

Introduction to Bayesian inference

Lecture 2: Key examples

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Lecture 2: Key examples

① Simple examples

Normal Distribution

Poisson Distribution

② Multilevel models for measurement error

③ Bayesian computation

Key examples

① Simple examples

Normal Distribution

Poisson Distribution

② Multilevel models for measurement error

③ Bayesian computation

Supplement

- Binary classification with binary data
- Bernoulli, binomial, negative binomial distributions
- Parameter estimation & model comparison
- Likelihood principle
- Relationships between probability & frequency

Inference With Normals/Gaussians

Gaussian PDF

$$p(x|\mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad \text{over } [-\infty, \infty]$$

Common abbreviated notation: $x \sim N(\mu, \sigma^2)$

Parameters

$$\mu = \langle x \rangle \equiv \int dx \, x p(x|\mu, \sigma)$$

$$\sigma^2 = \langle (x - \mu)^2 \rangle \equiv \int dx \, (x - \mu)^2 p(x|\mu, \sigma)$$

Gauss's Observation: Sufficiency

Suppose our data consist of N measurements, $d_i = \mu + \epsilon_i$.
Suppose the noise contributions are independent, and
 $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$.

$$\begin{aligned} p(D|\mu, \sigma, M) &= \prod_i p(d_i|\mu, \sigma, M) \\ &= \prod_i p(\epsilon_i = d_i - \mu|\mu, \sigma, M) \\ &= \prod_i \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(d_i - \mu)^2}{2\sigma^2}\right] \\ &= \frac{1}{\sigma^N(2\pi)^{N/2}} e^{-Q(\mu)/2\sigma^2} \end{aligned}$$

Find dependence of Q on μ by completing the square:

$$\begin{aligned} Q &= \sum_i (d_i - \mu)^2 && \text{[Note: } Q/\sigma^2 = \chi^2(\mu)\text{]} \\ &= \sum_i d_i^2 + \sum_i \mu^2 - 2 \sum_i d_i \mu \\ &= \left(\sum_i d_i^2 \right) + N\mu^2 - 2N\mu\bar{d} && \text{where } \bar{d} \equiv \frac{1}{N} \sum_i d_i \\ &= N(\mu - \bar{d})^2 + \left(\sum_i d_i^2 \right) - N\bar{d}^2 \\ &= N(\mu - \bar{d})^2 + Nr^2 && \text{where } r^2 \equiv \frac{1}{N} \sum_i (d_i - \bar{d})^2 \end{aligned}$$

Likelihood depends on $\{d_i\}$ **only through \bar{d} and r** :

$$\mathcal{L}(\mu, \sigma) = \frac{1}{\sigma^N (2\pi)^{N/2}} \exp\left(-\frac{Nr^2}{2\sigma^2}\right) \exp\left(-\frac{N(\mu - \bar{d})^2}{2\sigma^2}\right)$$

The sample mean and variance are *sufficient statistics*.

This is a miraculous compression of information—the normal dist'n is highly *abnormal* in this respect!

Estimating a Normal Mean

Problem specification

Model: $d_i = \mu + \epsilon_i$, $\epsilon_i \sim N(0, \sigma^2)$, σ is known $\rightarrow I = (\sigma, M)$.

Parameter space: μ ; seek $p(\mu|D, \sigma, M)$

Likelihood

$$\begin{aligned} p(D|\mu, \sigma, M) &= \frac{1}{\sigma^N (2\pi)^{N/2}} \exp\left(-\frac{Nr^2}{2\sigma^2}\right) \exp\left(-\frac{N(\mu - \bar{d})^2}{2\sigma^2}\right) \\ &\propto \exp\left(-\frac{N(\mu - \bar{d})^2}{2\sigma^2}\right) \end{aligned}$$

“Uninformative” prior

Translation invariance $\Rightarrow p(\mu) \propto C$, a constant.

This prior is *improper* unless bounded.

Prior predictive/normalization

$$\begin{aligned} p(D|\sigma, M) &= \int d\mu C \exp\left(-\frac{N(\mu - \bar{d})^2}{2\sigma^2}\right) \\ &= C(\sigma/\sqrt{N})\sqrt{2\pi} \end{aligned}$$

... minus a tiny bit from tails, using a proper prior.

Posterior

$$p(\mu|D, \sigma, M) = \frac{1}{(\sigma/\sqrt{N})\sqrt{2\pi}} \exp\left(-\frac{N(\mu - \bar{d})^2}{2\sigma^2}\right)$$

Posterior is $N(\bar{d}, w^2)$, with standard deviation $w = \sigma/\sqrt{N}$.

68.3% HPD credible region for μ is $\bar{d} \pm \sigma/\sqrt{N}$.

Note that C drops out \rightarrow limit of infinite prior range is well behaved.

Informative Conjugate Prior

Use a normal prior, $\mu \sim N(\mu_0, w_0^2)$.

Conjugate because the posterior turns out also to be normal.

Posterior

Normal $N(\tilde{\mu}, \tilde{w}^2)$, but mean, std. deviation “*shrink*” towards prior.

Define $B = \frac{w^2}{w^2 + w_0^2}$, so $B < 1$ and $B = 0$ when w_0 is large.

Then

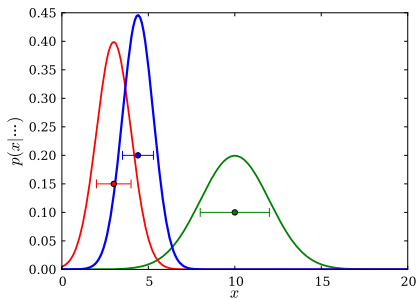
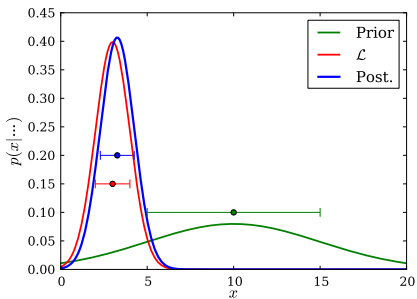
$$\tilde{\mu} = \bar{d} + B \cdot (\mu_0 - \bar{d})$$

$$\tilde{w} = w \cdot \sqrt{1 - B}$$

“*Principle of stable estimation*” — The prior affects estimates only when data are not informative relative to prior.

Conjugate normal examples:

- Data have $\bar{d} = 3$, $\sigma/\sqrt{N} = 1$
- Priors at $\mu_0 = 10$, with $w = \{5, 2\}$



Estimating a Normal Mean: Unknown σ

Supplement: Marginalize over $\sigma \rightarrow$ Student's t distribution

Gaussian Background Subtraction

Measure background rate $b = \hat{b} \pm \sigma_b$ with source off.

Measure total rate $r = \hat{r} \pm \sigma_r$ with source on.

Infer signal source strength s , where $r = s + b$.

With flat priors,

$$p(s, b|D, M) \propto \exp\left[-\frac{(b - \hat{b})^2}{2\sigma_b^2}\right] \times \exp\left[-\frac{(s + b - \hat{r})^2}{2\sigma_r^2}\right]$$

Marginalize b to summarize the results for s (complete the square to isolate b dependence; then do a simple Gaussian integral over b):

$$p(s|D, M) \propto \exp \left[-\frac{(s - \hat{s})^2}{2\sigma_s^2} \right] \quad \begin{aligned} \hat{s} &= \hat{r} - \hat{b} \\ \sigma_s^2 &= \sigma_r^2 + \sigma_b^2 \end{aligned}$$

\Rightarrow Background *subtraction* is a special case of background *marginalization*; i.e., marginalization “told us” to subtract a background estimate.

Recall the standard derivation of background uncertainty via “propagation of errors” based on Taylor expansion (statistician’s *Delta-method*).

Marginalization provides a generalization of error propagation—without approximation!

Supplement: Handling σ uncertainty by marginalizing over σ ;
Student's t distribution

Bayesian Curve Fitting & Least Squares

Setup

Data $D = \{d_i\}$ are measurements of an underlying function $f(x; \theta)$ at N sample points $\{x_i\}$. Let $f_i(\theta) \equiv f(x_i; \theta)$:

$$d_i = f_i(\theta) + \epsilon_i, \quad \epsilon_i \sim N(0, \sigma_i^2)$$

We seek learn θ , or to compare different functional forms (model choice, M).

Likelihood

$$\begin{aligned} p(D|\theta, M) &= \prod_{i=1}^N \frac{1}{\sigma_i \sqrt{2\pi}} \exp \left[-\frac{1}{2} \left(\frac{d_i - f_i(\theta)}{\sigma_i} \right)^2 \right] \\ &\propto \exp \left[-\frac{1}{2} \sum_i \left(\frac{d_i - f_i(\theta)}{\sigma_i} \right)^2 \right] \\ &= \exp \left[-\frac{\chi^2(\theta)}{2} \right] \end{aligned}$$

Bayesian Curve Fitting & Least Squares

Posterior

For prior density $\pi(\theta)$,

$$p(\theta|D, M) \propto \pi(\theta) \exp \left[-\frac{\chi^2(\theta)}{2} \right]$$

If you have a least-squares or χ^2 code:

- Think of $\chi^2(\theta)$ as $-2 \log \mathcal{L}(\theta)$.
- Bayesian inference amounts to exploration and numerical integration of $\pi(\theta)e^{-\chi^2(\theta)/2}$.

Important Case: Separable Nonlinear Models

A (linearly) separable model has parameters $\theta = (A, \psi)$:

- Linear amplitudes $A = \{A_\alpha\}$
- Nonlinear parameters ψ

$f(x; \theta)$ is a linear superposition of M nonlinear components $g_\alpha(x; \psi)$:

$$d_i = \sum_{\alpha=1}^M A_\alpha g_\alpha(x_i; \psi) + \epsilon_i$$

or

$$\vec{d} = \sum_{\alpha} A_\alpha \vec{g}_\alpha(\psi) + \vec{\epsilon}.$$

Why this is important: You can marginalize over A *analytically*
→ *Bretthorst algorithm* (“Bayesian Spectrum Analysis & Param. Est’n” 1988)

Algorithm is closely related to linear least squares, diagonalization, SVD; for sinusoidal g_α , generalizes periodograms.

Poisson Dist'n: Infer a Rate from Counts

Problem:

Observe n counts in T ; infer rate, r

Likelihood

$$\mathcal{L}(r) \equiv p(n|r, M) = p(n|r, M) = \frac{(rT)^n}{n!} e^{-rT}$$

Prior

Two simple standard choices (or conjugate gamma dist'n):

- r known to be nonzero; it is a scale parameter:

$$p(r|M) = \frac{1}{\ln(r_u/r_l)} \frac{1}{r}$$

- r may vanish; require $p(n|M) \sim \text{Const}$:

$$p(r|M) = \frac{1}{r_u}$$

Prior predictive

$$\begin{aligned} p(n|M) &= \frac{1}{r_u} \frac{1}{n!} \int_0^{r_u} dr (rT)^n e^{-rT} \\ &= \frac{1}{r_u T} \frac{1}{n!} \int_0^{r_u T} d(rT) (rT)^n e^{-rT} \\ &\approx \frac{1}{r_u T} \quad \text{for } r_u \gg \frac{n}{T} \end{aligned}$$

Posterior

A gamma distribution:

$$p(r|n, M) = \frac{T(rT)^n}{n!} e^{-rT}$$

Gamma Distributions

A 2-parameter family of distributions over nonnegative x , with shape parameter α and scale parameter s :

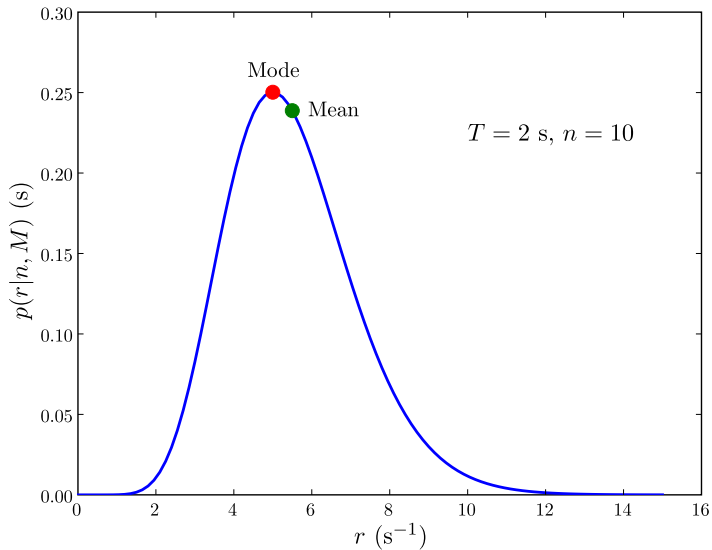
$$p_{\Gamma}(x|\alpha, s) = \frac{1}{s\Gamma(\alpha)} \left(\frac{x}{s}\right)^{\alpha-1} e^{-x/s}$$

Moments:

$$E(x) = s\alpha \quad \text{Var}(x) = s^2\alpha$$

Our posterior corresponds to $\alpha = n + 1$, $s = 1/T$.

- Mode $\hat{r} = \frac{n}{T}$; mean $\langle r \rangle = \frac{n+1}{T}$ (shift down 1 with $1/r$ prior)
- Std. dev'n $\sigma_r = \frac{\sqrt{n+1}}{T}$; credible regions found by integrating (can use incomplete gamma function)



The flat prior

Bayes's justification: *Not* that ignorance of $r \rightarrow p(r|I) = C$

Require (discrete) predictive distribution to be flat:

$$\begin{aligned} p(n|I) &= \int dr p(r|I)p(n|r, I) = C \\ &\rightarrow p(r|I) = C \end{aligned}$$

Useful conventions

- Use a flat prior for a rate that may be zero
- Use a log-flat prior ($\propto 1/r$) for a nonzero scale parameter
- Use proper (normalized, bounded) priors
- Plot posterior with abscissa that makes prior flat

The On/Off Problem

Basic problem

- Look off-source; unknown background rate b
Count N_{off} photons in interval T_{off}
- Look on-source; rate is $r = s + b$ with unknown signal s
Count N_{on} photons in interval T_{on}
- Infer s

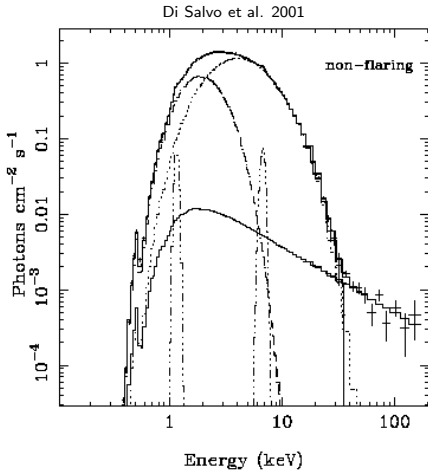
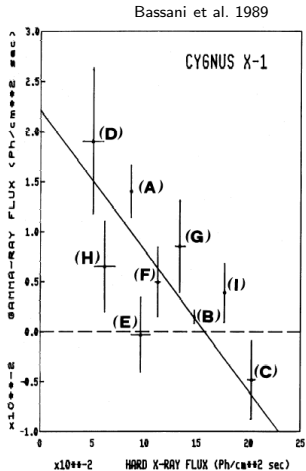
Conventional solution

$$\begin{aligned}\hat{b} &= N_{\text{off}}/T_{\text{off}}; & \sigma_b &= \sqrt{N_{\text{off}}/T_{\text{off}}} \\ \hat{r} &= N_{\text{on}}/T_{\text{on}}; & \sigma_r &= \sqrt{N_{\text{on}}/T_{\text{on}}} \\ \hat{s} &= \hat{r} - \hat{b}; & \sigma_s &= \sqrt{\sigma_r^2 + \sigma_b^2}\end{aligned}$$

But \hat{s} can be **negative!**

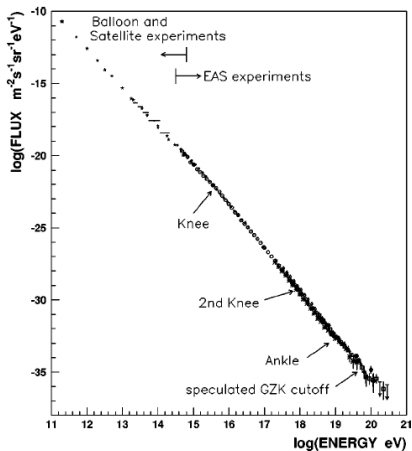
Examples

Spectra of X-Ray Sources

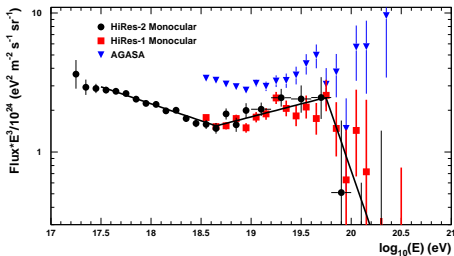


Spectrum of Ultrahigh-Energy Cosmic Rays

Nagano & Watson 2000



HiRes Team 2007



N is Never Large

Sample sizes are never large. If N is too small to get a sufficiently-precise estimate, you need to get more data (or make more assumptions). But once N is 'large enough,' you can start subdividing the data to learn more (for example, in a public opinion poll, once you have a good estimate for the entire country, you can estimate among men and women, northerners and southerners, different age groups, etc etc). N is never enough because if it were 'enough' you'd already be on to the next problem for which you need more data.

— Andrew Gelman (blog entry, 31 July 2005)

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Similarly, you never have quite enough money. But that's another story.

— Andrew Gelman (blog entry, 31 July 2005)

Bayesian Solution to On/Off Problem

First consider off-source data; use it to estimate b :

$$p(b|N_{\text{off}}, I_{\text{off}}) = \frac{T_{\text{off}}(bT_{\text{off}})^{N_{\text{off}}} e^{-bT_{\text{off}}}}{N_{\text{off}}!}$$

Use this as a prior for b to analyze on-source data. For on-source analysis $I_{\text{all}} = (I_{\text{on}}, N_{\text{off}}, I_{\text{off}})$:

$$p(s, b|N_{\text{on}}) \propto p(s)p(b)[(s+b)T_{\text{on}}]^{N_{\text{on}}} e^{-(s+b)T_{\text{on}}} \quad || \quad I_{\text{all}}$$

$p(s|I_{\text{all}})$ is flat, but $p(b|I_{\text{all}}) = p(b|N_{\text{off}}, I_{\text{off}})$, so

$$p(s, b|N_{\text{on}}, I_{\text{all}}) \propto (s+b)^{N_{\text{on}}} b^{N_{\text{off}}} e^{-sT_{\text{on}}} e^{-b(T_{\text{on}}+T_{\text{off}})}$$

Now marginalize over b ;

$$\begin{aligned} p(s|N_{\text{on}}, I_{\text{all}}) &= \int db \, p(s, b | N_{\text{on}}, I_{\text{all}}) \\ &\propto \int db \, (s + b)^{N_{\text{on}}} b^{N_{\text{off}}} e^{-sT_{\text{on}}} e^{-b(T_{\text{on}} + T_{\text{off}})} \end{aligned}$$

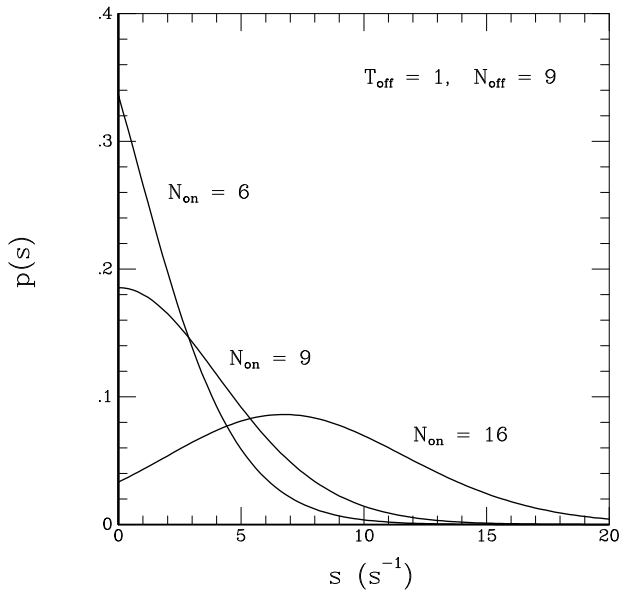
Expand $(s + b)^{N_{\text{on}}}$ and do the resulting Γ integrals:

$$\begin{aligned} p(s|N_{\text{on}}, I_{\text{all}}) &= \sum_{i=0}^{N_{\text{on}}} C_i \frac{T_{\text{on}}(sT_{\text{on}})^i e^{-sT_{\text{on}}}}{i!} \\ C_i &\propto \left(1 + \frac{T_{\text{off}}}{T_{\text{on}}}\right)^i \frac{(N_{\text{on}} + N_{\text{off}} - i)!}{(N_{\text{on}} - i)!} \end{aligned}$$

Posterior is a weighted sum of Gamma distributions, each assigning a different number of on-source counts to the source. (Evaluate via recursive algorithm or confluent hypergeometric function.)

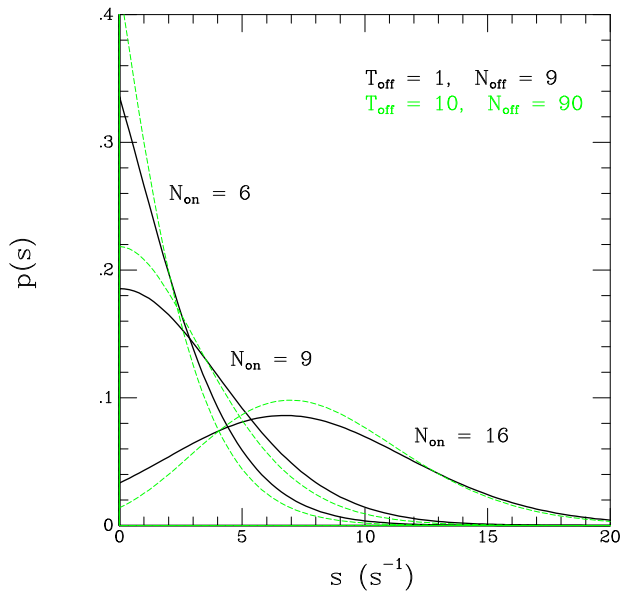
Example On/Off Posteriors—Short Integrations

$$T_{\text{on}} = 1$$



Example On/Off Posteriors—Long Background Integrations

$$T_{\text{on}} = 1$$



Supplement: Two more solutions of on/off problem (including data augmentation); multibin case

Recap of Key Ideas From Examples

- Sufficient statistic: Model-dependent summary of data
- Conjugate priors
- Marginalization: Generalizes background subtraction, propagation of errors
- Exact treatment of Poisson background uncertainty (don't subtract!)
- Likelihood principle
- Student's t for handling σ uncertainty

Key examples

① Simple examples

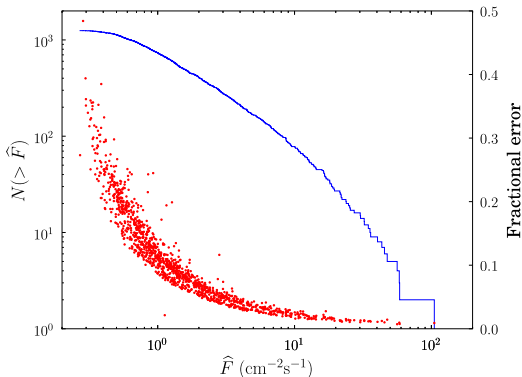
Normal Distribution

Poisson Distribution

② Multilevel models for measurement error

③ Bayesian computation

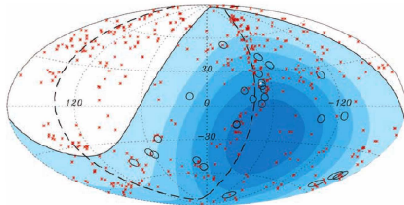
Complications With Survey Data



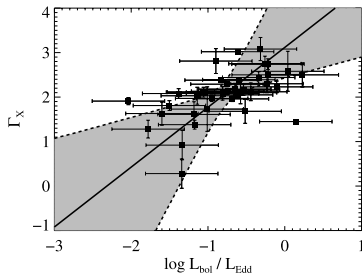
- *Selection effects* (truncation, censoring) — *obvious* (usually)
Typically treated by “correcting” data
Most sophisticated: product-limit estimators
- *“Scatter” effects* (measurement error, etc.) — *insidious*
Typically ignored (average out???)

Many Guises of Measurement Error

Auger data above GZK cutoff (PAO 2007; Soiaporn⁺ 2013)



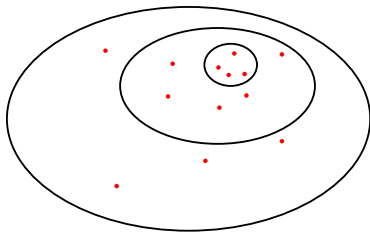
QSO hardness vs. luminosity (Kelly 2007, 2012)



Accounting For Measurement Error

Introduce latent/hidden/incidental parameters

Suppose $f(x|\theta)$ is a distribution for an observable, x .



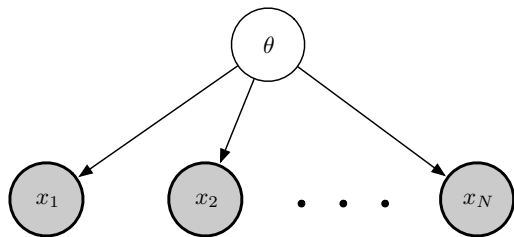
From N precisely measured samples, $\{x_i\}$, we can infer θ from

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

(A *binomial point process*)

Graphical representation

- Nodes/vertices = uncertain quantities (gray \rightarrow known)
- Edges specify conditional dependence
- Absence of an edge denotes *conditional independence*

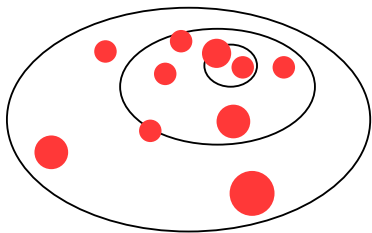


Graph specifies the form of the *joint distribution*:

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

Posterior from BT: $p(\theta|\{x_i\}) = p(\theta, \{x_i\})/p(\{x_i\})$

But what if the x data are *noisy*, $D_i = \{x_i + \epsilon_i\}$?



$\{x_i\}$ are now *uncertain (latent) parameters*

We should somehow incorporate $\ell_i(x_i) = p(D_i|x_i)$:

$$\begin{aligned} p(\theta, \{x_i\}, \{D_i\}) &= p(\theta) p(\{x_i\}|\theta) p(\{D_i\}|\{x_i\}) \\ &= p(\theta) \prod_i f(x_i|\theta) \ell_i(x_i) \end{aligned}$$

Marginalize over $\{x_i\}$ to summarize inferences for θ .

Marginalize over θ to summarize inferences for $\{x_i\}$.

Key point: *Maximizing over x_i and integrating over x_i can give very different results!*

To estimate x_1 :

$$\begin{aligned} p(x_1|\{x_2, \dots\}) &= \int d\theta p(\theta) f(x_1|\theta) l_1(x_1) \times \prod_{i=2}^N \int dx_i f(x_i|\theta) l_i(x_i) \\ &= l_1(x_1) \int d\theta p(\theta) f(x_1|\theta) \mathcal{L}_{m,\check{1}}(\theta) \\ &\approx l_1(x_1) f(x_1|\hat{\theta}) \end{aligned}$$

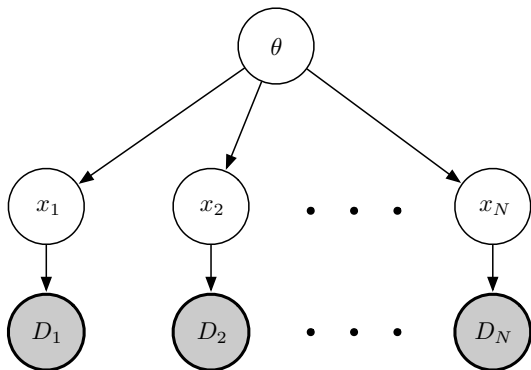
with $\hat{\theta}$ determined by the remaining data.

$f(x_1|\hat{\theta})$ behaves like a prior that shifts the x_1 estimate away from the peak of $l_1(x_i)$.

This generalizes the corrections derived by Eddington, Malmquist and Lutz-Kelker.

Landy & Szalay (1992) proposed adaptive Malmquist corrections that can be viewed as an approximation to this.

Graphical representation



$$\begin{aligned} p(\theta, \{x_i\}, \{D_i\}) &= p(\theta) p(\{x_i\}|\theta) p(\{D_i\}|\{x_i\}) \\ &= p(\theta) \prod_i f(x_i|\theta) p(D_i|x_i) = p(\theta) \prod_i f(x_i|\theta) \ell_i(x_i) \end{aligned}$$

A two-level *multi-level model* (MLM).

Bayesian MLMs in Astronomy

Surveys (number counts/“log N –log S ”/Malmquist):

- GRB peak flux dist'n (Loredo & Wasserman 1998)
- TNO/KBO magnitude distribution (Gladman⁺ 1998; Petit⁺ 2008)
- MLM tutorial; Malmquist-type biases in cosmology (*Loredo & Hendry 2009* in *BMIC* book)
- “Extreme deconvolution” for proper motion surveys (Bovy, Hogg, & Roweis 2011)

Directional & spatio-temporal coincidences:

- GRB repetition (Luo⁺ 1996; Graziani⁺ 1996)
- GRB host ID (Band 1998; Graziani⁺ 1999)
- VO cross-matching (Budavári & Szalay 2008)

Time series:

- SN 1987A neutrinos, uncertain energy vs. time (Loredo & Lamb 2002)
- Multivariate “Bayesian Blocks” (Dobigeon, Tourneret & Scargle 2007)
- SN Ia multicolor light curve modeling (Mandel⁺ 2009, 2011)

Linear & nonlinear regression with measurement error:

- QSO hardness vs. luminosity (Kelly 2007, 2012)
- Dust SEDs (Kelly⁺ 2012)

More information:

<http://astrostatistics.psu.edu/su10/surveys.html>

Overview of MLMs in astronomy: arXiv:1208.3036

In progress: GPU software (Budavari, Kelly, TJL)

Key examples

① Simple examples

Normal Distribution

Poisson Distribution

② Multilevel models for measurement error

③ Bayesian computation

Statistical Integrals

Inference with independent data

Consider N data, $D = \{x_i\}$; and model M with m parameters.

Suppose $\mathcal{L}(\theta) = p(x_1|\theta) p(x_2|\theta) \cdots p(x_N|\theta)$.

Frequentist integrals

Find long-run properties of procedures via sample space integrals:

$$\mathcal{I}(\theta) = \int dx_1 p(x_1|\theta) \int dx_2 p(x_2|\theta) \cdots \int dx_N p(x_N|\theta) f(D, \theta)$$

Rigorous analysis must explore the θ dependence; rarely done in practice.

“Plug-in” approximation: Report properties of procedure for $\theta = \hat{\theta}$. *Asymptotically* accurate (for large N , expect $\hat{\theta} \rightarrow \theta$).

“Plug-in” results are easy via Monte Carlo (due to independence).

Bayesian integrals

$$\int d^m \theta g(\theta) p(\theta|M) \mathcal{L}(\theta) = \int d^m \theta g(\theta) \overbrace{q(\theta)}^{p(\theta|M)} \mathcal{L}(\theta)$$

- $g(\theta) = 1 \rightarrow p(D|M)$ (norm. const., model likelihood)
- $g(\theta) = \text{'box'}$ \rightarrow credible region
- $g(\theta) = \theta \rightarrow$ posterior mean for θ

Such integrals are sometimes easy if analytic (especially in low dimensions), often easier than frequentist counterparts (e.g., normal credible regions, Student's t).

Asymptotic approximations: Require ingredients familiar from frequentist calculations. Bayesian calculation is *not significantly harder* than frequentist calculation in this limit.

Numerical calculation: For “large” m (> 4 is often enough!) the integrals are often very challenging because of structure (e.g., correlations) in parameter space. This is usually pursued *without making any procedural approximations*.

Bayesian Computation

Large sample size: Laplace approximation

- Approximate posterior as multivariate normal \rightarrow $\det(\text{covar})$ factors
- Uses ingredients available in χ^2 /ML fitting software (MLE, Hessian)
- Often accurate to $O(1/N)$

Modest-dimensional models ($d \lesssim 10$ to 20)

- Adaptive cubature
- Monte Carlo integration (importance & stratified sampling, adaptive importance sampling, quasirandom MC)

High-dimensional models ($d \gtrsim 5$)

- Posterior sampling — create RNG that samples posterior
- MCMC is most general framework — [Murali Haran's lab](#)



*See SCMA 5 Bayesian Computation tutorial notes,
and notes from next week's sessions,
for more on MLMs & computation!*

*See online resource list for an annotated list
of Bayesian books and software*