## **Hierarchical Bayesian modeling**

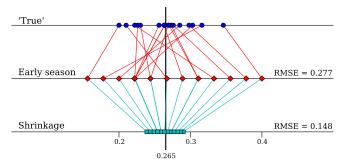
Tom Loredo Cornell Center for Astrophysics and Planetary Science http://www.astro.cornell.edu/staff/loredo/bayes/

SAMSI ASTRO — 19 Oct 2016

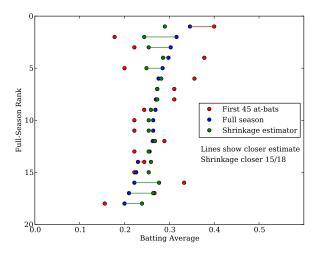
## 1970 baseball averages

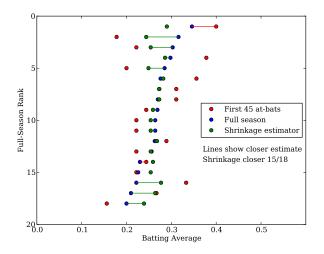
Efron & Morris looked at batting averages of baseball players who had N = 45 at-bats in May 1970 — 'large' N & includes Roberto Clemente (outlier!)

Red = n/N maximum likelihood estimates of true averages Blue = Remainder of season,  $N_{\rm rmdr} \approx 9N$ 



Cyan = James-Stein estimator: nonlinear, correlated, biased But *better*!





Theorem (independent Gaussian setting): In dimension  $\gtrsim$ 3, shrinkage estimators always beat independent MLEs in terms of expected RMS error

"The single most striking result of post-World War II statistical theory" — Brad Efron All 18 players are *humans playing baseball*—they are members of a population, not arbitrary, unrelated binomial random number generators!

In the absence of data about player *i*, we may use the performance of the other players to guide a guess about that player's performance—they provide *indirect evidence* (Efron) about player *i* 

But information that is relevant in the absence of data for i remains relevant when we additionally obtain that data; shrinkage estimators account for this

There is "mustering and *borrowing of strength*" (Tukey) across the population

*Hierarchical Bayesian modeling* is the most flexible framework for generalizing this lesson; *empirical Bayes* is an approximate version with a straightforward frequentist interpretation

## Agenda

#### **1** Basic Bayes recap

#### **2** Key idea in a nutshell

#### **3** Going deeper

Joint distributions and DAGs Conditional dependence/indepence Example: Binomial prediction Beta-binomial model Point estimation and shrinkage Gamma-Poisson model & Stan Algorithms

# Bayesian inference in one slide

Probability as generalized logic

Probability quantifies the *strength of arguments* 

To appraise hypotheses, calculate probabilities for arguments from data and modeling assumptions to each hypothesis

Use all of probability theory for this

Bayes's theorem

 $p(\text{Hypothesis} \mid \text{Data}) \propto p(\text{Hypothesis}) \times p(\text{Data} \mid \text{Hypothesis})$ 

Data *change* the support for a hypothesis  $\propto$  ability of hypothesis to *predict* the data

Law of total probability

 $p(\text{Hypothes}\underline{es} \mid \text{Data}) = \sum p(\text{Hypothes}\underline{is} \mid \text{Data})$ 

The support for a *compound/composite* hypothesis must account for all the ways it could be true

## **Bayes's theorem**

 $\mathcal{C} = \text{context}$ , initial set of premises

Consider  $P(H_i, D_{obs}|\mathcal{C})$  using the product rule:

$$P(H_i, D_{obs}|C) = P(H_i|C) P(D_{obs}|H_i, C)$$
  
=  $P(D_{obs}|C) P(H_i|D_{obs}, C)$ 

Solve for the *posterior probability* (expands the premises!):

$$P(H_i|D_{\text{obs}}, C) = P(H_i|C) \frac{P(D_{\text{obs}}|H_i, C)}{P(D_{\text{obs}}|C)}$$

Theorem holds for any propositions, but for hypotheses & data the factors have names:

posterior  $\propto$  prior  $\times$  likelihood norm. const.  $P(D_{obs}|\mathcal{C}) =$  prior predictive

## Law of Total Probability (LTP)

Consider exclusive, exhaustive  $\{B_i\}$  (C asserts one of them must be true),

$$\sum_{i} P(A, B_{i}|C) = \sum_{i} P(B_{i}|A, C)P(A|C) = P(A|C)$$
$$= \sum_{i} P(B_{i}|C)P(A|B_{i}, C)$$

If we do not see how to get  $P(A|\mathcal{P})$  directly, we can find a set  $\{B_i\}$  and use it as a "basis"—*extend the conversation*:

$$P(A|\mathcal{C}) = \sum_{i} P(B_i|\mathcal{C})P(A|B_i,\mathcal{C})$$

If our problem already has  $B_i$  in it, we can use LTP to get P(A|C) from the joint probabilities—*marginalization*:

$$P(A|C) = \sum_{i} P(A, B_i|C)$$

Example: Take  $A = D_{obs}$ ,  $B_i = H_i$ ; then  $P(D_{obs}|C) = \sum_i P(D_{obs}, H_i|C)$   $= \sum_i P(H_i|C)P(D_{obs}|H_i, C)$ 

> prior predictive for  $D_{obs}$  = Average likelihood for  $H_i$ (a.k.a. marginal likelihood)

#### **Parameter Estimation**

#### Problem statement

C = Model M with parameters  $\theta$  (+ any add'l info)

 $H_i$  = statements about  $\theta$ ; e.g. " $\theta \in [2.5, 3.5]$ ," or " $\theta > 0$ "

Probability for any such statement can be found using a probability density function (PDF) for  $\theta$ :

$$egin{aligned} & \mathcal{P}( heta \in [ heta, heta + d heta]| \cdots) &= f( heta) d heta \ &= p( heta| \cdots) d heta \end{aligned}$$

Posterior probability density

$$p(\theta|D,M) = \frac{p(\theta|M) \mathcal{L}(\theta)}{\int d\theta \ p(\theta|M) \mathcal{L}(\theta)}$$

#### Summaries of posterior

- "Best fit" values:
  - Mode,  $\hat{\theta}$ , maximizes  $p(\theta|D, M)$
  - Posterior mean,  $\langle \theta \rangle = \int d\theta \, \theta \, p(\theta | D, M)$
- Uncertainties:
  - Credible region Δ of probability C:
     C = P(θ ∈ Δ|D, M) = ∫<sub>Δ</sub> dθ p(θ|D, M)
     Highest Posterior Density (HPD) region has p(θ|D, M) higher inside than outside

Posterior standard deviation, variance, covariances

- Marginal distributions
  - Interesting parameters  $\phi$ , nuisance parameters  $\eta$
  - Marginal dist'n for  $\phi$ :  $p(\phi|D, M) = \int d\eta \, p(\phi, \eta|D, M)$

## Many Roles for Marginalization

Eliminate nuisance parameters

$$p(\phi|D,M) = \int d\eta \ p(\phi,\eta|D,M)$$

#### Propagate uncertainty

Model has parameters  $\theta$ ; what can we infer about  $F = f(\theta)$ ?

$$p(F|D, M) = \int d\theta \ p(F, \theta|D, M) = \int d\theta \ p(\theta|D, M) \ p(F|\theta, M)$$
$$= \int d\theta \ p(\theta|D, M) \ \delta[F - f(\theta)] \qquad [single-valued case]$$

#### Prediction

Given a model with parameters  $\theta$  and present data D, predict future data D' (e.g., for *experimental design*):

$$p(D'|D,M) = \int d\theta \ p(D',\theta|D,M) = \int d\theta \ p(\theta|D,M) \ p(D'|\theta,M)$$

#### Model comparison

Marginal likelihood for model  $M_i$ :

$$Z_i \equiv p(D|M_i) = \int d heta_i \ p( heta_i|M) \ \mathcal{L}_i( heta_i)$$

Bayes factor  $B_{ij} \equiv Z_i/Z_j$ Can write  $Z_i = \mathcal{L}_i(\hat{\theta}_i) \cdot \Omega_i$  with Ockham factor  $\Omega_i \approx \delta \theta / \Delta \theta = (\text{posterior volume})/(\text{prior volume})$ 

#### Hierarchical modeling, aka...

- Graphical models Hierarchical and other structures
- Multilevel models In regression, linear model settings
- Bayesian networks (Bayes nets) In AI/ML settings

## Agenda

#### **1** Basic Bayes recap

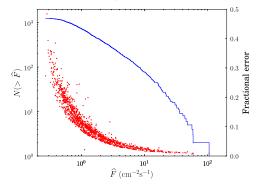
#### **2** Key idea in a nutshell

#### **3** Going deeper

Joint distributions and DAGs Conditional dependence/indepence Example: Binomial prediction Beta-binomial model Point estimation and shrinkage Gamma-Poisson model & Stan Algorithms

## Motivation: Measurement error in surveys

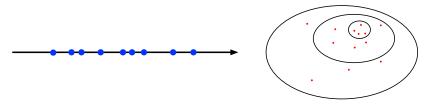
BATSE GRB peak flux estimates



- Selection effects (truncation, censoring) obvious (usually) Typically treated by "correcting" data Most sophisticated: product-limit estimators
- "Scatter" effects (measurement error, etc.) insidious Typically ignored (average out??? — No!)

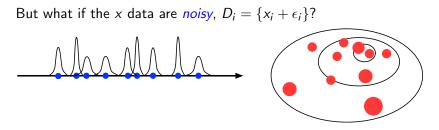
## **Accounting For Measurement Error**

Suppose  $f(x|\theta)$  is a distribution for an observable, x (scalar or vector,  $\vec{x} = (x, y, ...)$ ); and  $\theta$  is unknown



From N precisely measured samples,  $\{x_i\}$ , we can infer  $\theta$  from

$$\mathcal{L}(\theta) \equiv p(\{x_i\}|\theta) = \prod_i f(x_i|\theta)$$
$$p(\theta|\{x_i\}) \propto p(\theta)\mathcal{L}(\theta) = p(\theta, \{x_i\})$$



 $\{x_i\}$  are now uncertain (latent/hidden/incidental) parameters We should somehow incorporate  $\ell_i(x_i) = p(D_i|x_i)$ 

The joint PDF for everything is  $p(\theta, \{x_i\}, \{D_i\}) = p(\theta) p(\{x_i\}|\theta) p(\{D_i\}|\{x_i\})$   $= p(\theta) \prod_i f(x_i|\theta) \ell_i(x_i)$ 

The conditional (posterior) PDF for the unknowns is

$$p(\theta, \{x_i\} | \{D_i\}) = \frac{p(\theta, \{x_i\}, \{D_i\})}{p(\{D_i\})} \propto p(\theta, \{x_i\}, \{D_i\})$$

$$p(\theta, \{x_i\}|\{D_i\}) \propto p(\theta, \{x_i\}, \{D_i\})$$
  
=  $p(\theta) \prod_i f(x_i|\theta) \ell_i(x_i)$ 

*Marginalize over*  $\{x_i\}$  to summarize inferences for  $\theta$ 

*Marginalize over*  $\theta$  to summarize inferences for  $\{x_i\}$ 

Key point: Maximizing over  $x_i$  (i.e., just using best-fit  $\hat{x}_i$ ) and integrating over  $x_i$  can give very different results!

(See Loredo (2004) for tutorial examples)

To estimate  $x_1$ :

$$p(x_1|\{x_2,\ldots\}) = \int d\theta \ p(\theta) \ f(x_1|\theta) \ \ell_1(x_1) \times \prod_{i=2}^N \int dx_i \ f(x_i|\theta) \ \ell_i(x_i)$$
$$= \ell_1(x_1) \int d\theta \ p(\theta) \ f(x_1|\theta) \mathcal{L}_{m,\check{1}}(\theta)$$
$$\approx \ell_1(x_1) f(x_1|\hat{\theta}_{\check{1}})$$

with  $\hat{\theta}_{\check{1}}$  determined by the remaining data

 $f(x_1|\hat{\theta}_1)$  behaves like a "prior" that shifts the  $x_1$  estimate away from the peak of  $\ell_1(x_1)$ ; each member's prior depends on all of the rest of the data  $\rightarrow$  shrinkage

[*For astronomers*: This generalizes the corrections derived by Eddington, Malmquist and Lutz-Kelker (sans selection effects)]

## Agenda

#### **1** Basic Bayes recap

**②** Key idea in a nutshell

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## Joint and conditional distributions

Bayesian inference is largely about the interplay between *joint* and *conditional* distributions for related quantities

Ex: Bayes's theorem relating hypotheses and data (||C):

$$P(H_i|D) = \frac{P(H_i)P(D|H_i)}{P(D)} = \frac{P(H_i, D)}{P(D)} = \frac{\text{joint for everything}}{\text{marginal for knowns}}$$

The usual form identifies an available factorization of the joint

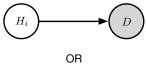
Express this via a *directed acyclic graph* (DAG):



## Joint distribution structure as a graph

- Graph = *nodes/vertices* connected by *edges/links*
- Circular/square nodes/vertices = a priori uncertain quantities (gray/square = becomes known as data)
- Directed edges specify conditional dependence
- Absence of an edge indicates conditional *in*dependence

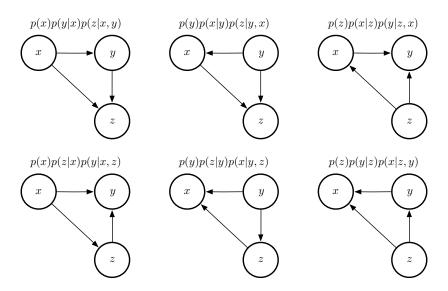
   *the most important edges are the missing ones*



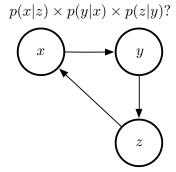


 $P(H_i, D) = P(H_i) \times P(D|H_i)$ 

#### p(x, y, z)



## Cycles not allowed

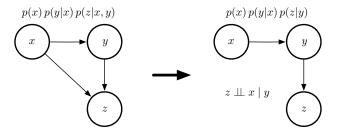


## **Conditional independence**

Suppose for the problem at hand z is independent of of x when y is known:

p(z|x,y) = p(z|y)

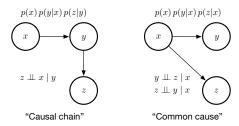
"z is conditionally independent of x, given y":  $z \perp x \mid y$ 



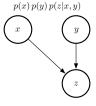
Absence of an edge indicates conditional *in*dependence Missing edges indicate simplification in structure  $\rightarrow$  *the most important edges are the missing ones* 

# DAGs with missing edges

#### **Conditional independence**



#### **Conditional dependence**



"Common effects"

## Conditional vs. complete independence

"z is conditionally independent of x, given y"  $\neq$ "z is independent of x"

(Complete) independence between z and x ("z  $\perp \perp$  x") would imply:

p(z|x) = p(z) (i.e., not a function of x)

Conditional independence given y ("z  $\perp \!\!\!\perp x \mid y$ ") is weaker:

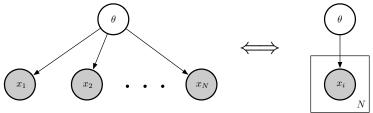
$$p(z|x) = \int dy \ p(z, y|x)$$
  
=  $\int dy \ p(y|x)p(z|x, y)$   
=  $\int dy \ p(y|x)p(z|y)$  since  $z \perp x \mid y$ 

Although x drops out of the last factor, x dependence remains in p(y|x)

x does provide information about z, but it only does so through the information it provides about y (which directly influences z)

#### Bayes's theorem with IID samples

For model with parameters  $\theta$  predicting data  $D = \{x_i\}$  that are IID given  $\theta$ :



$$p(\theta, D) = p(\theta)p(\{x_i\}|\theta) = p(\theta)\prod_{i=1}^{N} p(x_i|\theta)$$

To find the posterior for the unknowns ( $\theta$ ), divide the joint by the marginal for the knowns ({ $x_i$ }):

$$p(\theta|\{x_i\}) = \frac{p(\theta) \prod_{i=1}^{N} p(x_i|\theta)}{p(\{x_i\})} \quad \text{with} \quad p(\{x_i\}) = \int d\theta \, p(\theta) \prod_{i=1}^{N} p(x_i|\theta)$$

## **Binomial counts**







 $\bullet$   $\bullet$   $n_1$  heads in N flips



 $n_2$  heads in N flips

Suppose we know  $n_1$  and want to predict  $n_2$ 

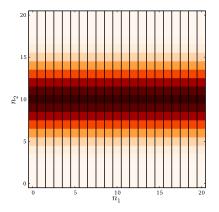
#### **Predicting binomial counts** — known $\alpha$

Success probability 
$$\alpha \to p(n|\alpha) = \frac{N!}{n!(N-n)!} \alpha^n (1-\alpha)^{N-n} \qquad || N$$

Consider two successive runs of N = 20 trials, known  $\alpha = 0.5$ 

$$p(n_2|n_1, \alpha) = p(n_2|\alpha) \qquad || N$$

 $n_1$  and  $n_2$  are conditionally independent



DAG for binomial prediction — known 
$$\alpha$$
  
 $a$   
 $p(\alpha, n_1, n_2) = p(\alpha)p(n_1|\alpha)p(n_2|\alpha)$   
 $p(n_2|\alpha, n_1) = \frac{p(\alpha, n_1, n_2)}{p(\alpha, n_1)}$   
 $= \frac{p(\alpha)p(n_1|\alpha)p(n_2|\alpha)}{p(\alpha)p(n_1|\alpha)\sum_{n_2}p(n_2|\alpha)}$   
 $= p(n_2|\alpha)$ 

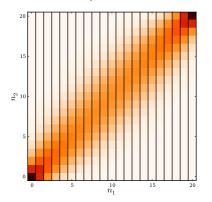
Knowing  $\alpha$  lets you predict each  $n_i$ , independently

#### **Predicting binomial counts** — uncertain $\alpha$

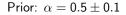
Consider the same setting, but with  $\alpha$  uncertain

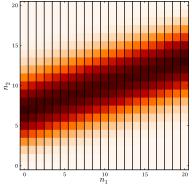
Outcomes are *physically* independent, but  $n_1$  tells us about  $\alpha \rightarrow$  outcomes are *marginally dependent* (see Lec 12 for calculation):

$$p(n_2|n_1,N) = \int d\alpha \ p(\alpha,n_2|n_1,N) = \int d\alpha \ p(\alpha|n_1,N) \ p(n_2|\alpha,N)$$

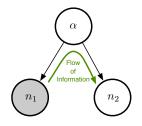


Flat prior on  $\alpha$ 





## DAG for binomial prediction



$$p(\alpha, n_1, n_2) = p(\alpha)p(n_1|\alpha)p(n_2|\alpha)$$

From joint to conditionals:

$$p(\alpha|n_1, n_2) = \frac{p(\alpha, n_1, n_2)}{p(n_1, n_2)} = \frac{p(\alpha)p(n_1|\alpha)p(n_2|\alpha)}{\int d\alpha \ p(\alpha)p(n_1|\alpha)p(n_2|\alpha)}$$
$$p(n_2|n_1) = \frac{\int d\alpha \ p(\alpha, n_1, n_2)}{p(n_1)}$$

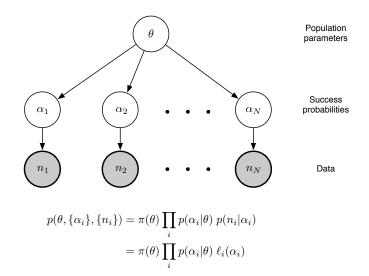
Observing  $n_1$  lets you learn about  $\alpha$ Knowledge of  $\alpha$  affects predictions for  $n_2 \rightarrow$  dependence on  $n_1$ 

# A population of coins/flippers



Each flipper+coin flips different number of times

- What do we learn about the *population* of coins—the distribution of *α*s?
- How does population membership effect inference for a single coin's  $\alpha$ ?

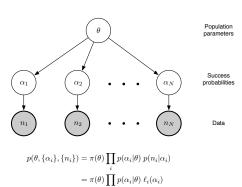


Terminology:  $\theta$  are hyperparameters,  $\pi(\theta)$  is the hyperprior

# A simple multilevel model: beta-binomial

Goals:

- Learn a population-level "prior" by pooling data
- Account for population membership in member inferences



Qualitative

$$\theta = (a, b) \text{ or } (\mu, \sigma)$$

Quantitative

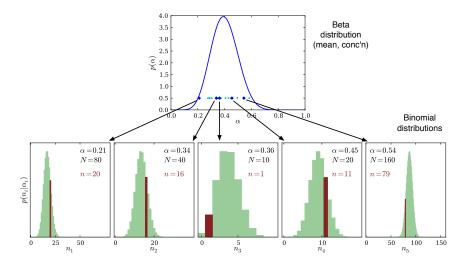
$$\pi(\theta) = \operatorname{Flat}(\mu, \sigma)$$

$$p(\alpha_i|\theta) = \text{Beta}(\alpha_i|\theta)$$

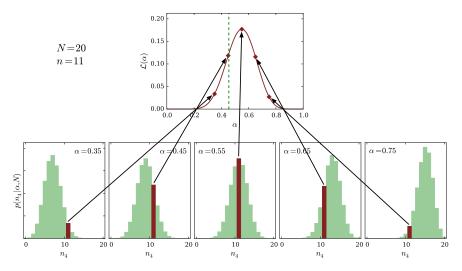
$$p(n_i | \alpha_i) = \binom{N_i}{n_i} \alpha_i^{n_i} (1 - \alpha_i)^{N_i - n_i}$$

36 / 51

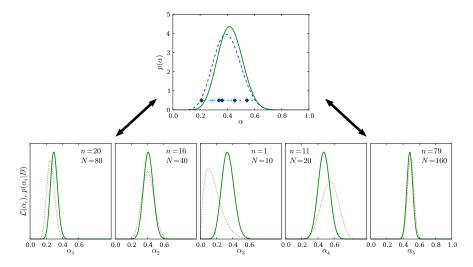
#### Generating the population & data



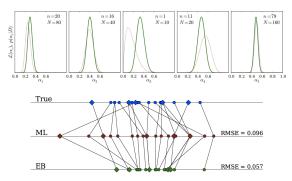
### Likelihood function for one member's $\boldsymbol{\alpha}$



### Learning the population distribution



#### Lower level estimates



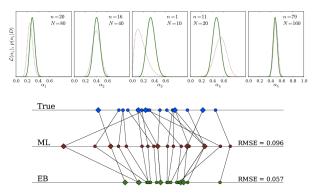
#### Two approaches

• Hierarchical Bayes (HB): Calculate marginals

$$p(\alpha_j|\{n_i\}) \propto \int d heta \, \pi( heta) \prod_{i \neq j} \int dlpha_i \, p(lpha_i| heta) \, p(n_i|lpha_i)$$

Empirical Bayes (EB): Plug in an optimum θ̂ and estimate {α<sub>i</sub>}
 View as approximation to HB, or a frequentist procedure that estimates a prior from the data

#### Lower level estimates



### Bayesian outlook

- Marginal posteriors are narrower than likelihoods
- Point estimates tend to be closer to true values than MLEs (averaged across the population)
- Joint distribution for  $\{\alpha_i\}$  is *dependent*

### Frequentist outlook

- Point estimates are biased
- Reduced variance  $\rightarrow$  estimates are closer to truth on average (lower MSE in repeated sampling)
- Bias for one member estimate depends on data for all other members

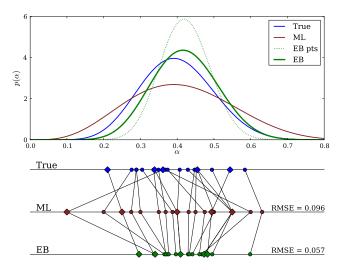
### Lingo

- Estimates *shrink* toward prior/population mean
- Estimates "muster and *borrow strength*" across population (Tukey's phrase); increases accuracy and precision of estimates
- Efron\* describes shrinkage as a consequence of accounting for *indirect evidence*

\*Bradley Efron (2010): "The Future of Indirect Evidence"

# Beware of point estimates!

Population and member estimates



## Competing data analysis goals

"Shrunken" member estimates provide improved & reliable estimate for population member properties

But they are *under-dispersed* in comparison to the true values  $\rightarrow$  not optimal for estimating *population* properties<sup>\*</sup>

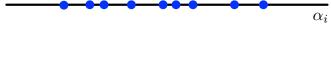
No point estimates of member properties are good for all tasks!

We should view population data tables/catalogs as providing descriptions of member likelihood functions, not "estimates with errors"

\*Louis (1984); Eddington noted this in 1940!

## Measurement error perspective

If the data provided *precise*  $\{\alpha_i\}$  values (coin measurements, flip physics), we could easily model them as points drawn from a (beta) population PDF with params  $\theta$ :

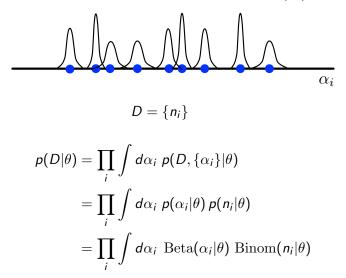


 $D = \{\alpha_i\}$ 

$$egin{aligned} p(D| heta) &= \prod_i p(lpha_i| heta) \ &= \prod_i ext{Beta}(lpha_i| heta) \end{aligned}$$

(A binomial point process)

Here the finite number of flips provide *noisy measurements of each*  $\alpha_i$ , described by the member likelihood functions  $\ell_i(\alpha_i)$ ;



This is a prototype for *measurement error problems* 

# Another conjugate MLM: Gamma-Poisson

Goal: Learn a rate dist'n from count data (E.g., learn a star or galaxy brightness dist'n from photon counts)

Population

parameters

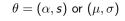
Qualitative

θ

 $F_1$ 

 $n_1$ 

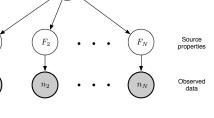
### Quantitative



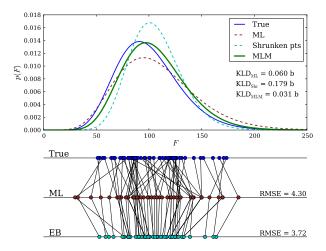
$$\pi(\theta) = \operatorname{Flat}(\mu, \sigma)$$

 $p(F_i|\theta) = \text{Gamma}(F_i|\theta)$ 

$$p(n_i|F_i) = \operatorname{Pois}(n_i|\epsilon_iF_i)$$



#### Gamma-Poisson population and member estimates



Simulations: N = 60 sources from gamma with  $\langle F \rangle = 100$  and  $\sigma_F = 30$ ; exposures spanning dynamic range of  $\times 16$ 

# Algorithms

Consider the posterior PDF for  $\theta$  and  $\{\alpha_i\}$  in the beta-binomial MLM:

$$p( heta, \{lpha_i\}|\{n_i\}) \propto \pi( heta) \prod_{i=1}^{N_{ ext{mem}}} ext{Beta}(lpha_i| heta) ext{ Binom}(n_i|lpha_i)$$

For each member, the Beta × Binom factor is  $\propto$  a beta distribution for  $\alpha_i$ ; but as a function of  $\theta$  (e.g., (a, b) or  $(\mu, \sigma)$ ) it is not simple

The full posterior has a product of  $N_{\rm mem}$  such factors specifying its  $\theta$  dependences  $\Rightarrow$  even for a conjugate model for the lower levels, the overall model is typically analytically intractable

Two approaches exploit *conditional independence of lower-level parameters* 

### Member marginalization

- Analytically or numerically integrate over {x<sub>i</sub>} → explore the reduced-dimension marginal for θ via MCMC
   → {θ<sub>i</sub>} ~ p(θ|D)
- If x<sub>i</sub> are of interest, sample them from their conditionals, conditioned on θ<sub>i</sub>:
  - $\blacktriangleright \text{ Pick a } \theta \text{ from } \{\theta_i\}$
  - Draw {x<sub>i</sub>} by independent sampling from their conditionals (give θ)
  - Iterate

GPUs can accelerate this for application to large datasets

Only useful for low-dimensional latent parameters  $x_i$ 

### Metropolis-within-Gibbs algorithm

Block the full parameter space:

- Block of m population parameters,  $\theta$
- N blocks of lower level (latent) parameters, x<sub>i</sub>

Get posterior samples by iterating back and forth between:

- *m*-D Metropolis-Hastings sampling of θ from p(θ|{x<sub>i</sub>}, D)
   This requires a problem-specific proposal distribution
- *N* independent samples of x<sub>i</sub> from the conditional p(x<sub>i</sub>|θ, D<sub>i</sub>)

This can often exploit conjugate structure

E.g., Beta-binomial:  $\alpha_i \sim \text{Beta}(\alpha_i | \theta) \text{ Binom}(n_i | \alpha_i)$ , which is just a Beta for  $\alpha_i$ 

MWG explicitly displays the feedback between population and member inference