# Introduction to Bayesian inference for astronomy, 2

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CASt Summer School

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# Agenda

1. **Probability theory for data analysis: Two theorems**

2. **Inference with parametric models**
   - Parameter Estimation
   - Model Uncertainty (Supp.)
   - Key role of LTP/marginalization

3. **Quick-looks**
   - Curve fitting & least squares (2 slides!)
   - Bayesian computation menu (1 slide!)

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# The Bayesian inference recipe

Assess hypotheses by calculating their probabilities $p(H_i|\ldots)$ conditional on known and/or presumed information (including observed data) using the rules of probability theory.

*Probability Theory Axioms*

$\mathcal{C} \equiv$ *context*, initial set of premises

$$\text{`OR' (sum rule):} \quad P(H_1 \vee H_2|\mathcal{C}) = P(H_1|\mathcal{C}) + P(H_2|\mathcal{C}) - P(H_1, H_2|\mathcal{C})$$

$$\begin{aligned} \text{`AND' (product rule):} \quad P(H_i, D_{\rm obs}|\mathcal{C}) &= P(H_i|\mathcal{C})\, P(D_{\rm obs}|H_i, \mathcal{C}) \\ &= P(D_{\rm obs}|\mathcal{C})\, P(H_i|D_{\rm obs}, \mathcal{C}) \end{aligned}$$

$$\text{`NOT':} \quad P(\overline{H_i}|\mathcal{C}) = 1 - P(H_i|\mathcal{C})$$

# Two Important Theorems

## *Bayes's Theorem (BT)*

Consider the *joint probability* for a hypothesis and the observed data, $P(H_i, D_{obs}|\mathcal{C})$, using the product rule:

$$\begin{aligned} P(H_i, D_{obs}|\mathcal{C}) &= P(H_i|\mathcal{C})\, P(D_{obs}|H_i, \mathcal{C}) \\ &= P(D_{obs}|\mathcal{C})\, P(H_i|D_{obs}, \mathcal{C}) \end{aligned}$$

Solve for the *posterior probability* for $H_i$ (adds a premise!):

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

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

*posterior* $\propto$ *prior* $\times$ *likelihood*

(all "for $H_i$")

norm. const. $P(D_{obs}|\mathcal{C}) =$ *prior predictive* for $D_{obs}$

## *Law of Total Probability (LTP)*

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

$$\begin{aligned}\sum_i P(A, B_i|\mathcal{C}) &= \sum_i P(B_i|A, \mathcal{C}) P(A|\mathcal{C}) = P(A|\mathcal{C}) \\ &= \sum_i P(B_i|\mathcal{C}) P(A|B_i, \mathcal{C})\end{aligned}$$

If we do not see how to get $P(A|\mathcal{C})$ 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 $P(A|\mathcal{P})$ from the joint probabilities—*marginalization*:

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

Joseph Blitzstein (Harvard statistician) on LTP (paraphrased):

> In most areas of math, when you're stuck, saying, "I wish I knew this or that" doesn't help you. In probability theory, saying "I wish I knew this" suggests what to condition on; then you condition on it, compute *as if* you knew it, and then average over those possibilities.
>
> *I didn't name the law of total probability, but if I had, I would have just called it* **wishful thinking**.
>
> — YouTube lecture on conditional probability (15:48)

**LTP example 1:** Take $\mathcal{C}$ to specify fair roll of a die, $A =$ "An even number comes up," $B_i =$ "face $i$ comes up" ($i = 1$ to 6)

$$
\begin{aligned}
P(A|\mathcal{C}) &= \sum_{i=1}^{6} P(A, B_i|\mathcal{C}) \\
&= \sum_{i=1}^{6} P(B_i|\mathcal{C}) P(A|B_i, \mathcal{C}) \\
&= \frac{1}{6} \times (0 + 1 + 0 + 1 + 0 + 1) = \frac{1}{2}
\end{aligned}
$$

**LTP example 2:** With context $\mathcal{C}$, take $A = D_{\text{obs}}$, $B_i = H_i$; then

$$
\begin{aligned}
P(D_{\text{obs}}|\mathcal{C}) &= \sum_{i} P(D_{\text{obs}}, H_i|\mathcal{C}) \\
&= \sum_{i} P(H_i|\mathcal{C}) P(D_{\text{obs}}|H_i, \mathcal{C})
\end{aligned}
$$

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

# Tabular/diagrammatic Bayesian inference

Simplest case: *Binary classification*

- 2 hypotheses: $\{C, \overline{C}\}$
- 2 possible data values: $\{-, +\}$

Concrete example: You test positive ($+$) for a medical condition. Do you have the condition ($C$) or not ($\overline{C}$)?

- Prior: Prevalence of the condition in your population is 0.1%
- Likelihood:
  - Test is 80% accurate if you have the condition:
    $P(+|C, \mathcal{C}) = 0.8$ ("sensitivity")
  - Test is 95% accurate if you are healthy:
    $P(-|\overline{C}, \mathcal{C}) = 0.95$ ("specificity," $1 - p(\text{false } +)$)

*Numbers roughly correspond to mammography screening for breast cancer in asymptomatic women*

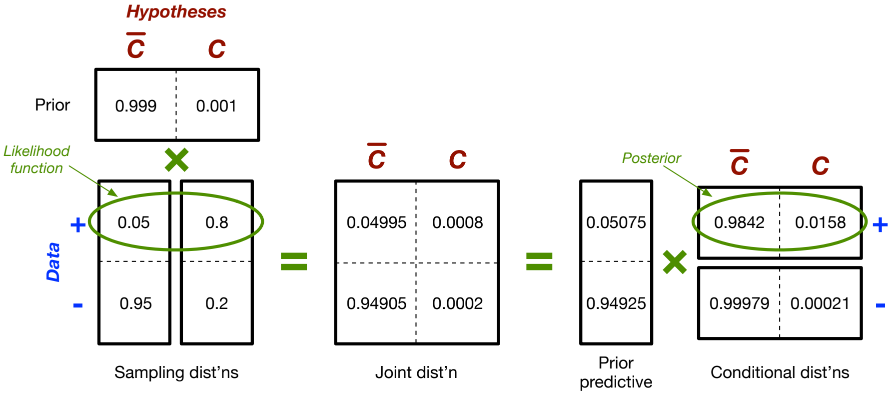
# *Tabular calculation*

| Hypothesis<br>$H_i$ | Prior<br>$\pi_i \equiv p(H_i)$ | Likelihood<br>$\mathcal{L}_i \equiv p(+\|H_i)$ | Joint<br>$\pi_i \times \mathcal{L}_i$ | Posterior<br>$p(H_i\|+)$ |
|---|---|---|---|---|
| $\overline{C}$ | 0.999 | 0.05 | 0.04995 | 0.9842 |
| $C$ | 0.001 | 0.8 | 0.0008 | 0.0158 |
| **Sums:** | 1.0 | **NA** | 0.05075<br>$= p(+)$ | 1.0 |

# *Inference as manipulation of the joint distribution*

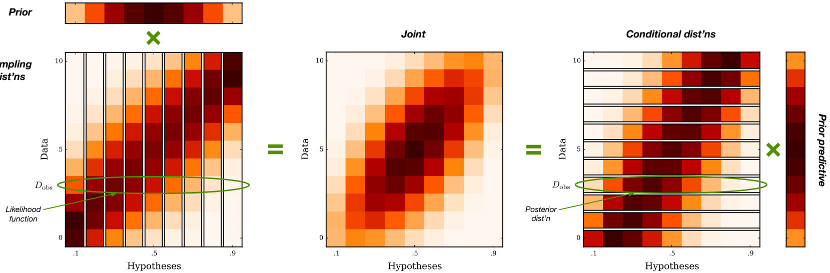
Bayes's theorem in terms of the *joint distribution*:

$$P(H_i|\mathcal{C}) \times P(D_{\rm obs}|H_i,\mathcal{C}) = P(H_i, D_{\rm obs}|\mathcal{C}) = P(H_i|D_{\rm obs},\mathcal{C}) \times P(D_{\rm obs}|\mathcal{C})$$



# Larger discrete case: Flip a coin 10 times (Binomial inference)

- 9 hypotheses: Prob. for heads is $\alpha = 0.1, 0.2, \ldots, 0.9$
- 11 possible data values: Number of heads, $n = 0, 1, \ldots, 10$
- Adopt a prior concentrated around $\alpha = 0.5$, with some spread




Joint ranks *"possible worlds"*—$(H_i, D)$ pairs—before observing data

Posterior adjusts the ranks once we learn the relevant possibilities must have $D = D_{obs}$ — focuses on the subset of possible worlds consistent with the real world

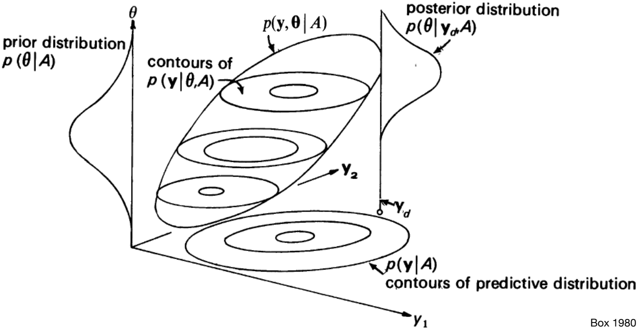
# Continuous data, parameter spaces

Prior $\times$ sampling distribution gives the *joint dist'n*:

$$p(\theta, D) = p(\theta) \times p(D|\theta);$$

Conditioning on $D = D_{\text{obs}}$ gives the posterior:

$$p(\theta|D) = p(\theta, D)/p(D)$$




Box 1980

Components of Bayes's theorem for a problem with a 1-D parameter space (θ) and a 2-D sample space (**y**), with observed data $\mathbf{y}_d$, and modeling assumptions *A*

# Recap of key ideas

*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 observed data

*Law of total probability*

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

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

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# Inference with parametric models

Models $M_i$ ($i = 1$ to $N$), each with parameters $\theta_i$, each imply a *sampling dist'n* (conditional predictive dist'n for possible data):

$$p(D|\theta_i, M_i)$$

The $\theta_i$ dependence when we fix attention on the *observed* data is the *likelihood function*:

$$\mathcal{L}_i(\theta_i) \equiv p(D_{\text{obs}}|\theta_i, M_i)$$

We may be uncertain about $i$ (model uncertainty) or $\theta_i$ (parameter uncertainty).

*Henceforth we will only consider the actually observed data, so we drop the cumbersome subscript: $D = D_{obs}$.*

# Classes of problems

*Single-model inference*

Premise = choice of single model (specific $i$)
*Parameter estimation*: What can we say about $\theta_i$ or $f(\theta_i)$?
*Prediction*: What can we say about future data $D'$?

*Multi-model inference*

Premise = $\{M_i\}$
*Model comparison/choice*: What can we say about $i$?
*Model averaging*:

- *Systematic error*: $\theta_i = \{\phi, \eta_i\}$; $\phi$ is common to all
  What can we say about $\phi$ w/o committing to one model?
- *Prediction*: What can we say about future $D'$, accounting for model uncertainty?

*Model checking*

Premise = $M_1 \vee$ "all" alternatives
Is $M_1$ adequate? (predictive tests, calibration, robustness)

# Parameter estimation

*Problem statement*

$\mathcal{C}$ = 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 $\theta$:

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

*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* $\Delta$ of probability $C$:
    $C = P(\theta \in \Delta|D, M) = \int_\Delta d\theta\, p(\theta|D, M)$
    *Highest Posterior Density (HPD) region* has $p(\theta|D, M)$ higher inside than outside
  - Posterior standard deviation, variance, covariances
- Marginal distributions
  - Interesting parameters $\phi$, nuisance parameters $\eta$
  - *Marginal dist'n* for $\phi$: $\quad p(\phi|D, M) = \int d\eta\, p(\phi, \eta|D, M)$

# Estimating a normal mean

*Problem specification*

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

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

*Likelihood*

$$\begin{aligned}
\mathcal{L}(\mu) &\equiv p(D|\mu, \sigma, M) \\
&= \prod_i \frac{1}{\sigma\sqrt{2\pi}} e^{-(d_i-\mu)^2/2\sigma^2}; \qquad \sigma = 1 \\
&\propto \exp\left(-\frac{N(\mu - \overline{d})^2}{2\sigma^2}\right)
\end{aligned}$$

Likelihood function is a Gaussian function at $\overline{d}$, width $w = \sigma/\sqrt{N}$

## Informative conjugate prior

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

Conjugate because the posterior turns out also to be normal

## Posterior

Normal $\mathcal{N}(\tilde{\mu}, \tilde{w}^2)$, but mean shifts towards prior, std. deviation decreases (reflecting add'l info from the prior)

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

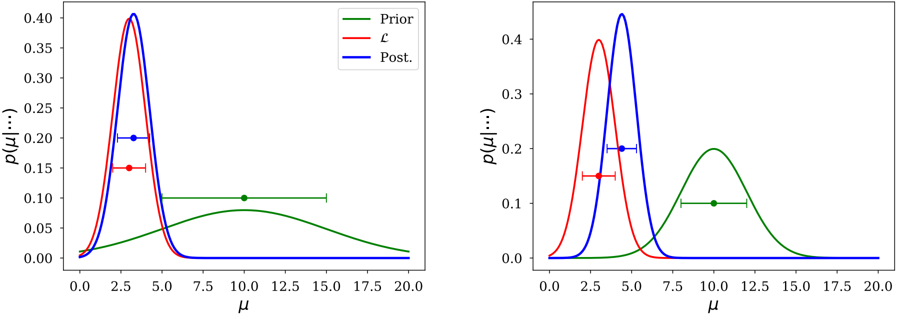
$$
\begin{aligned}
\widetilde{\mu} &= \overline{d} + B \cdot (\mu_0 - \overline{d}) \\
\widetilde{w} &= w \cdot \sqrt{1 - B}
\end{aligned}
$$

*Principle of stable estimation/precise measurement* — "If observations are precise... relative to the prior, then the form and properties of the prior distribution have negligible influence on the posterior distribution."

Edwards, Lindman, and Savage (1963), 'Bayesian Statistical Inference for Psychological Research,' reprinted in *Breakthroughs in Statistics*

Conjugate normal examples:

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



**Supplement:**

- Binomial example
  - Bernoulli trials: Bernoulli process & binomial sampling dist'ns
  - Beta-binomial conjugate model
- Normal example, cont'd
  - Analytical details for normal example
  - Sufficiency; sample mean and variance as sufficient statistics
  - Handling $\sigma$ uncertainty by marginalizing over $\sigma$; Student's $t$ distribution

# Nuisance parameters and marginalization

To model most data, we need to introduce parameters besides those of ultimate interest: *nuisance parameters*.

*Example*

> We have data from measuring a rate $r = s + b$ that is a sum of an interesting signal $s$ and a background $b$.
>
> We have additional data just about $b$.
>
> What do the data tell us about $s$?

# Marginal posterior distribution

To summarize implications for $s$, accounting for $b$ uncertainty, *marginalize*:

$$\begin{aligned} p(s|D,M) &= \int db\, p(s,b|D,M) \\ &\propto p(s|M) \int db\, p(b|s,M)\, \mathcal{L}(s,b) \\ &= p(s|M)\mathcal{L}_m(s) \end{aligned}$$

with $\mathcal{L}_m(s)$ the *marginal likelihood function for $s$*:

$$\mathcal{L}_m(s) \equiv \int db\, p(b|s)\, \mathcal{L}(s,b)$$

Maximum likelihood suggests instead computing the *profile likelihood*:

$$\mathcal{L}_p(s) \equiv \mathcal{L}(s,\hat{b}_s), \qquad \hat{b}_s = \text{best } b \text{ given } s$$

# Marginalization vs. profiling

*For insight:* Suppose the prior is broad compared to the likelihood $\rightarrow$ for a fixed $s$, we can accurately estimate $b$ with max likelihood $\hat{b}_s$, with small uncertainty $\delta b_s$.

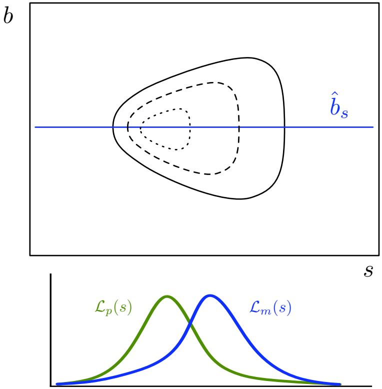
$$\begin{aligned}
\mathcal{L}_m(s) &\equiv \int db\; p(b|s)\, \mathcal{L}(s,b) \\
&\approx p(\hat{b}_s|s)\, \mathcal{L}(s, \underbrace{\boxed{\hat{b}_s}}_{\text{best } b \text{ given } s})\; \underbrace{\boxed{\delta b_s}}_{b \text{ uncertainty given } s}
\end{aligned}$$

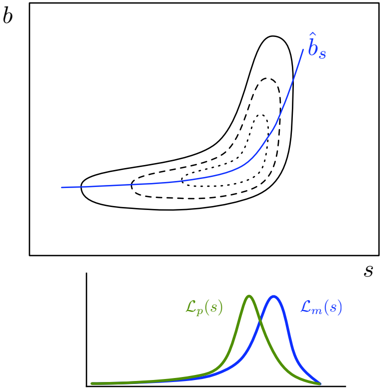
Profile likelihood $\mathcal{L}_p(s) \equiv \mathcal{L}(s, \hat{b}_s)$ gets weighted by a *parameter space volume factor*

E.g., Gaussians: $\hat{s} = \hat{r} - \hat{b}, \quad \sigma_s^2 = \sigma_r^2 + \sigma_b^2$

Background *subtraction* is a special case of background *marginalization*.

# Flared/skewed/bannana-shaped: $\mathcal{L}_m$ and $\mathcal{L}_p$ *differ*




General result: For a linear (in params) model sampled with Gaussian noise, and flat priors, $\mathcal{L}_m \propto \mathcal{L}_p$.
Otherwise, they will likely *differ*.

In *measurement error problems* the difference can have dramatic consequences (due to proliferation of latent parameters)

# The on/off problem for Poisson counting data

*Basic problem*

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

*Conventional solution*

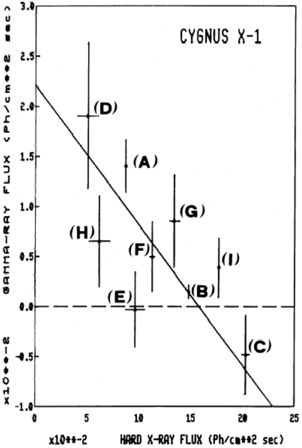
$$\begin{aligned}
\hat{b} &= N_{\rm off}/T_{\rm off}; & \sigma_b &= \sqrt{N_{\rm off}}/T_{\rm off} \\
\hat{r} &= N_{\rm on}/T_{\rm on}; & \sigma_r &= \sqrt{N_{\rm on}}/T_{\rm on} \\
\hat{s} &= \hat{r} - \hat{b}; & \sigma_s &= \sqrt{\sigma_r^2 + \sigma_b^2}
\end{aligned}$$

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

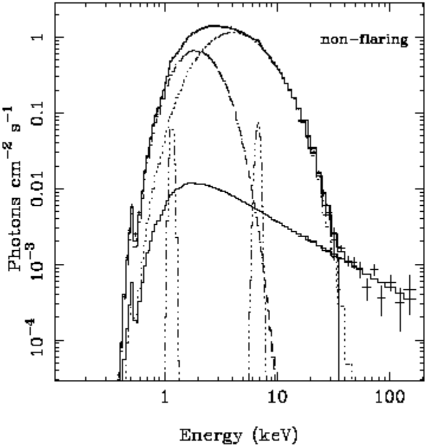
# Examples

Spectra of X-ray sources

Bassani et al. 1989

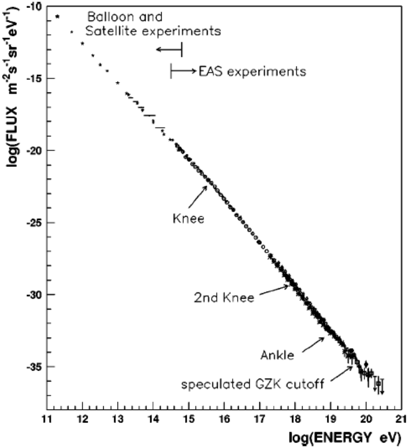



Di Salvo et al. 2001

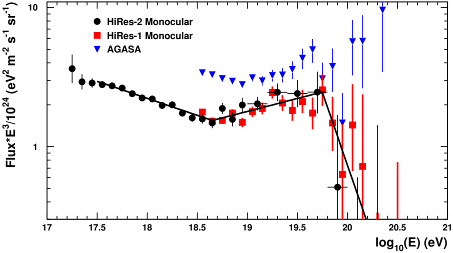


# Spectrum of ultrahigh-energy cosmic rays

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

The likelihood function is a product of separate Poisson distributions for the off-source and on-source data:

$$\mathcal{L}(s,b) = \frac{(bT_{\rm off})^{N_{\rm off}}}{N_{\rm off}!} e^{-bT_{\rm off}} \times \frac{[(s+b)T_{\rm on}]^{N_{\rm on}}}{N_{\rm on}!} e^{-(s+b)T_{\rm on}}$$

Adopting flat priors for $(s,b)$, the joint posterior is

$$p(s,b|N_{\rm on},N_{\rm off},\mathcal{C}) \quad \propto \quad (s+b)^{N_{\rm on}} b^{N_{\rm off}} e^{-sT_{\rm on}} e^{-b(T_{\rm on}+T_{\rm off})}$$

Note if $b=0$, the (normalized) posterior distribution is a gamma distribution,

$$p(s,b=0|N_{\rm on},N_{\rm off},\mathcal{C}) = \frac{T_{\rm on}(sT_{\rm on})^{N_{\rm on}}}{N_{\rm on}!} e^{-sT_{\rm on}}$$

Now marginalize over $b$;

$$
\begin{aligned}
p(s|N_{\rm on}, N_{\rm off}, \mathcal{C}) &= \int db\; p(s, b \mid N_{\rm on}, \mathcal{C}) \\
&\propto \int db\; (s+b)^{N_{\rm on}} b^{N_{\rm off}} e^{-sT_{\rm on}} e^{-b(T_{\rm on}+T_{\rm off})}
\end{aligned}
$$

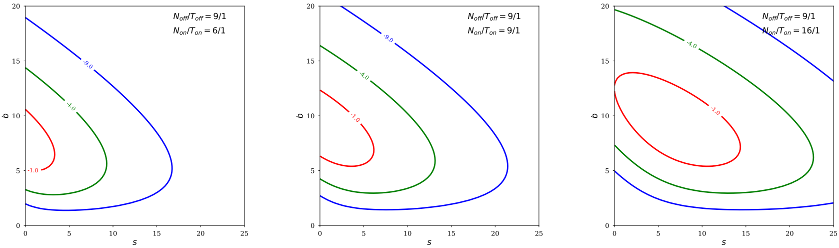
Expand $(s+b)^{N_{\rm on}}$ and do the resulting $\Gamma$ integrals:

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

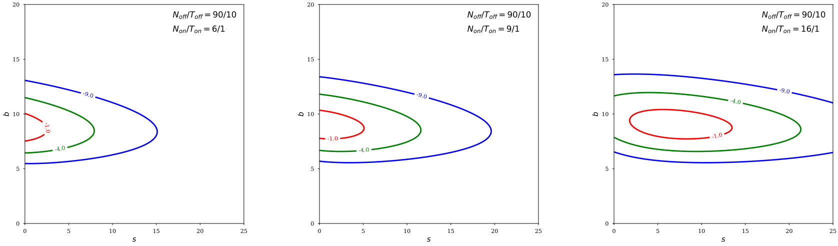
Posterior is a weighted sum of Gamma distributions, each assigning a different number of on-source counts to the source. (Evaluate via recursive algorithm or confluent hypergeometric function.)

# Example on/off joint PDFs

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

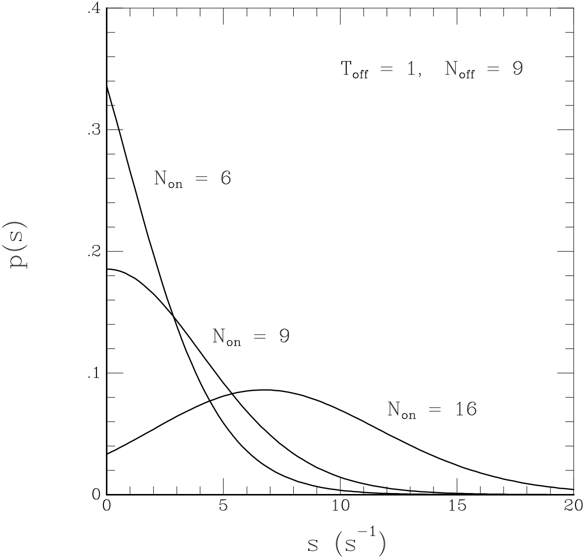



## $T_{\text{on}} = 1,\ T_{\text{off}} = 10$



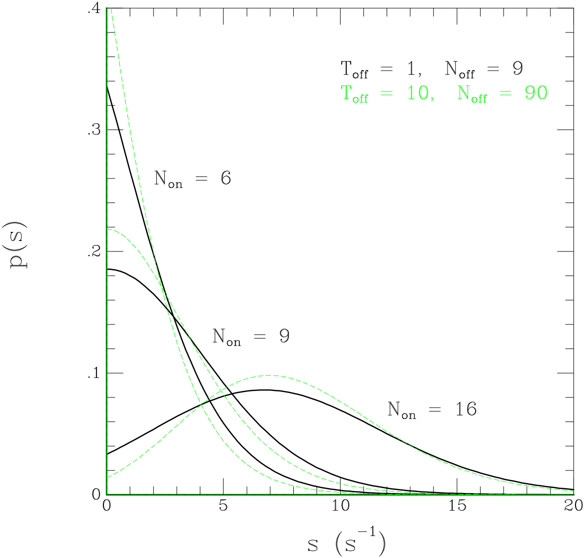
# Example on/off marginal PDFs—Short integrations

$T_{\rm on} = T_{\rm off} = 1$



# Example on/off marginal PDFs—Long background integrations

$T_{\rm on} = 1$, $T_{\rm off} = 10$



**Supplement:**

- Analytical details for Poisson dist'n inference
- Gamma-Poisson conjugate model
- Alternative (equivalent) solution to the on/off problem
- Multibin case

# Many roles for marginalization

*Many composite hypotheses are of interest...*

*Credible regions*

$$p(\theta \in \Delta|D, M) = \int_{\Delta} d\theta\; p(\theta|D, M)$$

*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 $F = f(\theta)$?

$$\begin{aligned} p(F|D, M) &= \int d\theta\; p(F, \theta|D, M) = \int d\theta\; p(\theta|D, M)\, p(F|\theta, M) \\ &= \int d\theta\; p(\theta|D, M)\, \delta[F - f(\theta)] \qquad \text{[\textit{single-valued case}]} \end{aligned}$$

## *Prediction*

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

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

## *Hierarchical modeling (graphical models, multilevel models)*

Learn population parameters by marginalizing over latent parameters for each member's actual (vs. measured) properties.

Learn a member's parameters by marginalizing over pop'n model and other members' parameters $\rightarrow$ *shrinkage* (beneficial bias!) — "the single most striking result of post-World War II statistical theory" (Efron 2010).

[See Supp. for brief intro.]

## *Model uncertainty & multi-model inference...*

# Agenda

1. **Probability theory for data analysis: Two theorems**
2. **Inference with parametric models**
   - Parameter Estimation
   - Model Uncertainty (Supp.)
   - Key role of LTP/marginalization
3. **Quick-looks**
   - Curve fitting & least squares (2 slides!)
   - Bayesian computation menu (1 slide!)

# Model uncertainty & multi-model inference

**Supplement:**

- Odds and Bayes factors: Compare models using *marginal* (average) likelihoods, not *maximum* likelihoods
- Bayesian Ockham's razor and Ockham factors
- Bayesian model averaging

In a nutshell:

Marginal likelihood for model $M_i$:

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

Bayes factor $B_{ij} \equiv Z_i/Z_j$ (ratio of *average*, not *max* likelihoods)
Can write $Z_i = \mathcal{L}_i(\hat{\theta}_i) \cdot \Omega_i$ = maximum likelihood $\times$ *Ockham factor*
$\Omega_i \approx \delta\theta/\Delta\theta =$ (posterior volume)/(prior volume)

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# A misconception

Bayesian data analysis gets its name from ***Bayes's theorem***:

$$
\begin{aligned}
p(\theta|D_{\rm obs}) &= \frac{p(\theta)\, p(D_{\rm obs}|\theta)}{p(D_{\rm obs})} \\
&= \frac{p(\theta)\, \mathcal{L}(\theta)}{p(D_{\rm obs})}
\end{aligned}
$$

So it's basically about ***modulating maximum likelihood with priors***…

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$$

So it's basically about ***modulating maximum likelihood with priors***...

Computing the posterior is just the *starting point*—we then have to do calculations, using all of probability theory to get answers to our questions from the posterior.

We'll find ourselves using the *law of total probability* over and over again—**marginalization** (summing/integrating probabilities).

*Integrating over parameter space is the key feature distinguishing Bayesian from frequentist data analysis*

(frequentist methods typically **optimize** over parameter space)

# On the key role of marginalization

Bayesian statistics uses all of probability theory, not just Bayes's theorem, and not even primarily Bayes's theorem. . . . Perhaps the most important theorem for doing Bayesian calculations is the *law of total probability* (LTP) that relates marginal probabilities to joint and conditional probabilities. . . . Arguably, if this approach to inference is to be named for a theorem, "total probability inference" would be a more appropriate appellation than "Bayesian statistics." It is probably too late to change the name. But it is not too late to change the emphasis.

— Loredo (2013)

The key distinguishing property of a Bayesian approach is marginalization instead of optimization, not the prior, or Bayes rule. . . . Broadly speaking, what makes Bayesian approaches distinctive is a posterior weighted marginalization over parameters. . . . Moreover, basic probability theory indicates that marginalization is desirable.

— Wilson (2020), Wilson & Izmailov (2020)

# Roles of the prior

*Prior has two roles*

- Modulate the likelihood to incorporate relevant prior information
- Convert likelihood from "intensity" to "measure"
  → enable accounting for *size of parameter space*

*Physical analogy*

$$\text{Heat} \quad Q = \int d\vec{r}\, c_v(\vec{r}) T(\vec{r})$$

$$\text{Probability} \quad P \propto \int d\theta\, p(\theta)\mathcal{L}(\theta)$$

Maximum likelihood focuses on the "hottest" parameters.
Bayes focuses on the parameters with the most "heat."

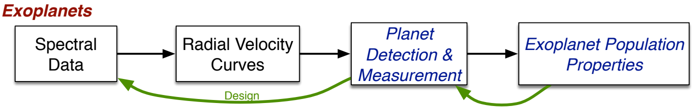
A high-$T$ region may contain little heat if its $c_v$ is low or if its volume is small.

A high-$\mathcal{L}$ region may contain little probability if its prior is low or if its volume is small.

Priors are like initial conditions/boundary conditions in physics: sometimes a nuisance, sometimes crucially important, always required by the theory

By converting likelihood to probability, priors provide two crucial capabilities:

- Accumulation of evidence (learning) $\rightarrow$ *discovery chains*




- Automatic accounting for the sizes of parameter/hypothesis spaces: nuisance parameters, uncertainty propagation, prediction, model comparison...

If your problem needs particularly careful and thorough implementation of these capabilities, you should consider Bayesian methods

**Supplement:**

- Typical sets (from MOO to MOE)
    - Priors do more than penalize/shift the mode
    - "Typical" samples can be very different from the mode (sample space examples: biased coin flips, $\chi^2 \approx \nu$)
    - Exploration/marginalization vs. optimization
- Assigning priors
- Rule-based "objective" priors: Jeffreys, reference

Also see Stan's "Prior Choice Recommendations" Wiki

# Theme: Parameter space volume

*Bayesian calculations sum/integrate over parameter/hypothesis space!*

(Frequentist calculations average over *sample* space & typically *optimize* over parameter space.)

- Credible regions integrate over parameter space
- Marginalization weights the profile likelihood by a volume factor for the nuisance parameters
- Model marginal likelihoods have parameter space volume factors that can penalize models for unncecessary complexity
- Prediction, uncertainty propagation, model averaging...

Many virtues of Bayesian methods can be attributed to this accounting for the "size" of parameter space. This idea does not arise naturally in frequentist statistics (but it can be added "by hand"—ignoring Fisher!).

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# 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 $f_i(\theta) \equiv f(x_i;\theta)$:

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

We seek to learn $\theta$, or to compare different functional forms (model choice, $M$)

*Likelihood*

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

## *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 $\chi^2$ code:

- Treat $\chi^2(\theta)$ as $-2 \log \mathcal{L}(\theta)$
- Bayesian inference amounts to *exploration and numerical integration* (by quadrature or Monte Carlo) of $\pi(\theta)e^{-\chi^2(\theta)/2}$

Forthcoming Python *Parametric Inference Engine* (PIE):

```
class MyData(PredictorSet):
    d1 =  SampledGaussianPred(data1, doc="Sampled")
    d2 =  BinnedGaussianPred(data2, doc="Binned")


class PowerLaw(SignalModel):
    A = PosParam(1., 'Amplitude')
    alpha = RealParam(range=(-5,-1), 'Index')

    def signal(self, E):
        return self.A * E**self.alpha
```

```
class PowerLawInference(BayesianInference,
                        PowerLaw, MyData):
    def log_prior(self):
        return 0.  # const. prior


inf = PowerLawInference()

inf.A.vary()
inf.alpha.step(0., 5., 50)

grid1 = laplace()  # Laplace approx.
grid2 = marg()     # Marg. via cubature
```

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# Bayesian computation menu

*Large sample size, $N$: Laplace approximation*

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

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

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

*High-dimensional models ($m \gtrsim 5$): Non-IID Monte Carlo*

- Posterior sampling — create RNG that samples posterior
    - Markov Chain Monte Carlo (MCMC) is the most general framework
- Nested sampling
- Sequential Monte Carlo (SMC)
- Approximate(ly) Bayesian computation (ABC)/Likelihood-free inference (LFI)
- ...

# Recap of key ideas

*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 observed data

*Law of total probability*

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

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