Bayesian inference in a nutshell

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Bayesian inference in a nutshell

1. Probability as logic

2. Three theorems

3. Inference with parametric models
   - Parameter Estimation
   - Model Uncertainty
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1 Probability as logic

2 Three theorems

3 Inference with parametric models
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   Model Uncertainty
Scientists argue!

Argument ≡ Collection of statements comprising an act of reasoning from premises to a (hypothetical) conclusion

A key goal of science: Explain or predict quantitative measurements (data!)

Data analysis: Constructing and appraising arguments that reason from data to interesting scientific conclusions (explanations, predictions)
The role of data

*Data do not speak for themselves!*

“No body of data tells us all we need to know about its own analysis.”
— John Tukey, *EDA*

We don’t just *tabulate* data, we *analyze* data

We gather data so they may speak for or against existing hypotheses, and guide the formation of new hypotheses

A key role of data in science is to be among the premises in scientific arguments

Bayesian inference uses probability theory to *quantify uncertainty* in such arguments
Frequentist vs. Bayesian probabilities

**Frequentist probability**

\[ p(E) = \text{frequency of occurrence of event } E \text{ in a hypothetical infinite ensemble, e.g., outcomes of repeated experiment} \]

Probability quantifies *variability*

**Bayesian probability**

\[ p(H|\mathcal{P}) = \text{strength of an argument } H|\mathcal{P} \text{ reasoning from premises } \mathcal{P} \text{ to hypothetical conclusion } H \text{ on } [0, 1] \text{ scale} \]

Probability quantifies *uncertainty*

\( \mathcal{F} \) definition appears more concrete and leads to an obvious calculus of probabilities; issues arise with definitions of events and ensembles

\( \mathcal{B} \) definition appears more abstract \( \rightarrow \) broader applicability but more explicit subjectivity and less obvious calculus
Frequentist vs. Bayesian statements

“The data $D_{obs}$ support conclusion $C$ . . . ”

**Frequentist assessment**

“$C$ was selected with a procedure that’s right 95% of the time over a set $\{D_{hyp}\}$ that includes $D_{obs}$.”

Probabilities are properties of *procedures*, not of particular results.

**Bayesian assessment**

“The strength of the chain of reasoning from the model and $D_{obs}$ to $C$ is 0.95, on a scale where 1= certainty.”

Probabilities are associated with *specific, observed data*. Long-run performance must be separately evaluated (and is typically good by frequentist criteria).
Logic—some essentials

“Logic can be defined as *the analysis and appraisal of arguments*”
—Gensler, *Intro to Logic*

Build arguments with propositions and logical operators/connectives:

- **Propositions**: Statements that may be true or false
  - $\mathcal{P}$: Universe can be modeled with ΛCDM
  - $A$: $\Omega_{\text{tot}} \in [0.9, 1.1]$
  - $B$: $\Omega_{\Lambda}$ is not 0
  - $\overline{B}$: “not $B$,” i.e., $\Omega_{\Lambda} = 0$

- **Connectives**:
  - $A \land B$: *A and B are both* true
  - $A \lor B$: *A or B is true, or both are*
Arguments

Argument: Assertion that an hypothesized conclusion, $H$, follows from premises, $P = \{A, B, C, \ldots\}$ (take “,” = “and”)

Notation:

\[ H \models P : \quad \text{Premises } P \text{ imply } H \]
\[ H \text{ may be deduced from } P \]
\[ H \text{ follows from } P \]
\[ H \text{ is true given that } P \text{ is true} \]

Arguments are (compound) propositions.

Central role of arguments → special terminology for true/false:

- A true argument is \textit{valid}
- A false argument is \textit{invalid} or \textit{fallacious}
Valid vs. sound arguments

Content vs. form

- An argument is *factually correct* iff all of its *premises are true* (it has “good content”).

- An argument is *valid* iff its conclusion *follows from* its premises (it has “good form”).

- An argument is *sound* iff it is both *factually correct and valid* (it has good form and content).

Deductive logic (and probability theory) addresses *validity*.

We want to make *sound* arguments. There is no formal approach for addressing factual correctness → there is always a subjective element to an argument.
Factual correctness

Passing the buck
Although logic can teach us something about validity and invalidity, it can teach us very little about factual correctness. The question of the truth or falsity of individual statements is primarily the subject matter of the sciences.

— Hardegree, *Symbolic Logic*

An open issue
To test the truth or falsehood of premises is the task of science. . . . But as a matter of fact we are interested in, and must often depend upon, the correctness of arguments whose premises are not known to be true.

— Copi, *Introduction to Logic*
Premises

- **Facts** — Things known to be true, e.g. *observed data*

- *“Obvious” assumptions* — Axioms, postulates, e.g., Euclid’s first 4 postulates (line segment b/t 2 points; congruency of right angles . . . )

- *“Reasonable” or “working” assumptions* — E.g., Euclid’s fifth postulate (parallel lines)

- *Desperate presumption!*

- **Conclusions from other arguments** → chains of discovery

Every argument has a set of premises defining a fixed *context* in which the argument is assessed.

Premises are considered “given”—if only for the sake of the argument!
Deductive and inductive inference

**Deduction**—*Syllogism as prototype*

Premise 1: $A$ implies $H$
Premise 2: $A$ is true
Deduction: $\therefore H$ is true
$H \models \mathcal{P}$ is valid

**Induction**—*Analogy as prototype*

Premise 1: $A, B, C, D, E$ all share properties $x, y, z$
Premise 2: $F$ has properties $x, y$
Induction: $F$ has property $z$

"$F$ has $z$" $\models \mathcal{P}$ is not strictly valid, but may still be rational
(likely, plausible, probable); some such arguments are stronger than others

*Boolean algebra* (and/or/not over $\{0, 1\}$) quantifies deduction.

*Bayesian probability theory* (and/or/not over $[0, 1]$) generalizes this to quantify the strength of inductive arguments.
Representing induction with \([0, 1]\) calculus

\[ P(H|\mathcal{P}) \equiv \text{strength of argument } H|\mathcal{P} \]

\[ P = 1 \rightarrow \text{Argument is deductively valid} \]
\[ = 0 \rightarrow \text{Premises imply } \overline{H} \]
\[ \in (0, 1) \rightarrow \text{Degree of deducibility} \]

**Mathematical model for induction**

‘AND’ (product rule):
\[ P(A \land B|\mathcal{P}) = P(A|\mathcal{P}) P(B|A \land \mathcal{P}) \]
\[ = P(B|\mathcal{P}) P(A|B \land \mathcal{P}) \]

‘OR’ (sum rule):
\[ P(A \lor B|\mathcal{P}) = P(A|\mathcal{P}) + P(B|\mathcal{P}) \]
\[ - P(A \land B|\mathcal{P}) \]

‘NOT’:
\[ P(\overline{A}|\mathcal{P}) = 1 - P(A|\mathcal{P}) \]
Firm foundations

Many different formal lines of argument derive induction-as-probability from various simple and appealing requirements:

- Consistency with logic + internal consistency (Cox; Jaynes)
- “Coherence” /optimal betting (Ramsey; DeFinetti; Wald; Savage)
- Algorithmic information theory (Rissanen; Wallace & Freeman)
- Optimal information processing (Zellner)
- Avoiding problems with frequentist methods:
  - Avoiding recognizable subsets (Cornfield)
  - Avoiding stopping rule problems → likelihood principle (Birnbaum; Berger & Wolpert)
Pierre Simon Laplace (1819)

Probability theory is nothing but *common sense reduced to calculation*.

James Clerk Maxwell (1850)

They say that Understanding ought to work by the rules of right reason. These rules are, or ought to be, contained in Logic, but the actual science of *Logic is conversant at present only with things either certain, impossible, or entirely doubtful*, none of which (fortunately) we have to reason on. Therefore *the true logic of this world is the calculus of Probabilities*, which takes account of the magnitude of the probability which is, or ought to be, in a reasonable man’s mind.

Harold Jeffreys (1931)

If we like there is no harm in saying that a probability expresses a degree of reasonable belief. . . . ‘Degree of confirmation’ has been used by Carnap, and possibly avoids some confusion. But whatever verbal expression we use to try to convey the primitive idea, this expression cannot amount to a definition. *Essentially the notion can only be described by reference to instances where it is used*. It is intended to express *a kind of relation between data and consequence* that habitually arises in science and in everyday life, and the reader should be able to recognize the relation from examples of the circumstances when it arises.
Interpreting Bayesian probabilities

Physics uses words drawn from ordinary language—mass, weight, momentum, force, temperature, heat, etc.—but their technical meaning is more abstract than their colloquial meaning. We can map between the colloquial and abstract meanings associated with specific values by using specific instances as “calibrators.”

### A Thermal Analogy

<table>
<thead>
<tr>
<th>Intuitive notion</th>
<th>Quantification</th>
<th>Calibration</th>
</tr>
</thead>
</table>
| Hot, cold        | Temperature, $T$ | Cold as ice = 273K  
Boiling hot = 373K |
| uncertainty      | Probability, $P$ | Certainty = 0, 1  
$p = 1/36$: plausible as “snake’s eyes”  
$p = 1/1024$: plausible as 10 heads |


Interpreting PDFs

**Bayesian**

Probability *quantifies uncertainty* in an inductive inference. $p(x)$ describes how *probability* is distributed over the possible values $x$ might have taken in the single case before us:

![Bayesian Diagram](image)

**Frequentist**

Probabilities are always (limiting) rates/proportions/frequencies that *quantify variability* in a sequence of trials. $p(x)$ describes how the *values of $x$* would be distributed among infinitely many trials:

![Frequentist Diagram](image)
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The Bayesian 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:*

- ’OR’ (sum rule): \[ P(H_1 \lor H_2|I) = P(H_1|I) + P(H_2|I) - P(H_1, H_2|I) \]

- ’AND’ (product rule): \[ P(H_1, D_{obs}|I) = P(H_1|I)P(D_{obs}|H_1, I) \]
  \[ = P(D_{obs}|I)P(H_1|D_{obs}, I) \]

- ’NOT’: \[ P(\overline{H_1}|I) = 1 - P(H_1|I) \]
Bayes’s Theorem (BT)

Consider \( P(H_i, D_{\text{obs}}|I) \) using the product rule:

\[
P(H_i, D_{\text{obs}}|I) = P(H_i|I) P(D_{\text{obs}}|H_i, I) = P(D_{\text{obs}}|I) P(H_i|D_{\text{obs}}, I)
\]

Solve for the posterior probability:

\[
P(H_i|D_{\text{obs}}, I) = P(H_i|I) \frac{P(D_{\text{obs}}|H_i, I)}{P(D_{\text{obs}}|I)}
\]

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

\[
\text{posterior } \propto \text{ prior } \times \text{ likelihood}
\]

norm. const. \( P(D_{\text{obs}}|I) = \text{ prior predictive} \)
Law of Total Probability (LTP)

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

\[
\sum_i P(A, B_i | I) = \sum_i P(B_i | A, I)P(A | I) = P(A | I)
\]

\[
= \sum_i P(B_i | I)P(A | B_i, I)
\]

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

\[
P(A | I) = \sum_i P(B_i | I)P(A | B_i, I)
\]

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

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

$$P(D_{\text{obs}}|I) = \sum_i P(D_{\text{obs}}, H_i|I)$$

$$= \sum_i P(H_i|I) P(D_{\text{obs}}|H_i, I)$$

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

**Normalization**

For exclusive, exhaustive $H_i$,

$$\sum_i P(H_i|\cdots) = 1$$
Well-Posed Problems

The rules express desired probabilities in terms of other probabilities.

To get a numerical value *out*, at some point we have to put numerical values *in*.

*Direct probabilities* are probabilities with numerical values determined directly by premises (via modeling assumptions, symmetry arguments, previous calculations, desperate presumption . . . ).

An inference problem is *well posed* only if all the needed probabilities are assignable based on the premises. We may need to add new assumptions as we see what needs to be assigned. We may not be entirely comfortable with what we need to assume! (Remember Euclid’s fifth postulate!)

Should explore how results depend on uncomfortable assumptions ("robustness").
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Inference With Parametric Models

Models $M_i$ ($i = 1 \text{ to } N$), 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: $D = D_{\text{obs}}$.***
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 = $M_1 \lor$ “all” alternatives

Is $M_1$ adequate? (predictive tests, calibration, robustness)
Parameter Estimation

Problem statement

\( I = \) 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 \( \theta \):

\[
P(\theta \in [\theta, \theta + d\theta] | \cdots) = f(\theta)d\theta
\]

\[
= p(\theta | \cdots) d\theta
\]

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 \( \phi \):
    \[ p(\phi|D, M) = \int d\eta p(\phi, \eta|D, M) \]
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 $s$?
To summarize implications for $s$, accounting for $b$ uncertainty, marginalize:

$$p(s|D, M) = \int db \ p(s, b|D, M)$$

$$\propto p(s|M) \int db \ p(b|s) \mathcal{L}(s, b)$$

$$= p(s|M) \mathcal{L}_m(s)$$

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

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

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

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

$$\approx p(\hat{b}_s|s) \mathcal{L}(s, \hat{b}_s) \delta b_s$$

Profile likelihood $L_p(s) \equiv \mathcal{L}(s, \hat{b}_s)$ 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.
Bivariate normals: $\mathcal{L}_m \propto \mathcal{L}_p$

$\delta b_s$ is const. vs. $s$

$\Rightarrow \mathcal{L}_m \propto \mathcal{L}_p$
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 (future lecture!) the difference can be dramatic.
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 \( F = f(\theta) \)?

\[ p(F|D, M) = \int d\theta \ p(F, \theta|D, M) = \int d\theta \ p(\theta|D, M) \ p(F|\theta, M) \]
\[ = \int d\theta \ p(\theta|D, M) \delta[F - f(\theta)] \quad [\text{single-valued case}] \]

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...
Model Comparison

Problem statement

\[ I = (M_1 \lor M_2 \lor \ldots) \] — Specify a set of models.

\[ H_i = M_i \] — Hypothesis chooses a model.

Posterior probability for a model

\[
p(M_i|D, I) = \frac{p(M_i|I) p(D|M_i, I)}{p(D|I)} \propto p(M_i|I) \mathcal{L}(M_i)
\]

But \( \mathcal{L}(M_i) = p(D|M_i) = \int d\theta_i p(\theta_i|M_i) p(D|\theta_i, M_i) \).

Likelihood for model = Average likelihood for its parameters

\[
\mathcal{L}(M_i) = \langle \mathcal{L}(\theta_i) \rangle
\]

Varied terminology: Prior predictive = Average likelihood = Global likelihood = Marginal likelihood = (Weight of) Evidence for model
Odds and Bayes factors

A ratio of probabilities for two propositions using the same premises is called the **odds** favoring one over the other:

\[
O_{ij} \equiv \frac{p(M_i|D, I)}{p(M_j|D, I)}
\]

\[
= \frac{p(M_i|I)}{p(M_j|I)} \times \frac{p(D|M_i, I)}{p(D|M_j, I)}
\]

The data-dependent part is called the **Bayes factor**:

\[
B_{ij} \equiv \frac{p(D|M_i, I)}{p(D|M_j, I)}
\]

It is a *likelihood ratio*; the BF terminology is usually reserved for cases when the likelihoods are marginal/average likelihoods.
An Automatic Ockham’s Razor

Predictive probabilities can favor simpler models

\[ p(D|M_i) = \int d\theta_i \, p(\theta_i|M) \, L(\theta_i) \]
The Ockham Factor

\[ p(D|M_i) = \int d\theta_i \ p(\theta_i|M) \ L(\theta_i) \approx p(\hat{\theta}_i|M) L(\hat{\theta}_i) \delta\theta_i \]

\[ \approx \ L(\hat{\theta}_i) \frac{\delta\theta_i}{\Delta\theta_i} \]

\[ = \ \text{Maximum Likelihood} \times \text{Ockham Factor} \]

Models with more parameters often make the data more probable — for the best fit

Ockham factor penalizes models for “wasted” volume of parameter space

Quantifies intuition that models shouldn’t require fine-tuning
Model Averaging

Problem statement

\( l = (M_1 \lor M_2 \lor \ldots) \) — Specify a set of models
Models all share a set of “interesting” parameters, \( \phi \)
Each has different set of nuisance parameters \( \eta_i \) (or different prior info about them)
\( H_i = \) statements about \( \phi \)

Model averaging

Calculate posterior PDF for \( \phi \):

\[
p(\phi|D, l) = \sum_i p(M_i|D, l) p(\phi|D, M_i)
\]

\[
\propto \sum_i \mathcal{L}(M_i) \int d\eta_i p(\phi, \eta_i|D, M_i)
\]

The model choice is a (discrete) nuisance parameter here.
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 likelihoods have Ockham factors resulting from parameter space volume factors.

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”).
Roles of the prior

*Prior has two roles*

- Incorporate any relevant prior information
- Convert likelihood from “intensity” to “measure” → account for *size of parameter space*

*Physical analogy*

\[
Q = \int d\mathbf{r} \ c_v(\mathbf{r}) \ T(\mathbf{r})
\]

\[
P \propto \int d\theta \ p(\theta) \mathcal{L}(\theta)
\]

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.
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 data

**Law of total probability**

\[ p(\text{Hypotheses} \mid \text{Data}) = \sum p(\text{Hypothesis} \mid \text{Data}) \]

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