

BAYESIAN COMPUTATION IN COLOR-MAGNITUDE DIAGRAMS

SA, AA, PT, EE, MCMC AND ASIS IN CMDs

Paul Baines

Department of Statistics
Harvard University

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OVERVIEW

- ▶ Motivation and Introduction
- ▶ Modelling Color-Magnitude Diagrams
- ▶ Bayesian Statistical Computation
- ▶ Acronyms in SC: MH, ASIS, EE, PT

STELLAR POPULATIONS

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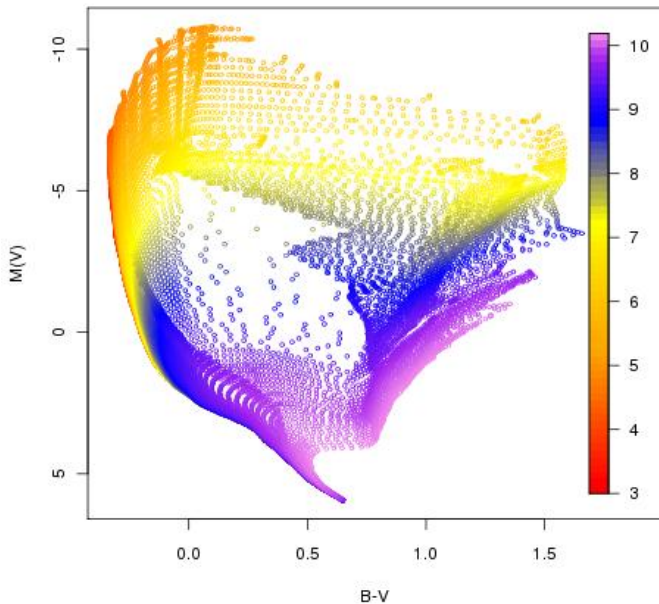
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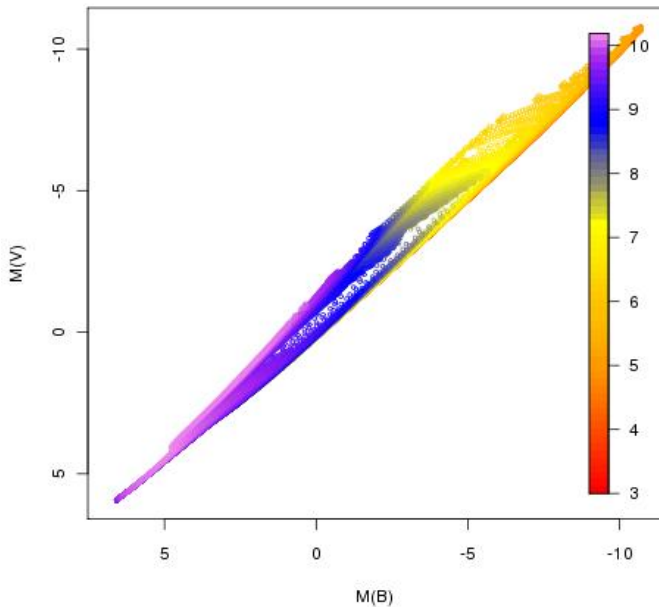
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- ... doesn't utilize any knowledge of underlying structure, propagation of error, hard to extend coherently...

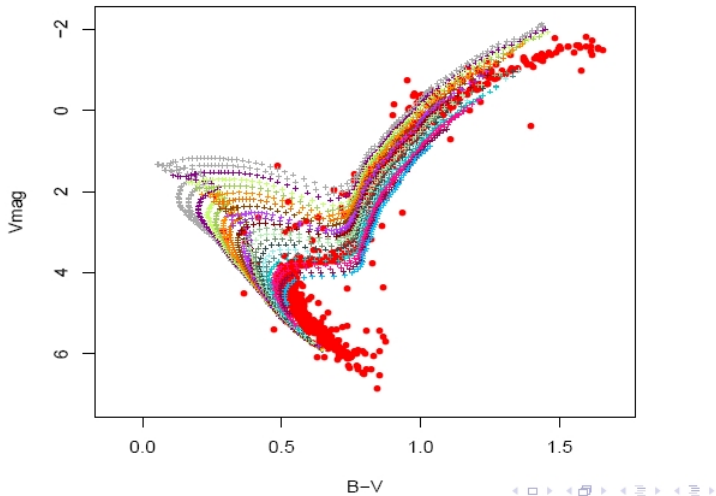
Isochrones: Metallicity = 4



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NGC 104 (47 Tuc)



Hyunsook Lee, Harvard Smithsonian Center for Astrophysics

GAUSSIAN ERRORS

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(Mechanically unimportant)

THE LIKELIHOOD

Assuming gaussian errors with common correlation matrix:

$$y_i \mid A_i, M_i, Z \sim N(\tilde{f}_i, \mathbf{R}) \quad i = 1, \dots, n \quad (1)$$

Where,

$$y_i = \begin{pmatrix} \frac{1}{\sigma_i^{(B)}} B_i \\ \frac{1}{\sigma_i^{(V)}} V_i \\ \frac{1}{\sigma_i^{(I)}} I_i \end{pmatrix}, \tilde{f}_i = \begin{pmatrix} \frac{1}{\sigma_{Bi}} \cdot f_b(M_i, A_i, Z) \\ \frac{1}{\sigma_{Vi}} \cdot f_v(M_i, A_i, Z) \\ \frac{1}{\sigma_{Ii}} \cdot f_i(M_i, A_i, Z) \end{pmatrix}, \mathbf{R} = \begin{pmatrix} 1 & \rho^{(BV)} & \rho^{(BI)} \\ \rho^{(BV)} & 1 & \rho^{(VI)} \\ \rho^{(BI)} & \rho^{(VI)} & 1 \end{pmatrix} .$$

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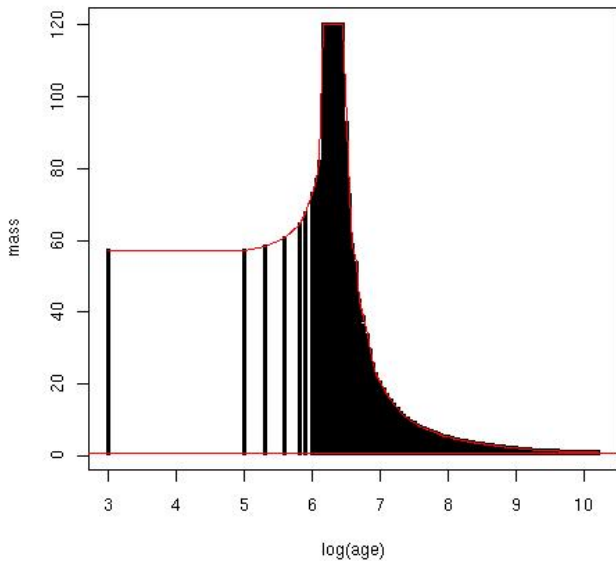
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Now, we assume a hierarchical Bayesian model on the mass, age, and metallicities.

Isochrone table layout (support)



JOINT DISTRIBUTION OF MASS AND AGE

Even before we observe any data, we know that the distributions of stellar mass and age are not independent. We know *a priori* that, (for a star to be in the population of all possibly observable stars), old stars cannot have large mass, likewise for very young stars. Hence, we specify the prior on mass conditional on age:

$$p(M_i | A_i, M_{min}, M_{max}(A_i), \alpha) \propto \frac{1}{M_i^\alpha} \cdot \mathbf{1}_{\{M_i \in [M_{min}, M_{max}(A_i)]\}} \quad (2)$$

i.e. $M_i | A_i, M_{min}, M_{max}(A_i), \alpha \sim \text{Truncated-Pareto}$.

AGE

For age we assume the following hierarchical structure:

$$A_i | \mu_A, \sigma_A^2 \stackrel{iid}{\sim} N(\mu_A, \sigma_A^2) \quad (3)$$

where $A_i = \log_{10}(\text{Age})$, with μ_A and σ_A^2 hyperparameters. . .

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Idea: Allow greater flexibility/reduce dimensionality, investigate strength of assumptions, capture underlying structure, correlation etc

HYPERPARAMETERS

Next, we model the hyperparameters with the simple conjugate form:

$$\mu_A | \sigma_A^2 \sim N \left(\mu_0, \frac{\sigma_A^2}{\kappa_0} \right), \quad \sigma_A^2 \sim \text{Inv} - \chi^2 (\nu_0, \sigma_0^2) \quad (4)$$

Where μ_0, κ_0, ν_0 and σ_0^2 are fixed by the user to represent prior knowledge (or lack of).

Sensitivity (or robustness) to the prior is of great interest.

CORRELATION

We assume a uniform prior over the space of positive definite correlation matrices.

This isn't quite uniform on each of $\rho^{(BV)}$, $\rho^{(BI)}$ and $\rho^{(VI)}$, but it is close for low dimensions.

PUTTING IT ALL TOGETHER

$$y_i = \begin{pmatrix} \frac{1}{\sigma_i^{(B)}} B_i \\ \frac{1}{\sigma_i^{(V)}} V_i \\ \frac{1}{\sigma_i^{(I)}} I_i \end{pmatrix} \Bigg| A_i, M_i, Z \sim N(\tilde{f}_i, \mathbf{R}) \quad i = 1, \dots, n.$$

$$M_i | A_i, M_{min}, \alpha \sim \text{Truncated-Pareto}(\alpha - 1, M_{min}, M_{max}(A_i))$$

$$A_i | \mu_A, \sigma_A^2 \stackrel{iid}{\sim} N(\mu_A, \sigma_A^2)$$

$$\mu_A | \sigma_A^2 \sim N\left(\mu_0, \frac{\sigma_A^2}{\kappa_0}\right), \quad \sigma_A^2 \sim \text{Inv} - \chi^2(\nu_0, \sigma_0^2)$$

$$p(\mathbf{R}) \propto \mathbf{1}_{\{\mathbf{R}p.d.\}}$$

MCMC TOOLBOX

(Almost) everything must use a Gibbs sampler (or conditional maximization) if it has lots of parameters. Gibbs is great but its failings are well documented. Three top-of-the-range tools for building your MCMC scheme:

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We now take a 'hands on' look at these in developing a robust algorithm for analysis Color-Magnitude data.

DEFAULT MCMC

ALGORITHM

Let $\Theta^{(t)} = \{(M_i^{(t)}, A_i^{(t)}) : i = 1, \dots, n\}$.

0. Set $t = 0$. Choose starting states $\Theta^{(0)}, \mu_a^{(0)}, \sigma_a^{(0)}$.
1. Draw $\Theta^{(t+1)}$ from $\{M_i, A_i\}_{i=1, \dots, n} | \mu_a^{(t)}, \sigma_a^{(t)}, \mathbf{Y}$.
2. Draw $\mu_a^{(t+1)}, \sigma_a^{(t+1)}$ from $\mu_a, \sigma_a | \Theta^{(t+1)}, \mathbf{Y}$.
3. Increment $t \mapsto t + 1$, return to 1.

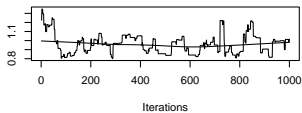
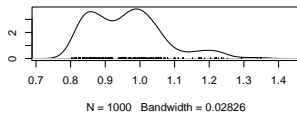
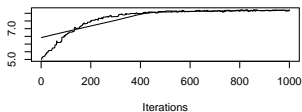
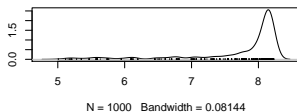
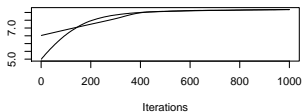
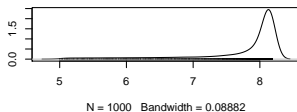
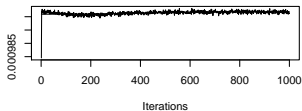
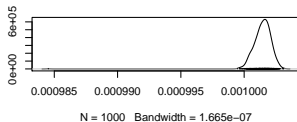
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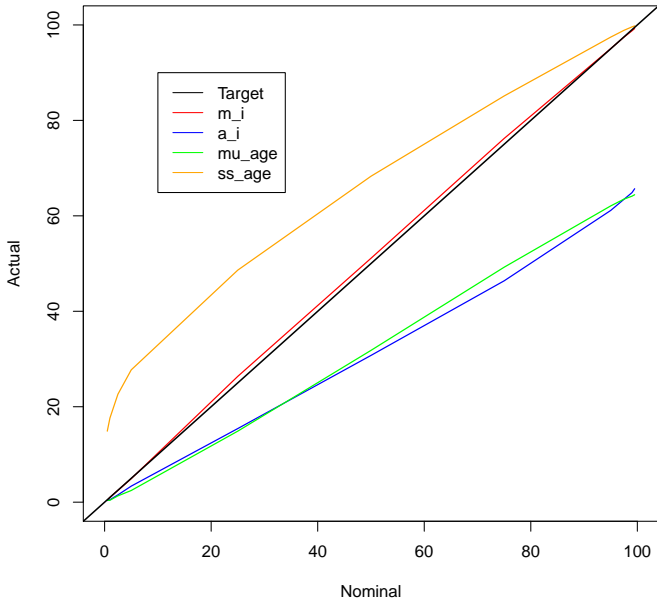
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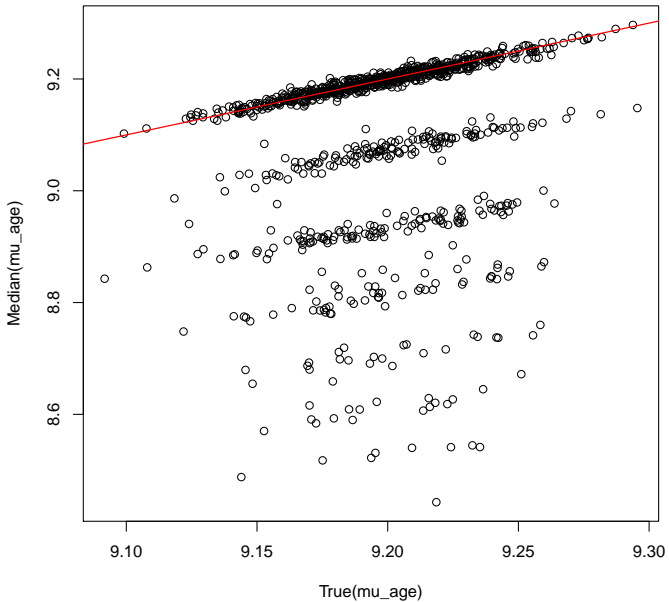
The samples $(\Theta^{(t)}, \mu_a^{(t)}, \sigma_a^{(t)})$, for $t = B + 1, \dots, B + N$ form a sample from the target distribution (approximately)...

Trace of m_0**Density of m_0****Trace of a_0****Density of a_0****Trace of mu_age****Density of mu_age****Trace of ss_age****Density of ss_age**

Actual vs. Nominal Coverage



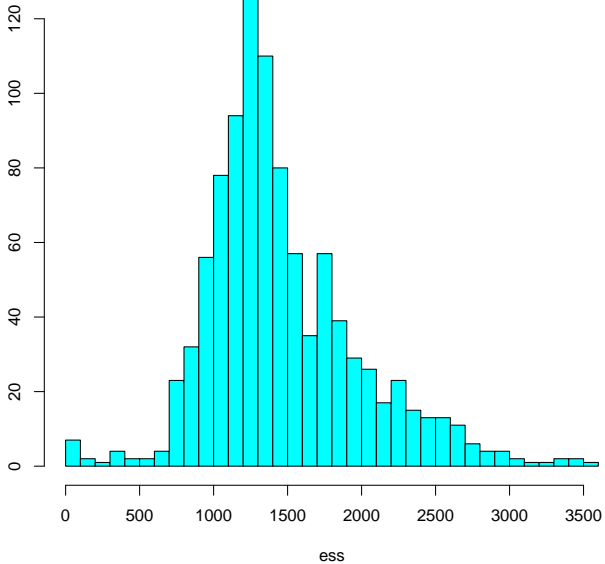
mu_age: Posterior medians vs. Truth



	1%	2.5%	5%	25%	50%	75%	95%	97.5%	99%
m_i	1.0	2.5	4.9	26.4	51.1	76.2	95.0	97.5	98.8
a_i	0.5	1.5	3.4	15.4	30.8	46.4	61.1	63.5	64.9
μ_a	0.4	1.3	2.4	14.9	31.8	49.2	62.1	63.5	64.1
σ_a^2	17.6	22.6	27.7	48.6	68.3	85.1	97.5	98.9	99.6

TABLE: Coverage table for the standard SA sampler and synthetic isochrones

MCMC: Effective Sample Sizes



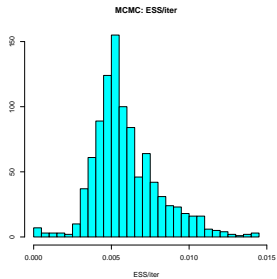
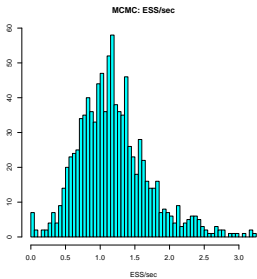
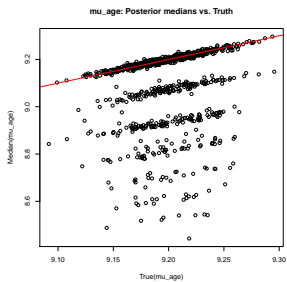


FIGURE: Convergence plots for standard sampler (synthetic isochrones)

INTRO TO INTERWEAVING

From Yu & Meng (2009): Consider,

$$Y_{obs}|\theta, Y_{mis} \sim N(Y_{mis}, 1) \quad (5)$$

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The standard Gibbs sampler iterates between:

$$Y_{mis}|\theta, Y_{obs} \sim N\left(\frac{\theta + VY_{obs}}{1 + V}, \frac{V}{1 + V}\right) \quad (7)$$

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It is easy to show that the geometric convergence rate for this scheme is $1/(1 + V)$ i.e., very slow for small V .

PROBLEMS WITH THE SA

By analogy, the very small variance among the stellar ages causes high autocorrelations across the draws and slow convergence.

This standard scheme is known as the **sufficient augmentation (SA)**, since Y_{mis} is a sufficient statistic for μ in the complete-data model.

ANCILLARY AUGMENTATION

However, by letting $\tilde{Y}_{mis} = Y_{mis} - \theta$ the complete-data model becomes:

$$Y_{obs} | \tilde{Y}_{mis}, \theta \sim N(\tilde{Y}_{mis} + \theta, 1), \quad (9)$$

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The Gibbs sampler for this **Ancillary Augmentation (AA)** is:

$$\tilde{Y}_{mis} | \theta, Y_{obs} \sim N\left(\frac{V(Y_{obs} - \theta)}{1 + V}, \frac{V}{1 + V}\right) \quad (11)$$

$$\theta | \tilde{Y}_{mis}, Y_{obs} \sim N\left(Y_{obs} - \tilde{Y}_{mis}, 1\right), \quad (12)$$

with convergence rate $1/(1 + V)$ i.e., extremely fast for small V .

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ASIS SAMPLER

The Gibbs sampler forms a conditional SA, and it can be shown that:

$$\tilde{A}_i = \Phi\left(\frac{A_i - \mu_A}{\sigma_A}\right), \quad \tilde{M}_i = \frac{M_{min}^{-(\alpha-1)} - M_i^{-(\alpha-1)}}{M_{min}^{-(\alpha-1)} - M_{max}(A_i)^{-(\alpha-1)}}, \quad (13)$$

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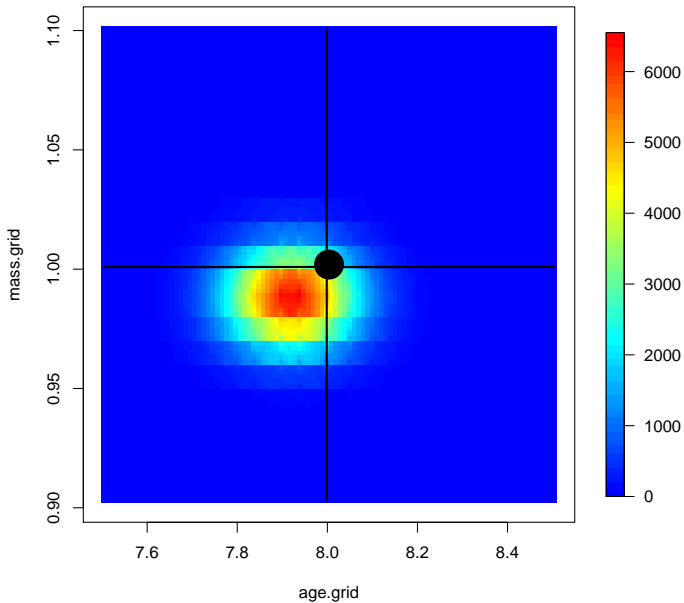
forms an AA:

$$Y_i | \tilde{\mathbf{M}}, \tilde{\mathbf{A}}, \mathbf{R}, \mu_A, \sigma_A^2 \sim N\left(f(M_i(\tilde{M}_i), \tilde{A}_i; \mu_A, \sigma_A), A_i(\tilde{M}_i, \tilde{A}_i; \mu_A, \sigma_A), Z), \mathbf{R}\right)$$

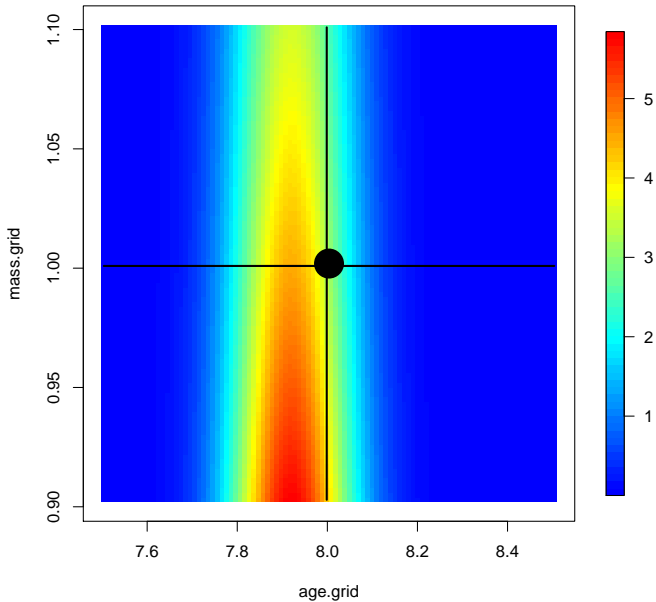
$$\tilde{A}_i | \mu_A, \sigma_A^2 \sim N[0, 1], \quad \tilde{M}_i | \tilde{A}_i, \mu_A, \sigma_A^2 \sim U[0, 1]$$

$$\mu_A | \sigma_A^2 \sim N\left(\mu_0, \frac{\sigma_A^2}{\kappa_0}\right), \quad \sigma_A^2 \sim \text{Inv-}\chi^2(\nu_0, \sigma_0^2).$$

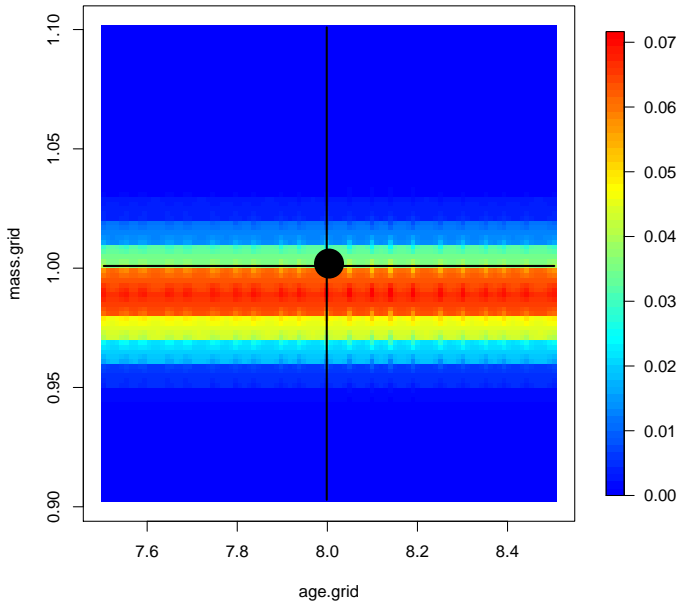
Posterior distribution



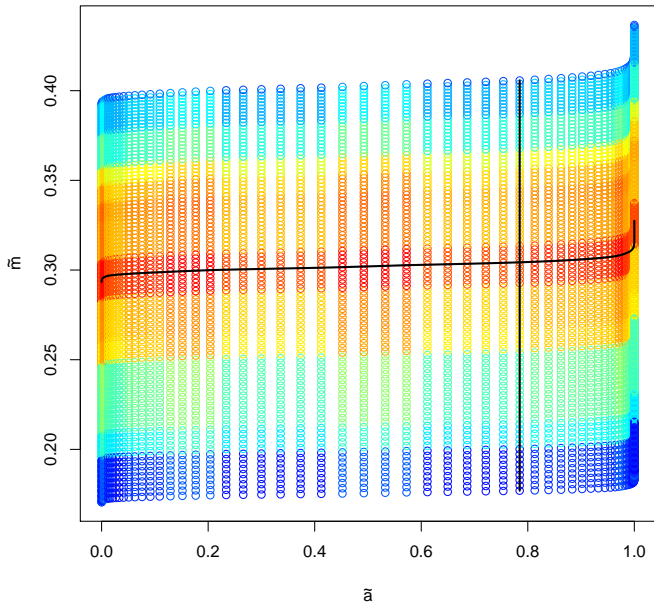
Prior distribution



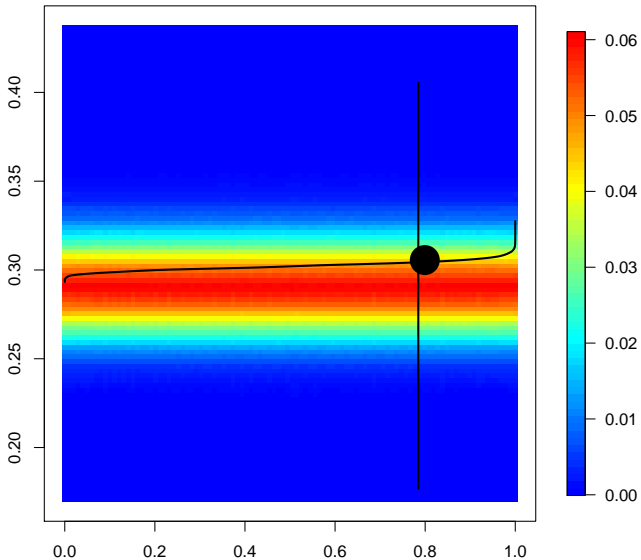
Likelihood Surface



Transformation: SA→AA (transition)



Posterior in AA-parametrization



AN ASIS FOR THE CMD PROBLEM

1. Draw $(\mathbf{M}^{(t+0.5)}, \mathbf{A}^{(t+0.5)})$ from SA: $\mathbf{M}, \mathbf{A} | \mathbf{Y}, \mu_A^{(t)}, \sigma_A^{(t)}, \delta^{(t)}$.
2. Compute:
 $(\tilde{\mathbf{M}}^{(t+0.5)}, \tilde{\mathbf{A}}^{(t+0.5)}) = H(\mathbf{M}^{(t+0.5)}, \mathbf{A}^{(t+0.5)}; \mu_A^{(t)}, \sigma_A^{(t)})$.
3. Draw $(\mu_A^{(t+0.5)}, \sigma_A^{(t+0.5)})$ from AA:
 $\mu_A, \sigma_A^2 | \mathbf{Y}, \tilde{\mathbf{M}}^{(t+0.5)}, \tilde{\mathbf{A}}^{(t+0.5)}, \delta^{(t)}$.
4. Compute:
 $(\mathbf{M}^{(t+1)}, \mathbf{A}^{(t+1)}) = H(\tilde{\mathbf{M}}^{(t+0.5)}, \tilde{\mathbf{A}}^{(t+0.5)}; \mu_A^{(t+0.5)}, \sigma_A^{(t+0.5)})$.
5. Redraw $(\mu_A^{(t+1)}, \sigma_A^{(t+1)})$ from SA:
 $\mu_A, \sigma_A^2 | \mathbf{Y}, \mathbf{M}^{(t+1)}, \mathbf{A}^{(t+1)}, \delta^{(t)}$.

BEAUTY AND THE BEAST

The conditional posterior for (μ_a, σ_a^2) under the AA scheme is given by:

$$p(\mu_A, \sigma_A^2 | \tilde{\mathbf{M}}, \tilde{\mathbf{A}}, \mathbf{R}, \mathbf{Y}, \phi) \propto \det(\mathbf{R})^{-n/2} \exp \left\{ -\frac{1}{2} \left[\frac{\kappa_0}{\sigma_A^2} (\mu_A - \mu_0)^2 + \text{tr}(\mathbf{R}^{-1} \mathbf{F}) \right] \right\} p(\mu_a, \sigma_a^2)$$

BEAUTY AND THE BEAST

The conditional posterior for (μ_a, σ_a^2) under the AA scheme is given by:

$$p(\mu_A, \sigma_A^2 | \tilde{\mathbf{M}}, \tilde{\mathbf{A}}, \mathbf{R}, \mathbf{Y}, \phi) \propto \det(\mathbf{R})^{-n/2} \exp \left\{ -\frac{1}{2} \left[\frac{\kappa_0}{\sigma_A^2} (\mu_A - \mu_0)^2 + \text{tr}(\mathbf{R}^{-1} \mathbf{F}) \right] \right\} p(\mu_a, \sigma_a^2)$$

Shifting (μ_a, σ_a^2) and mapping back to the AA will shift every single mass and age, but at a price. . .

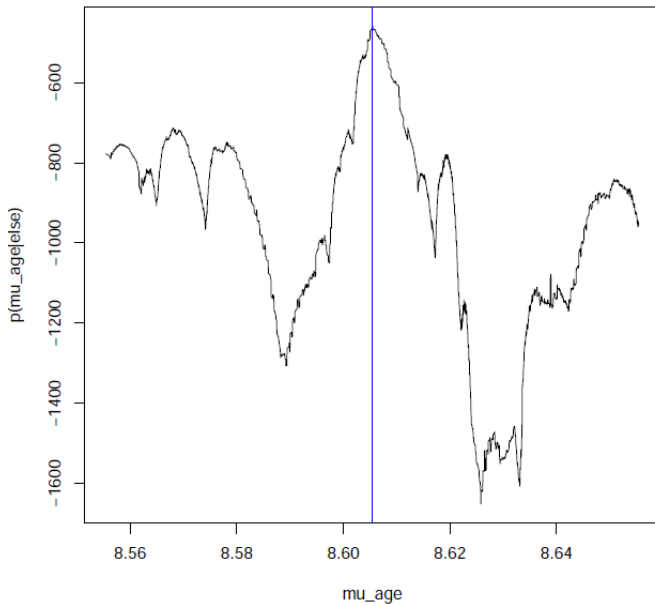


FIGURE: Full conditional log-posterior for μ_a in the AA-sampler.

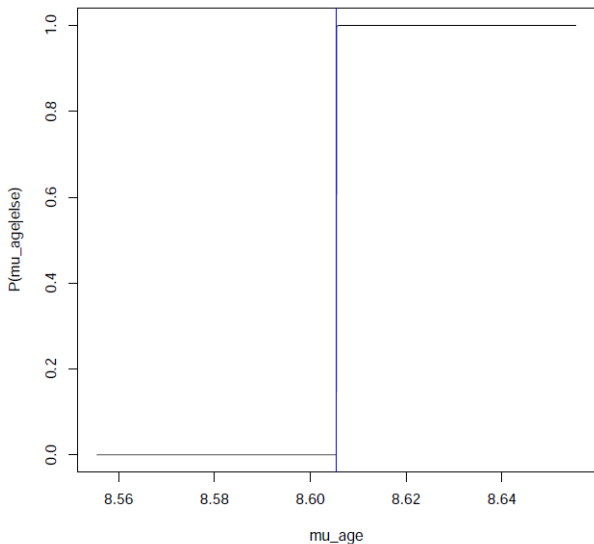


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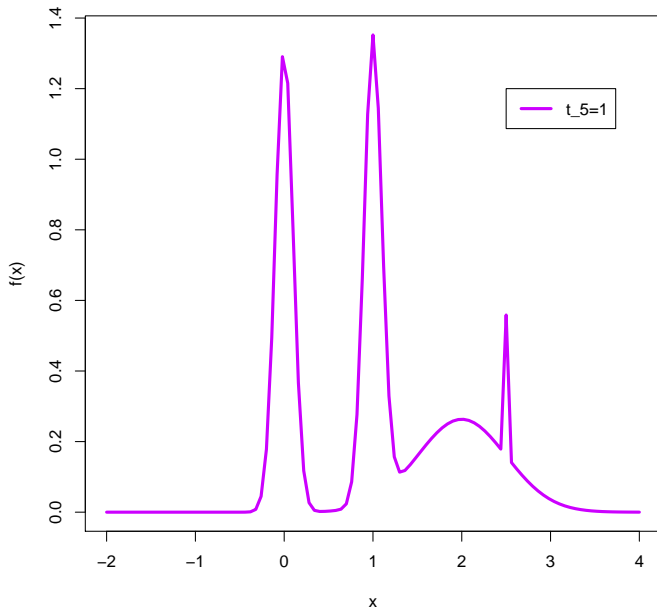
SAMPLING (M,A)

Sampling individual masses and ages is itself a complicated task, given the irregular and non-linear nature of the isochrone tables.

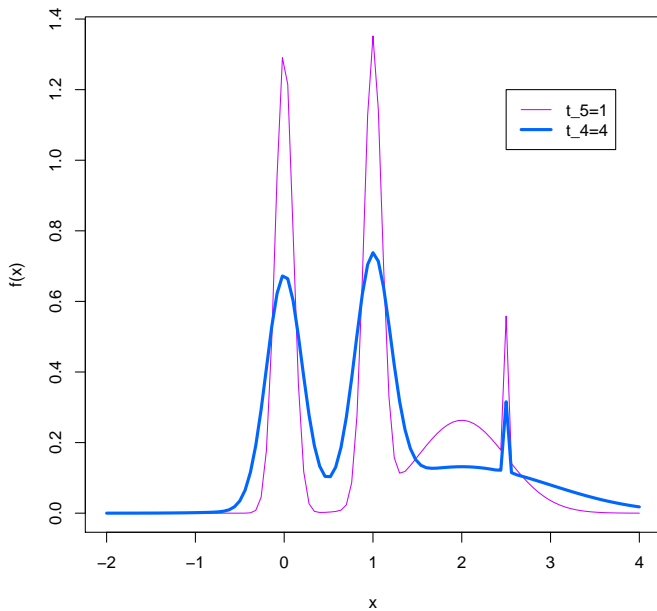
We construct an efficient, energy-based proposal distribution, in the spirit of Equi-Energy sampling (Kou, Zhou and Wong, 2006).

The entire scheme is then embedded within a Parallel Tempering framework (Geyer, 1991).

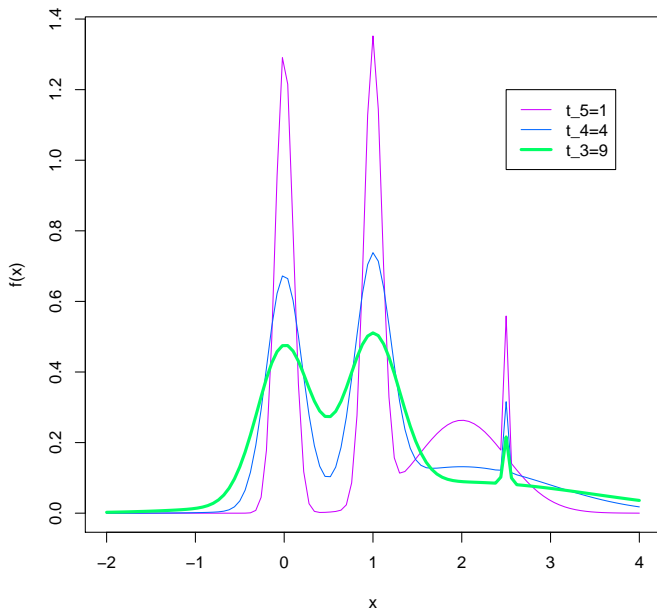
PT Example



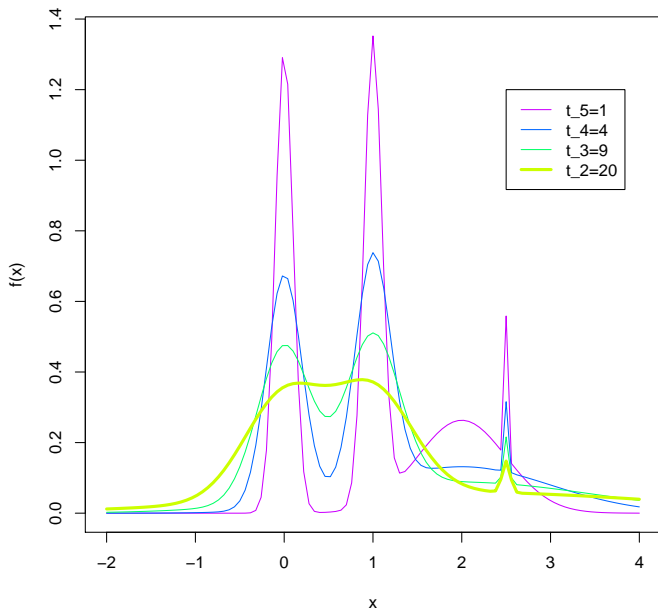
PT Example



PT Example



PT Example



PARALLEL TEMPERING

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(1) **Energy function:** $h(x) \propto -\log \pi(x)$ (i.e. $T = 1$)

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(4) Hotter chains are easier to sample from (flatter), allow for a filtering of states from higher to lower temperatures (random exchange) to avoid local modes etc.

EQUI-ENERGY SAMPLING

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(4) **Per-level energy functions:**

$$h_i(x) = \frac{1}{T_i} \max\{h(x), H_i\} \quad \text{i.e.} \quad \pi_i(x) \propto \begin{cases} e^{-h(x)/T_i} & \text{if } h(x) > H_i \\ e^{-H_i/T_i} & \text{if } h(x) \leq H_i \end{cases}$$

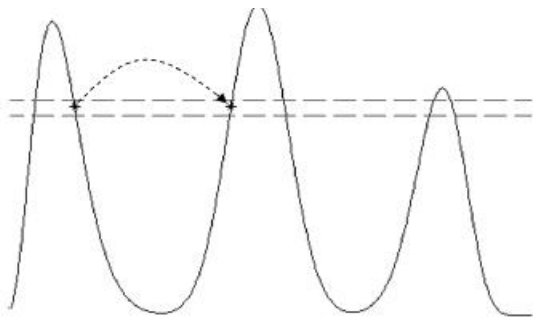


FIGURE: The equi-energy jump

ENERGY LEVELS: A CLOSER LOOK

For those who are unfamiliar with temperature-scaling it may be helpful to look at exactly what we have in the familiar setting:

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$$\pi_i(x) = \begin{cases} (\pi(x))^{1/T_i} & \text{if } \pi(x) > e^{-H_i} \\ \text{constant} & \text{if } \pi(x) \leq e^{-H_i} \end{cases}$$

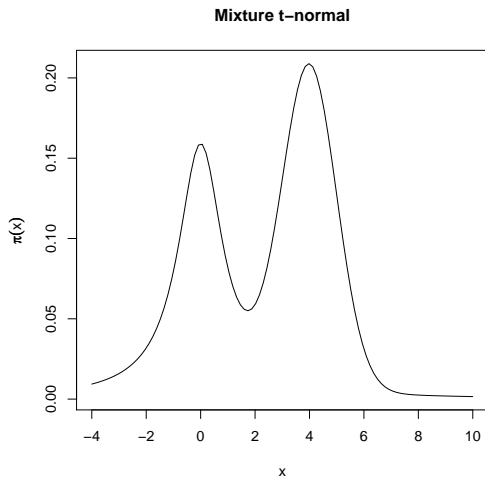
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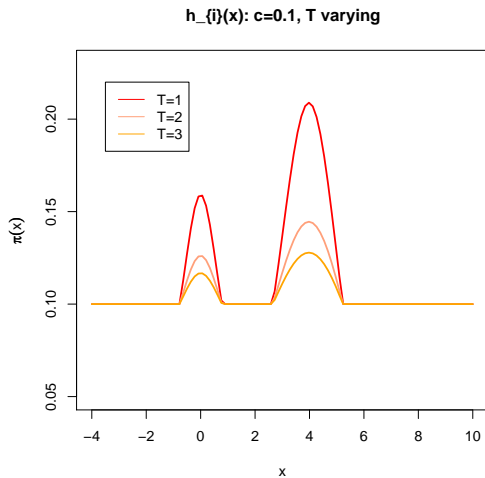
$$\pi_i(x) = \begin{cases} (\pi(x))^{1/T_i} & \text{if } \pi(x) > e^{-H_i} \\ \text{constant} & \text{if } \pi(x) \leq e^{-H_i} \end{cases}$$

- ▶ So the i^{th} -level target densities are **(lower-)truncated and flattened** versions of the original density

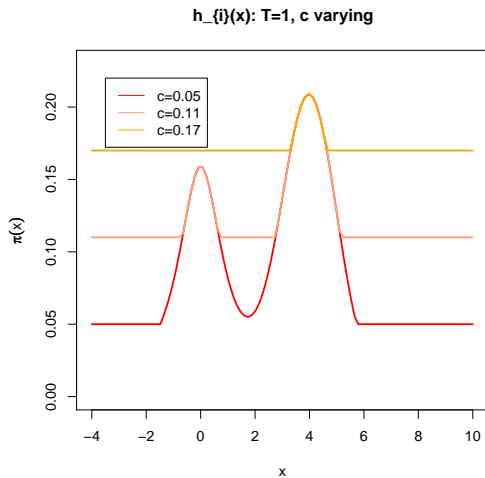
AN EXAMPLE



TEMPERATURE EFFECT



TRUNCATION EFFECT



THE DETAILS

- ▶ **Idea:** Construct empirical energy rings $\hat{D}_j^{(K)}$ for $j = 0, 1, \dots, K$
i.e. compute set membership $l(x)$ for each sampled state:

$$l(x) = j \quad \text{if} \quad h(x) \in [H_j, H_{j+1}) \quad \left(\text{i.e. } \pi(x) \in [e^{-H_j}, e^{-H_{j+1}}) \right)$$

EE-INSPIRED PROPOSAL CONSTRUCTION

The driving force of the posterior in the ancillary augmentation is the likelihood, as determined primarily by the isochrone tables.

- ▶ EE constructs energy bins in joint space. . .

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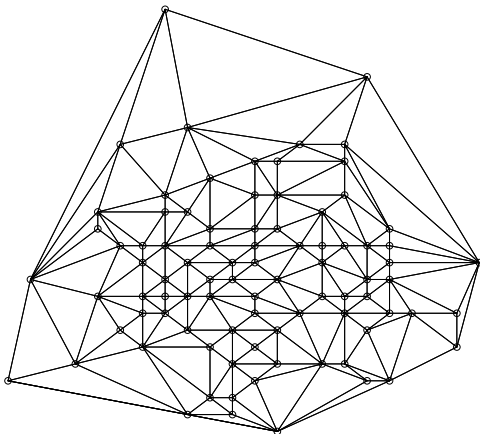
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- ▶ EE constructs energy bins in joint space. . .
here $2n + 2 + p(p - 1)/2$ ☹
- ▶ For Gibbs step drawing (M_i, A_i) , we can utilize the common structure of the isochrone tables
- ▶ We have a map ahead of time of which parameter combinations map to 'similar' regions of the observation space
- ▶ Construct 'energy-based' proposal based on this
- ▶ Partition parameter space into 'boxes' and characterize distance between boxes. . .

Delaunay triangulation



```
tri.mesh(rpois(100, lambda = 20), rpois(100, lambda = 20), duplicate = "remove")
```

FIGURE: Example of Delaunay Triangulation

Delaunay triangulation

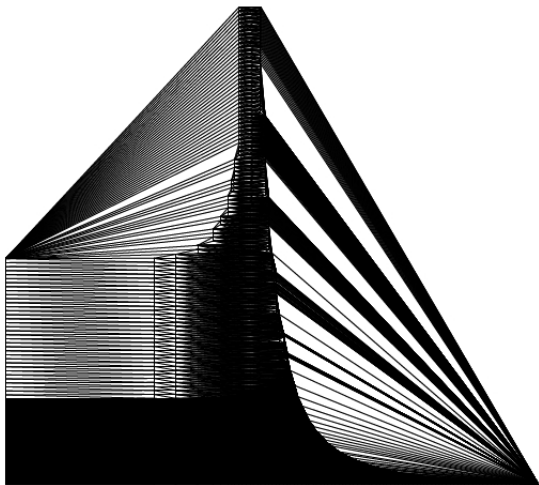


FIGURE: Delaunay Triangulation of (M, A)

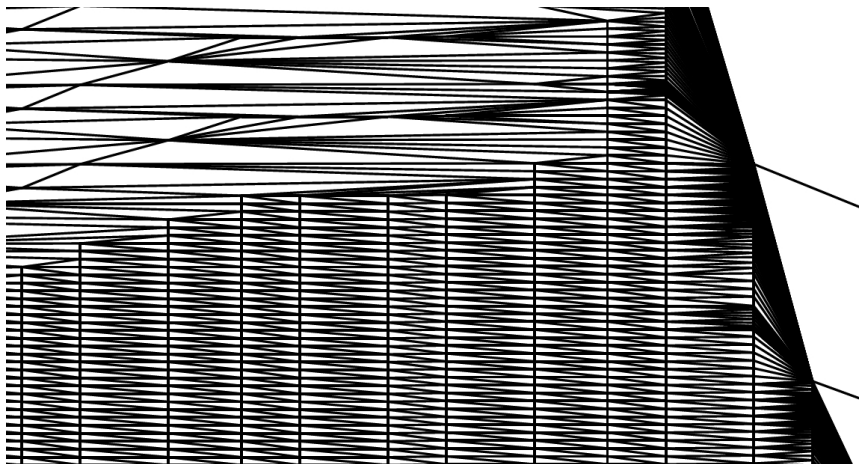


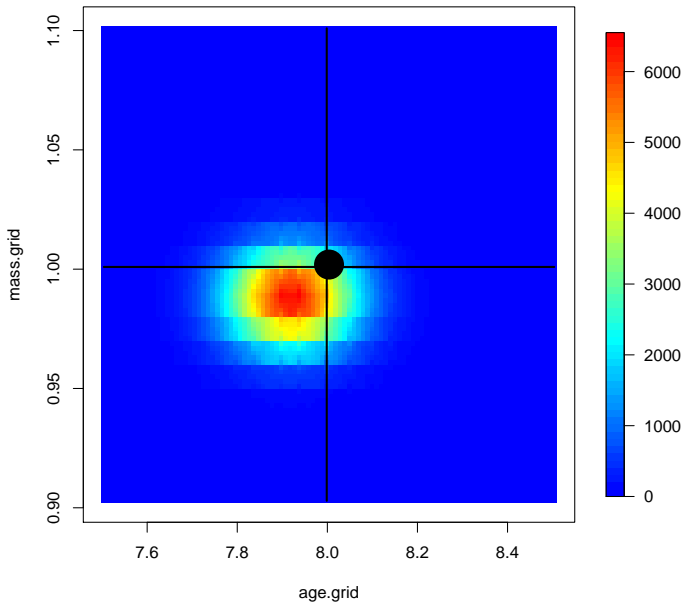
FIGURE: Close up view of the partition

PARSIMONIOUS REPRESENTATION

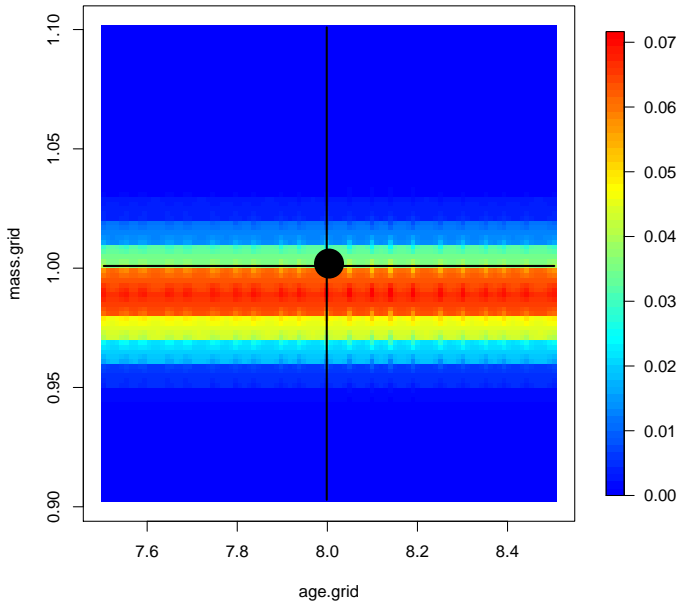
Storing a 'box-to-box' proposal weight matrix is a little cumbersome as the number of boxes is relatively large ($\approx 193,000$).

Instead we cluster the boxes into 'clusters' of boxes that are 'close' in color/magnitude space, then propose (uniformly) within the clusters, and store a much smaller cluster-to-cluster proposal.

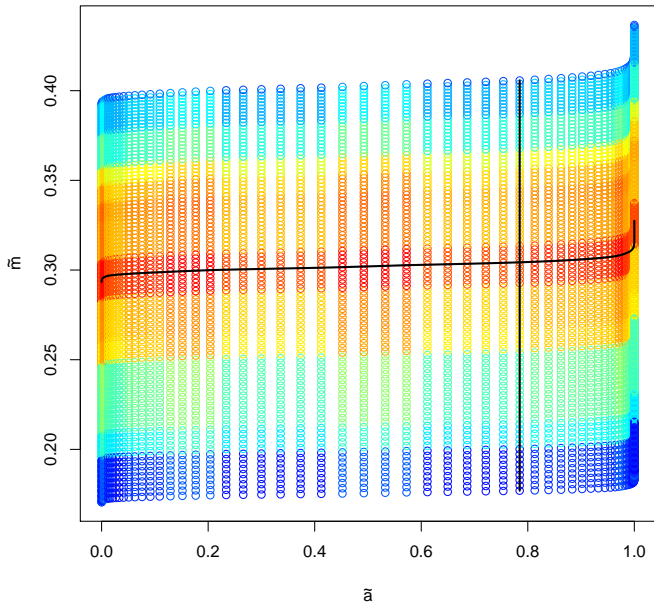
Posterior distribution



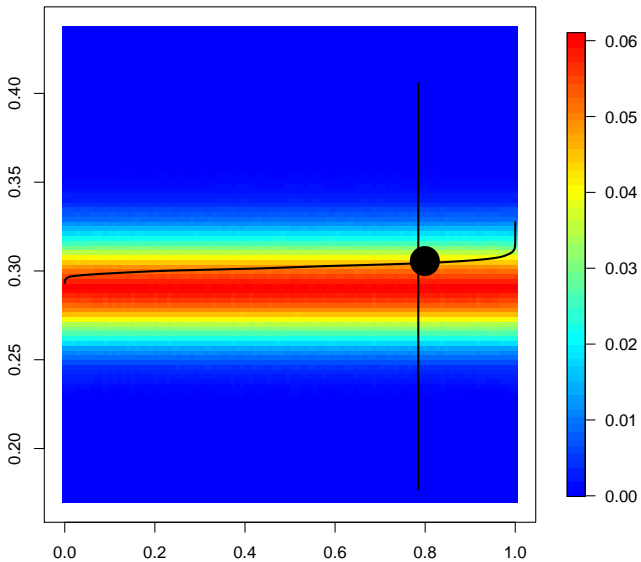
Likelihood Surface



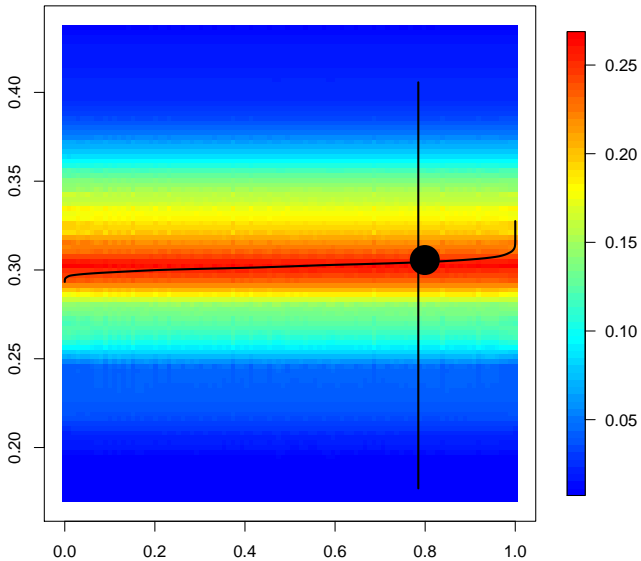
Transformation: SA→AA (transition)



Posterior in AA-parametrization



Proposal distribution in AA-parametrization



IMPLEMENTATION

The goal was a general purpose methodology for CMD-esque analysis, for which we have developed (and are developing) an R package `cmd`, complete with other computational and graphical tools for CMD-analysis.

The algorithm is implemented in C, and can effectively datasets up to $\approx 2,000,000$ observations.

The package can be run in standard form or, for more intensive analyses, a multi-threaded implementation is available for parallel computation.

Python front end expected in the future. . .

RESULTS

Simulating from the model and fitting, we check the sampling scheme validates (on average)...

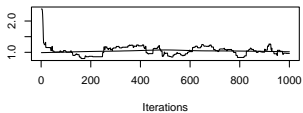
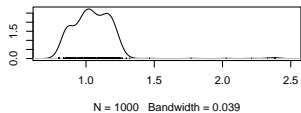
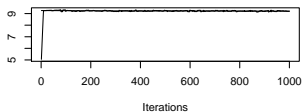
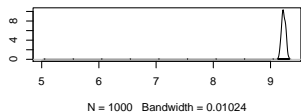
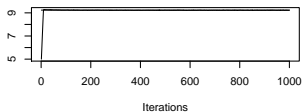
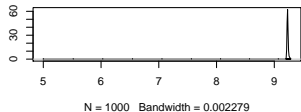
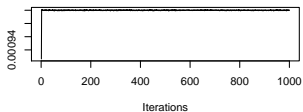
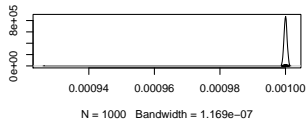
RESULTS

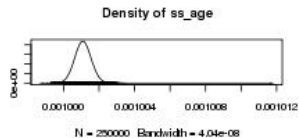
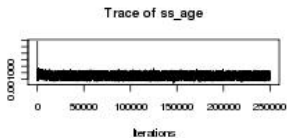
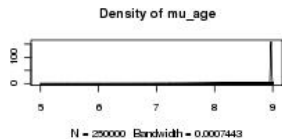
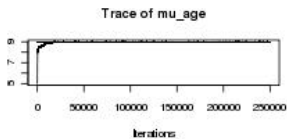
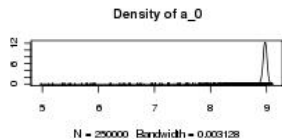
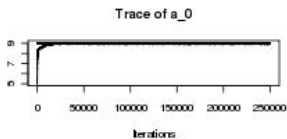
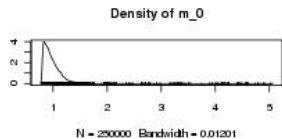
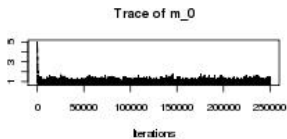
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VALIDATION RECIPE (AGGREGATE)

1. *Simulate parameters from the prior distribution, M times,*
2. *For each parameter combination, simulate a dataset conditional on these,*
3. *Compute the posterior interval(s) for each of these datasets,*
4. *Compute whether or not each interval covers the truth.*

Coverage rates of 95% interval (etc) should agree with nominal level.

Trace of m_0**Density of m_0****Trace of a_0****Density of a_0****Trace of mu_age****Density of mu_age****Trace of ss_age****Density of ss_age**



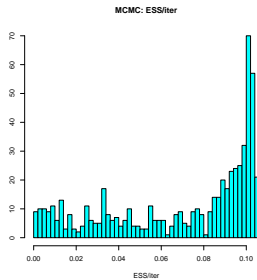
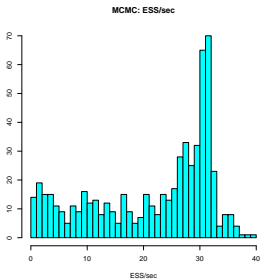
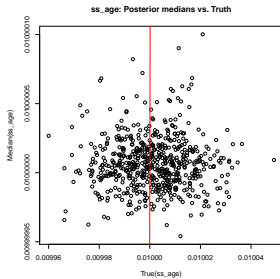
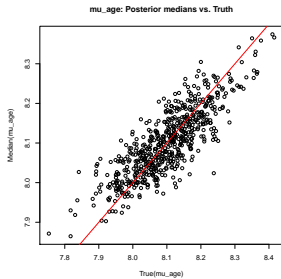


FIGURE: Convergence plots for sampler with Parallel Tempering

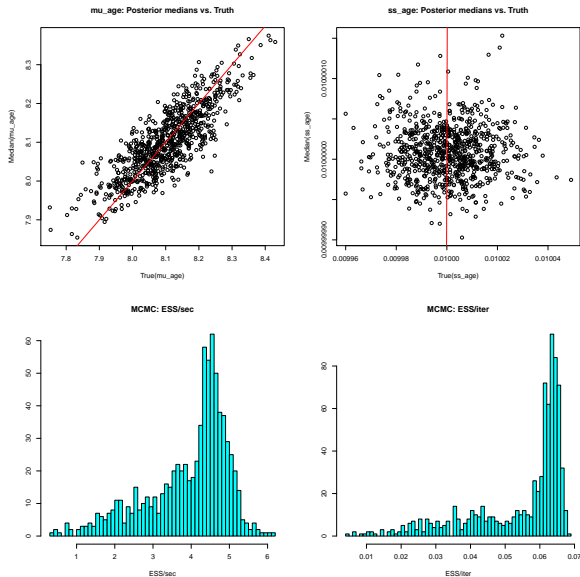
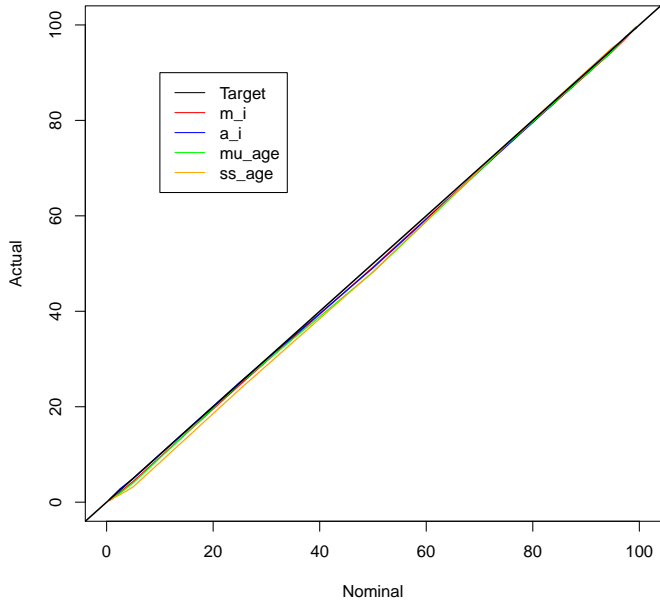


FIGURE: Convergence plots for sampler with box-and-cluster proposal in the ancillary augmentation

Actual vs. Nominal Coverage



COVERAGE TABLE

	1%	2.5%	5%	25%	50%	75%	95%	97.5%	99%
m_i	0.7	2.1	4.4	24.6	49.3	74.6	94.5	97.2	99.2
a_i	1.1	2.8	5.0	25.1	49.1	74.5	94.8	97.6	99.0
mu_a	0.7	1.9	4.0	24.9	48.2	74.8	94.6	97.4	99.1
sigmasq_a	0.7	1.6	3.2	23.7	48.3	75.0	95.3	97.3	99.3

TABLE: Coverage table for the standard SA+AA box+cluster sampler with Geneva isochrones.

SUMMARY

- ▶ Use a flexible hierarchical Bayesian model to make inference about properties of stellar clusters
- ▶ The complex 'black-box' nature of the lookup table presents computation challenges
- ▶ By interweaving two complementary parametrizations we can gain relative to each individual scheme
- ▶ Distinction between inferential and computational parametrizations
- ▶ Combination of several heavy-hitting MCMC techniques allows us to effectively sample from the posterior for wide range of lookup tables

REFERENCES

Acknowledgments

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3. Baines, P.D., Meng, X.-L., Zezas, A., Kashyap, V.K., Lee, H. (2009) Bayesian Analysis of Color-Magnitude Diagrams (in progress)
4. Yu, Y., Meng, X.-L. (2009) To Center or Not To Center: That Is Not The Question, (in progress)