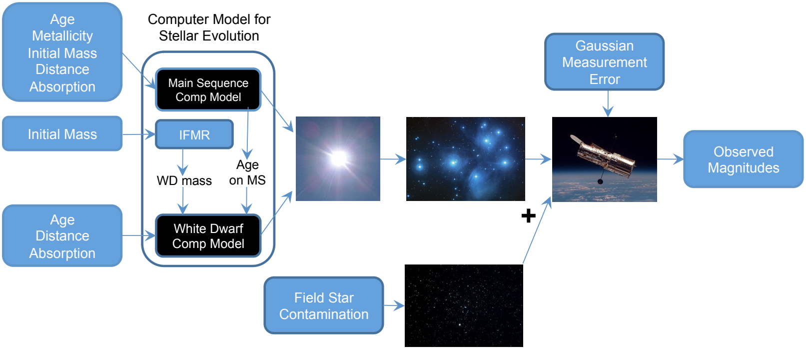
Traditional Method for Fitting IFMR

A Sequence of Independent Analyses:

- *Total (cluster) age:* Fit the color-magnitude diagram to the MS / RG model using chi-by-eye.
- *White Dwarf Mass and Age:* Spectroscopy to determine temperature and surface gravity. Age and mass are backed out using computer model for white dwarf cooling.
- *Progenitor Age:* Subtract white dwarf age from total age.
- *Initial Mass:* Progenitor age with fitted MS / RG model.
- *Errors in fitted line are difficult to evaluate!!*

We aim to fit the IFMR with a coherent statistical model without expensive star-by-star spectrography.

Opening Up the Black Box: The Final Model



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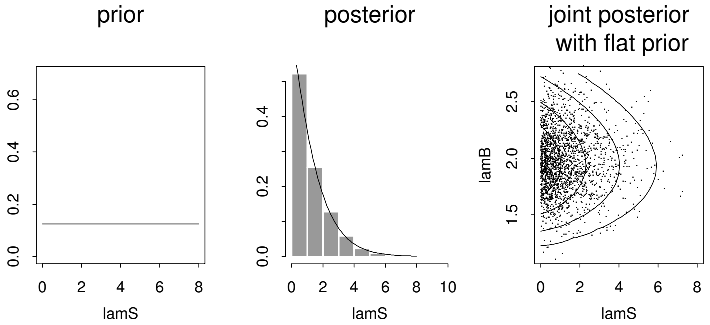
Markov Chain Monte Carlo

Exploring the posterior distribution via Monte Carlo.



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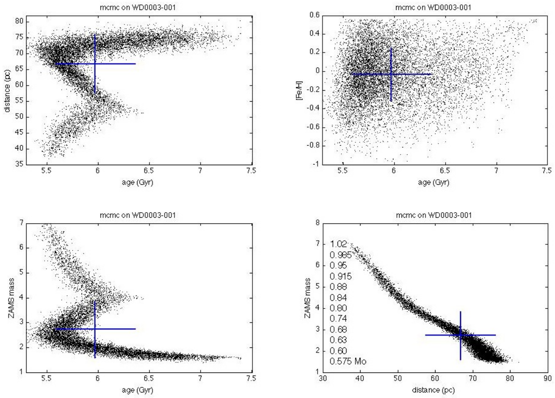
Model Fitting: Complex Posterior Distributions



Highly non-linear relationship among stellar parameters.

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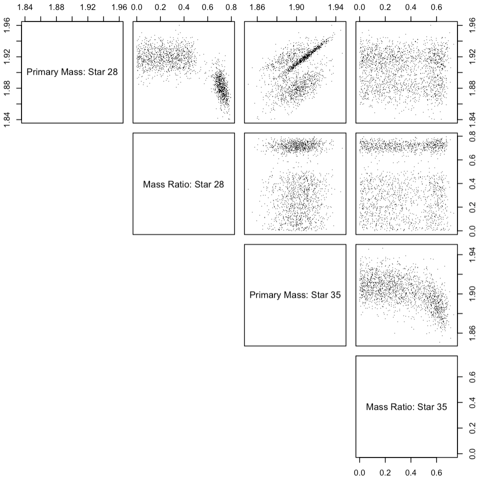
Model Fitting: Complex Posterior Distributions



The classification of certain stars as field or cluster stars can cause multiple modes in the distributions of other parameters.

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Statistical Computation

- Hundreds of parameters

  Stellar: Mass, Mass Ratio, Cluster Membership
  Cluster: Age, Metallicity, Distance, Absorption
  General: IFMR slope, IFMR intercept

- Strategy: numerically integrate out stellar parameters and use Metropolis on remaining six parameters.
- Marginal posterior factors into N_{stars} 2D integrals.
- Computer code for MCMC is easy to parallelize.

Result: Fast Mixing but computationally expensive code.

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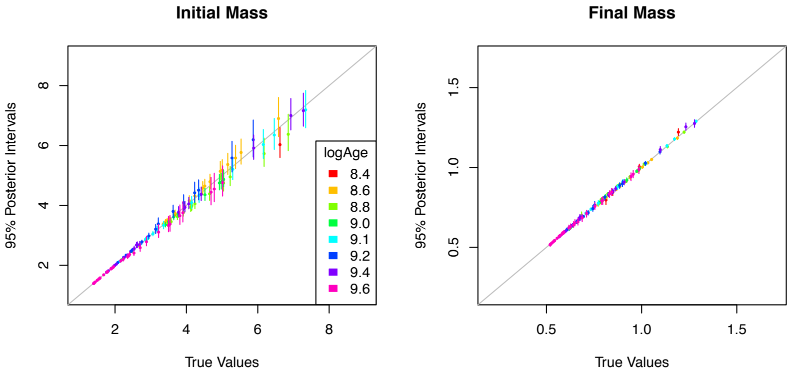
Simulation: Recovering the Masses



- Simulated 8 clusters of varying age–and white dwarf mass.
- Resulting fits recover of the masses well.

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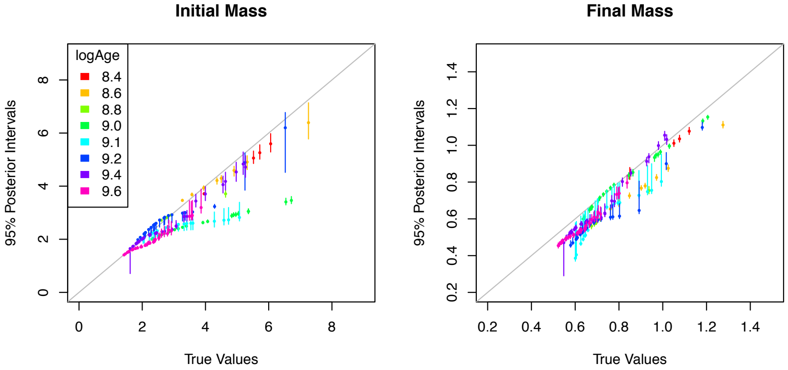
Simulation: Sensitivity to MS / RG Model Choice



- Checking Computer Models: Use different computer models in simulation (YY) and fit (Dotter et al.).
- Measure of bias relative to “True Model”?

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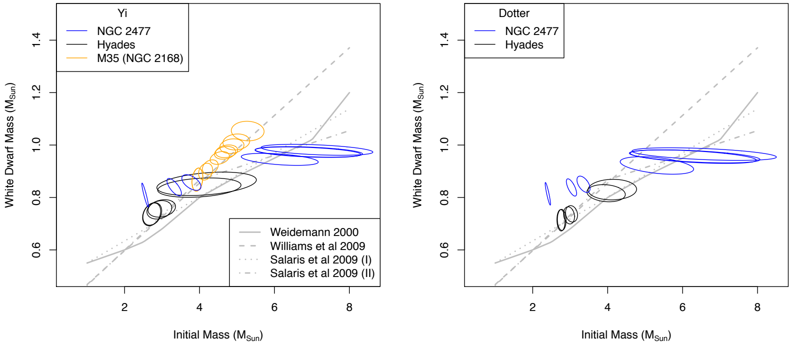
FItting the IFMR



- How best to combine results from three clusters?
- Is there one relationship? Depend on other variables?

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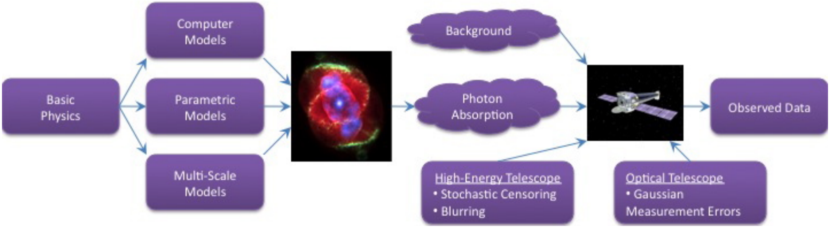
The Basic Statistical Model



- Embed physics models into multi-level statistical models.
- X-ray and γ-ray detectors count a typically *small number of photons* in each of a *large number of pixels*.
- Must account for complexities of data generation.
- State of the art data and computational techniques enable us to fit the resulting complex model.

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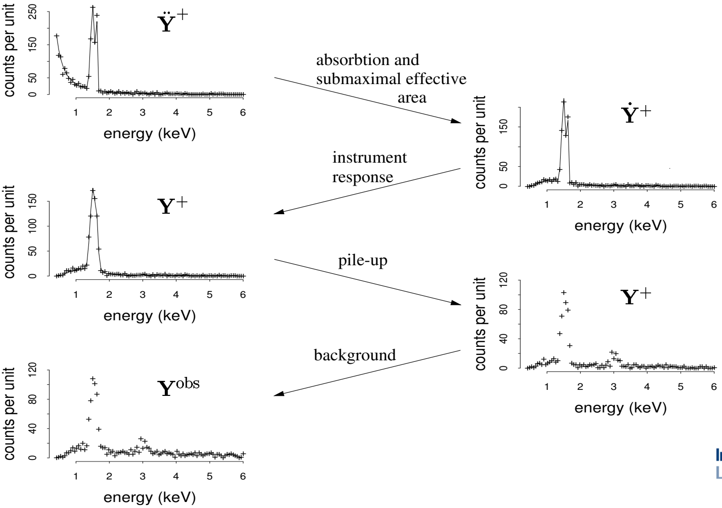
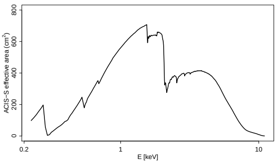
Degradation of the Photon Counts

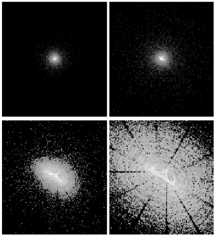


Calibration Products

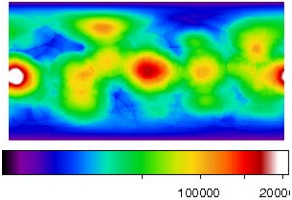
- Analysis is highly dependent on *Calibration Products:*
  - Effective area records sensitivity as a function of energy
  - Energy redistribution matrix can vary with energy/location
  - Point Spread Functions can vary with energy and location
  - Exposure Map shows how effective area varies in an image
- In this talk we focus on uncertainty in the effective area.



A *CHANDRA* effective area.



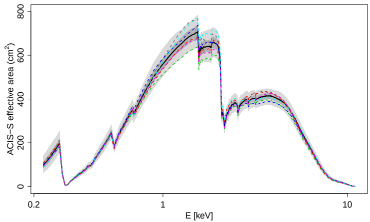
Sample Chandra psf's
(Karovska et al., ADASS X)

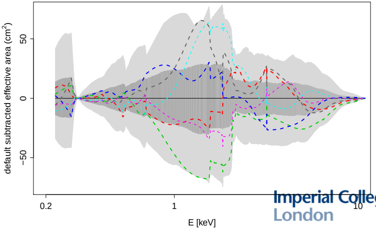


EGERT exposure map
(area $\times$ time)

Derivation of Calibration Products

- Prelaunch ground-based and post-launch space-based empirical assessments.
- Aim to capture deterioration of detectors over time.
- Complex computer models of subassembly components.
- Calibration scientists provide a sample representing uncertainty
- *Calibration Sample* is typically of size $M \approx 1000$.





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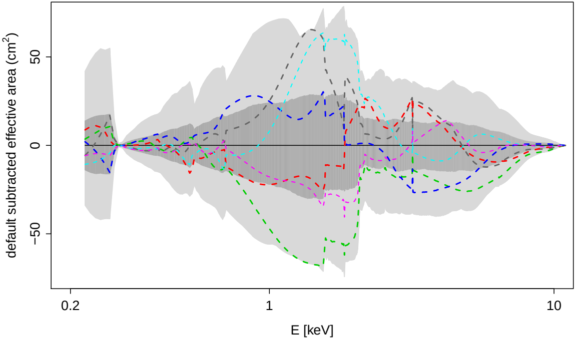
Complex Variability

Computer model generated calibration sample requires:

1. *running the computer model on the fly, or*
2. *storing many high dimensional calibration products.*



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Simple Emulation of Computer Model

We use *Principal Component Analysis* to represent uncertainly:

$$A \sim A_0 + \bar{\delta} + \sum_{j=1}^{m} e_j r_j \boldsymbol{v}_j,$$

A_0: default effective area,

$\bar{\delta}$: mean deviation from A_0,

r_j and $\boldsymbol{v}_j$: first m principle component eigenvalues & vectors,

e_j: independent standard normal deviations.

Capture 95% of variability with $m = 6 - 9$.

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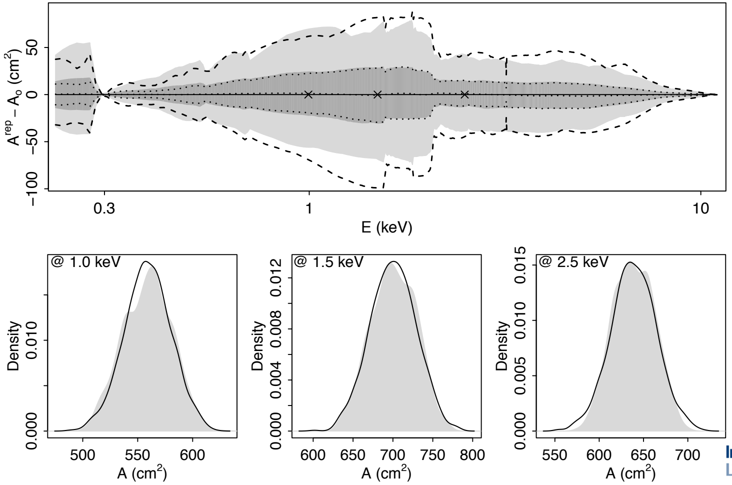
Checking the PCA Emulator



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Using Monte Carlo to Account for Uncertainty

1. Drake et al. (2006) propose a bootstrap-like method:
   - Simulate M spectra under fit model & default effective area.
   - Fit each spectra with effective area from calibration sample.
2. A simpler solution involves Multiple Imputation:
   - Treat $m \ll M$ effective areas from calibration sample as imputations and fit the model m times.
   - Use MI *Combining Rules* to compute estimates and errors.
3. When using MCMC in a Bayesian setting we can:
   - Sample a different effective area from calibration sample at each iteration according to its conditional distribution.
   - Effectively average over the calibration uncertainty.

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Two Possible Target Distributions

We consider inference under:

A PRAGMATIC BAYESIAN TARGET: $\pi_0(A, \theta) = p(A)p(\theta|A, Y)$.

THE FULLY BAYESIAN POSTERIOR: $\pi(A, \theta) = p(A|Y)p(\theta|A, Y)$.

Concerns:

- **Statistical** Fully Bayesian target is "correct".
- **Cultural** Astronomers have concerns about letting the current data influence calibration products.
- **Computational** Both targets pose challenges, but pragmatic Bayesian target is easier to sample.
- **Practical** How different are $p(A)$ and $p(A|Y)$?

Drake (2006) and MI are approximations to π_0.

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Sampling the Full Posterior Distribution

- Sampling $\pi(A, \theta) = p(A, \theta | Y)$ is complicated because we only have a computer-model generated sample of $p(A)$ rather than an analytic form.
- But PCA gives a *degenerate normal* approximation:

$$A \sim A_0 + \bar{\delta} + \sum_{j=1}^{m} e_j r_j \boldsymbol{v}_j,$$

  where e_j are independent standard normals.
- PCA represents A as deterministic function of $e = (e_1, \ldots, e_m)$.
- We can construct an MCMC sampler of $p(e, \theta | Y)$.

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A Prototype Fully Bayesian Sampler

An MH within Gibbs Sampler:

STEP 1: $e \sim \mathcal{K}(e|e', \theta')$ via MH with limiting dist'n $p(e|\theta, Y)$

STEP 2: $\theta \sim \mathcal{K}(\theta|e', \theta')$ via MH with limiting dist'n $p(\theta|e, Y)$

- STEP 1: Gaussian Metropolis jumping rule centered at e'.
- STEP 2: Simplified pyBLoCXS (no rmf or background).

A Simulation.

- Sampled 10^5 counts from a power law spectrum: E^{-2}.
- A_{true} is 1.5σ from the center of the calibration sample.

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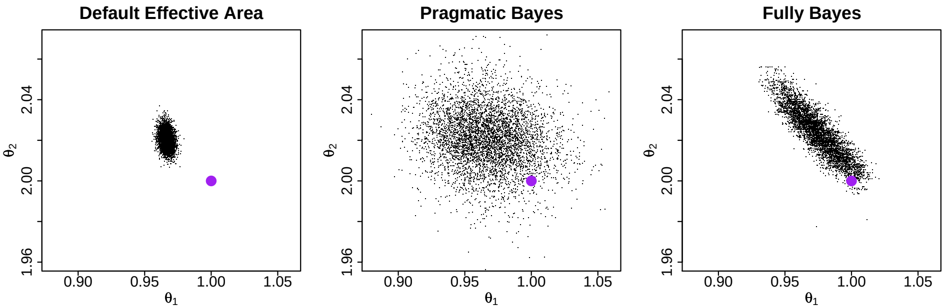
Sampling From the Full Posterior



Spectral Model (purple bullet = truth):

$$f(E_j) = \theta_1 e^{-\theta_3 x(E_j)} E_j^{-\theta_2}$$

Pragmatic Bayes is clearly better than current practice, but a Fully Bayesian Method is the ultimate goal.

Implementing the Fully Bayesian Analysis

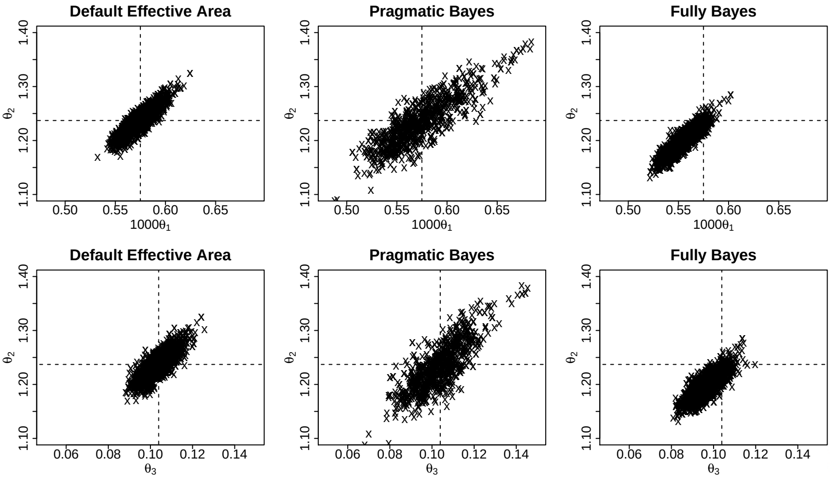
An MH within Gibbs Sampler:

STEP 1: $e \sim \mathcal{K}(e|e', \theta')$ via MH with limiting dist'n $p(e|\theta, Y)$

STEP 2: $\theta \sim \mathcal{K}(\theta|e', \theta')$ via MH with limiting dist'n $p(\theta|e, Y)$

- We use a mixture of two jumping rules in each step:
  - STEP 1: Gaussian Metropolis jump centered at e' and
    MH jump from the prior.
  - STEP 2: T Metropolis jump centered at θ' and
    MH jump from an approximation to the posterior.
- Six tuning parameters: three scale parameters, two proportions (M vs MH jump), and *df* for T.
- Tuning parameters must be adjusted.

The Effect in an Analysis of a Quasar Spectrum



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Thanks...

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- Elizabeth Jeffery
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- Ted von Hippel

Instrument Calibration

- Vinay Kashyap
- Jin Xu
- Alanna Connors
- Hyunsook Lee
- Aneta Siegminowska
- California-Harvard Astro-Statistics Collaboration

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For Further Reading I

- Stein, N, van Dyk, D., von Hippel, T., DeGennaro, S., Jeffery, E., Jeffreys, W. H.
  Combining Computer Models in a Principled Bayesian Analysis: From Normal Stars to White Dwarf Cinders. Submitted.
- Jeffery, E., von Hippel, T., DeGennaro, S., van Dyk, D., Stein, N., and Jefferys, W.
  The White Dwarf Age of NGC 2477. *Astrophysical Journal*, **730**, 35–43, 2011.
- Lee, H., Kashyap, V., van Dyk, D., Connors, A., Drake, J., Izem, R., Min, S., Park, T., Ratzlaff, P., Siemiginowska, A., and Zezas, A.
  Accounting for Calibration Uncertainties in X-ray Analysis: Effective Area in Spectral Fitting. *The Astrophysical Journal*, **731**, 126–144, 2011.
- van Dyk, D. A., DeGennaro, S., Stein, N., Jefferys, W. H., von Hippel, T.
  Statistical Analysis of Stellar Evolution *The Annals of Applied Statistics* **3**, 117-143, 2009.
- DeGennaro, S., von Hippel, T., Jefferys, W., Stein, N., van Dyk, D., and Jeffery, E.
  Inverting Color-Magnitude Diagrams to Access Precise Cluster Parameters: A New White Dwarf Age for the Hyades. *Astrophysical Journal*, **696**, 12–23, 2009.

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The Simulation Studies

Simulated Spectra

- Spectra were sampled using an absorbed power law,

$$f(E_j) = \alpha e^{-N_H x(E_j)} E_j^{-\Gamma},$$

  accounting for instrumental effects; E_j is the energy of bin j.
- Parameters (Γ and N_H) and sample size/exposure times:

	Effective Area		Nominal Counts		Spectal Model	
	Default	Extreme	10^5	10^4	Hard†	Soft‡
SIM 1	X		X		X	
SIM 2	X		X			X
SIM 3	X			X	X	

†An absorbed powerlaw with $\Gamma = 2$, $N_{\rm H} = 10^{23}/{\rm cm}^2$

‡An absorbed powerlaw with $\Gamma = 1$, $N_{\rm H} = 10^{21}/{\rm cm}^2$

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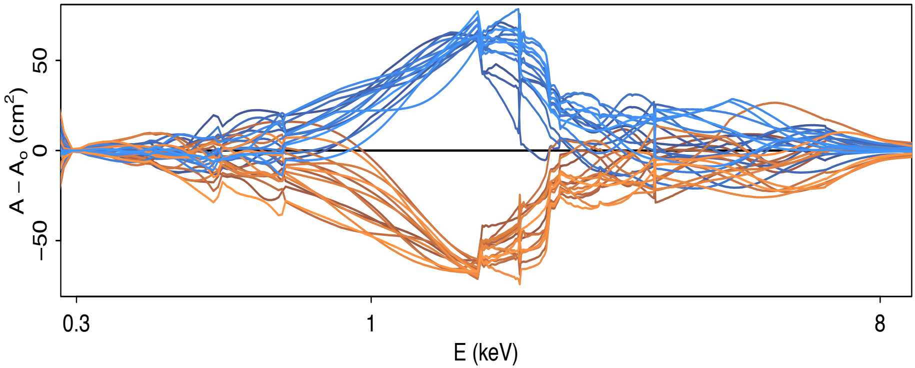
30 Most Extreme Effective Areas in Calibration Sample



15 largest and 15 smallest determined by maximum value

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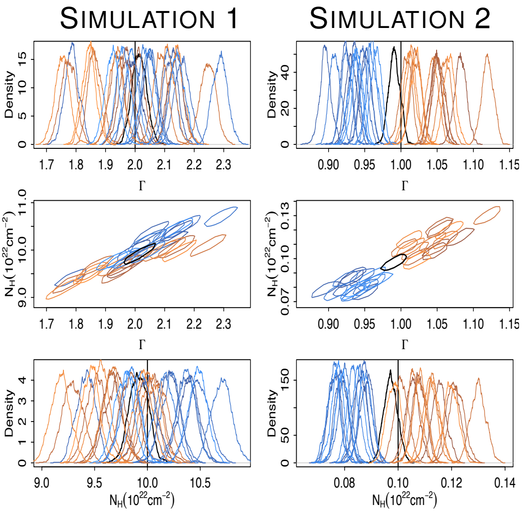
The Effect of Calibration Uncertainty



- Columns represent two simulated spectra.
- True parameters are horizontal lines.
- Posterior under default calibration is plotted in black.
- The posterior is highly sensitive to the choice of effective area!

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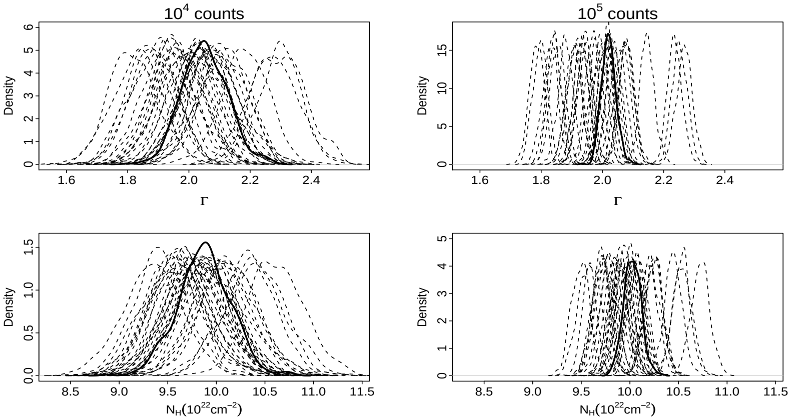
The Effect of Sample Size



The effect of Calibration Uncertainty is more pronounced with larger sample sizes.