Bayesian Workshop: How to use Bayesian methods in Pumas

Jose Storopoli and Mohamed Tarek {jose.storopoli,mohamed}@pumas.ai
PumasAI

Outline

Bayesian Statistics - Recommended References

- Gelman et al. [1] - Chapter 1: Probability and inference
- McElreath [2] - Chapter 1: The Golem of Prague
- Gelman, Hill, and Vehtari [3] - Chapter 3: Some basic methods in mathematics and probability
- Khan and Rue [4]
- **Probability**:
  - A great textbook - Bertsekas and Tsitsiklis [5]
  - Also a great textbook (skip the frequentist part)- Dekking et al. [6]
  - Bayesian point-of-view and also a philosophical approach- Jaynes [7]
  - Bayesian point-of-view with a simple and playful approach - Kurt [8]
  - Philosophical approach not so focused on mathematical rigor - Diaconis and Skyrms [9]

What is Bayesian Statistics?

Bayesian statistics is a **data analysis approach based on Bayes' theorem** where available knowledge about the parameters of a statistical model is updated with the information of observed data. [1]. Previous knowledge is expressed as a **prior** distribution and combined with the observed data in the form of a **likelihood** function to generate a **posterior** distribution. The posterior can also be used to make predictions about future events.

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What changes from Frequentist Statistics?

- **Flexibility** - probabilistic building blocks to construct a model[i]:
  - Probabilistic conjectures about parameters:
    - Prior
    - Likelihood
- Better **uncertainty** treatment:
  - Coherence
  - Propagation
  - We don't use *"if we sampled infinite times from a population that we do not observe..."*
- No p**-values**:
  - All statistical intuitions makes **sense**
  - 95% certainty that θ's parameter value is between x and y
  - Almost **impossible** to perform p-hacking

[i] like LEGO

A little bit more formal

- Bayesian Statistics uses probabilistic statements:
  - one or more parameters θ
  - unobserved data $\tilde{y}$

- These statements are conditioned on the observed values of y:
  - $P(\theta \mid y)$
  - $P(\tilde{y} \mid y)$

- We also, implicitly, conditioned on the observed data from any covariate x

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Definition of Bayesian Statistics

Definition (Bayesian Statistics)

The use of Bayes theorem as the procedure to ***estimate parameters of interest*** θ ***or unobserved data*** $\tilde{y}$. *[1]*

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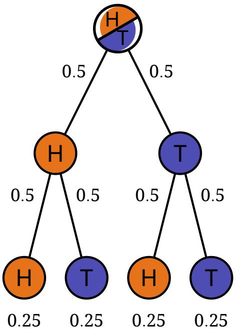
PROBABILITY DOES NOT EXIST![ii]

- Yes, probability does not exist ...
- Or even better, probability as a physical quantity, objective chance, **does NOT exist**
- if we disregard objetive chance *nothing is lost*
- The math of inductive rationality remains **exactly the same**

[ii] de Finetti [10]

PROBABILITY DOES NOT EXIST![iii]

- Consider flipping a biased coin
- The trials are considered independent and, as a result, have an important property: **the order does not matter**
- The frequency is considered a **sufficient statistic**
- Saying that order does not matter or saying that the only thing that matters is frequency are two ways of saying the same thing
- We say that the probability is **invariant under permutations**



[iii] de Finetti [10]

Probability Interpretations

- **Objective** - frequency in the long run for an event:
  - $P(\text{rain}) = \frac{\text{days that rained}}{\text{total days}}$
  - $P(\text{me being elected president}) = 0$ (never occurred)

- **Subjective** - degrees of belief in an event:
  - $P(\text{rain}) = \text{degree of belief that will rain}$
  - $P(\text{me being elected president}) = 10^{-10}$ (highly unlikely)

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What is Probability?

Definition (Probability)

We define A is an event and $P(A)$ the probability of event A. $P(A)$ has to be between 0 and 1, where higher values defines higher probability of A happening.

$$P(A) \in \mathbb{R}$$

$$P(A) \in [0, 1]$$

$$0 \leq P(A) \leq 1$$

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Probability Axioms[iv]

- **Non-negativity**: For every A:

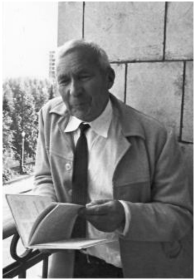
$$P(A) \geq 0$$

- **Additivity**: For every two *mutually exclusive* A and B:

$$P(A) = 1 - P(B) \text{ and } P(B) = 1 - P(A)$$

- **Normalization**: The probability of all possible events $A_1, A_2, \dots$ must sum up to 1:

$$\sum A_n = 1$$



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Sample Space

- Discrete

$$\Theta = \{1, 2, \ldots\}$$

- Continuous

$$\Theta \in (-\infty, \infty)$$

Discrete Sample Space

8 planets in our solar system:

- Mercury - ☿
- Venus - ♀
- Earth - ♁
- Mars ♂
- Jupiter - ♃
- Saturn ♄
- Uranus - ⛢
- Neptune ⯉

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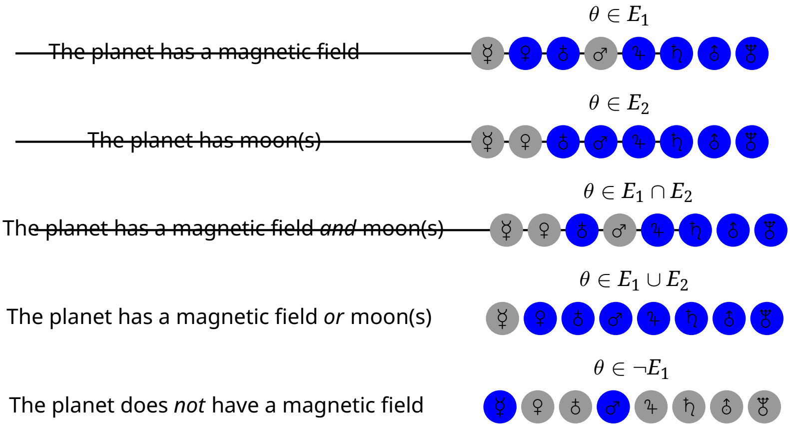
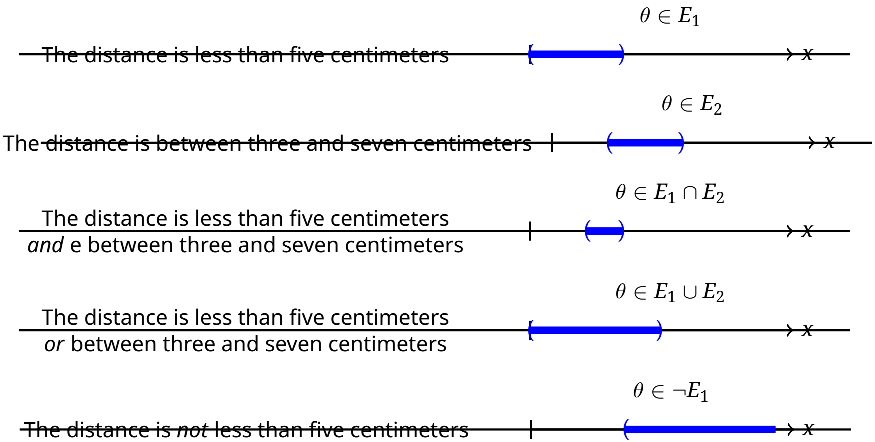
Discrete Sample Space[v]



[v]figure adapted from Michael Betancourt (CC-BY-SA-4.0)

Continuous Sample Space[vi]



[vi] figure adapted from Michael Betancourt (CC-BY-SA-4.0)

Discrete versus Continuous Parameters

Everything that has been exposed here was under the assumption that the parameters are discrete. This was done with the intent to provide an intuition what is probability. Not always we work with discrete parameters. Parameters can be continuous, such as: age, height, weight etc. But don't despair! All probability rules and axioms are valid also for continuous parameters. The only thing we have to do is to change all sum $\sum$ for integrals $\int$. For example, the third axiom of **Normalization** for *continuous* random variables becomes:

$$\int_{x \in X} p(x) dx = 1.$$

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Conditional Probability

Definition (Conditional Probability)

Probability of an event occurring in case another has occurred or not.

The notation we use is $P(A \mid B)$, that read as "the probability of observing A given that we already observed B".

$$P(A \mid B) = \frac{\text{number of elements in } A \text{ and } B}{\text{number of elements in } B}$$

$$P(A \mid B) = \frac{P(A \cap B)}{P(B)}$$

assuming that $P(B) > 0$.

Example of Conditional Probability

Example (Poker Texas Hold'em)

- **Sample Space**: 52 cards in a deck, 13 types of cards and 4 types of suits.
- $P(A)$: Probability of being dealt an Ace $\left(\frac{4}{52} = \frac{1}{13}\right)$
- $P(K)$: Probability of being dealt a King $\left(\frac{4}{52} = \frac{1}{13}\right)$
- $P(A \mid K)$: Probability of being dealt an Ace, given that you have already a King $\left(\frac{4}{51} \approx 0.078\right)$
- $P(K \mid A)$: Probability of being dealt a King, given that you have already an Ace $\left(\frac{4}{51} \approx 0.078\right)$

Caution! Not always $P(A \mid B) = P(B \mid A)$

In the previous example we have the symmetry $P(A \mid K) = P(K \mid A)$, **but not always this is true**[vii]

Example (The Pope is catholic)

- $P(\text{pope})$: Probability of some random person being the Pope, something really small, 1 in 8 billion $\left(\frac{1}{8 \cdot 10^9}\right)$
- $P(\text{catholic})$: Probability of some random person being catholic, 1.34 billion in 8 billion $\left(\frac{1.34}{8} \approx 0.17\right)$
- $P(\text{catholic} \mid \text{pope})$: Probability of the Pope being catholic $\left(\frac{999}{1000} = 0.999\right)$
- $P(\text{pope} \mid \text{catholic})$: Probability of a catholic person being the Pope $\left(\frac{1}{1.34 \cdot 10^9} \cdot 0.999 \approx 7.46 \cdot 10^{-10}\right)$
- **Hence**: $P(\text{catholic} \mid \text{pope}) \neq P(\text{pope} \mid \text{catholic})$

[vii] More specific, if the basal rates $P(A)$ and $P(B)$ aren't equal, the symmetry is broken $P(A \mid B) \neq P(B \mid A)$

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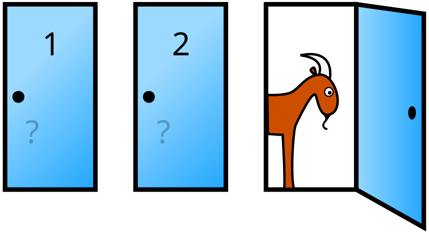
A Probability Textbook Classic

Example (Monty Hall)

- A TV presenter shows you 3 doors
- One of them has a prize: a car! The others have a goat
- You must choose a door (that is not open or revealed)
- In this moment, the presenter opens one of the other two doors that you did not choose, revealing one of the two goats
- The presenter then asks you “Do you want to change your door or stay with your choice?”



Solution for the Monty Hall Problem

Idea (Probability of winning a car)

$$P(car \mid C_i) = \frac{1}{3}$$

$$P(car) = \frac{1}{3} \cdot P(car \mid C_1) + \frac{1}{3} \cdot P(car \mid C_2) + \frac{1}{3} \cdot P(car \mid C_3)$$

$$P(car) = \frac{\sum_{i=1}^{3} P(car \mid C_i)}{3}$$

$$P(car) = \frac{1}{3}$$

C_i is the event that the car is behind door i, $i = 1, 2, 3$

Solution for the Monty Hall Problem

Scenario 1: Don't change doors

Simple:

$$\frac{1}{3}$$

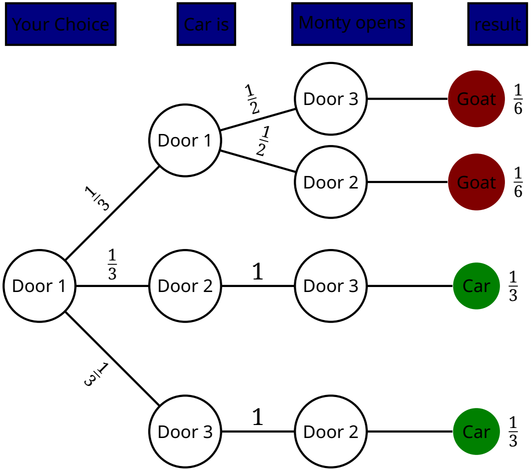
Scenario 2: Change doors

Choose any door i to be $C_i = 0$

$$P(\text{car}) = 0 \cdot P(\text{car} \mid C_i) + \frac{1}{3} + \frac{1}{3}$$

$$P(\text{car}) = \frac{2}{3}$$

Visualization of the Monty Hall Problem



Joint Probability

Definition (Joint Probability)

Probability of two or more events occurring.

The notation we use
is $P(A, B)$, that read as "the probability of observing A and also observing B".

$$
\begin{aligned}
P(A, B) &= \textit{number of elements in } A \textit{ or } B \\
P(A, B) &= P(A \cup B) \\
P(A, B) &= P(B, A)
\end{aligned}
$$

Example of Joint Probability

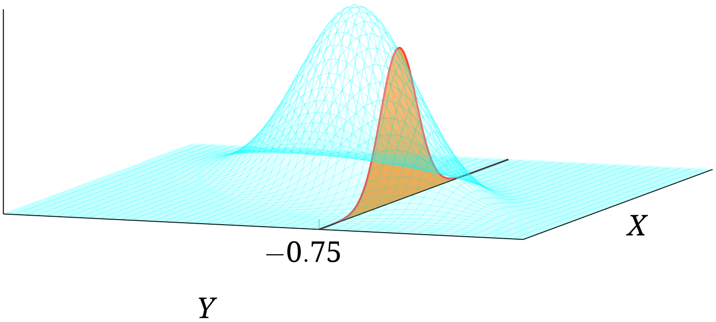
Example (Revisiting Poker Texas Hold'em)

- **Sample Space**: 52 cards in a deck, 13 types of cards and 4 types of suits.
- $P(A)$: Probability of being dealt an Ace $\left(\frac{4}{52} = \frac{1}{13}\right)$
- $P(K)$: Probability of being dealt a King $\left(\frac{4}{52} = \frac{1}{13}\right)$
- $P(A \mid K)$: Probability of being dealt an Ace, given that you have already a King $\left(\frac{4}{51} \approx 0.078\right)$
- $P(K \mid A)$: Probability of being dealt a King, given that you have already an Ace $\left(\frac{4}{51} \approx 0.078\right)$
- $P(A, K)$: Probability of being dealt an Ace *and* being dealt a King

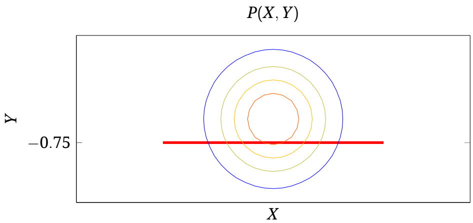
$$P(A, K) = P(K, A)$$
$$P(A) \cdot P(K \mid A) = P(K) \cdot P(A \mid K)$$
$$\frac{1}{13} \cdot \frac{4}{51} = \frac{1}{13} \cdot \frac{4}{51}$$

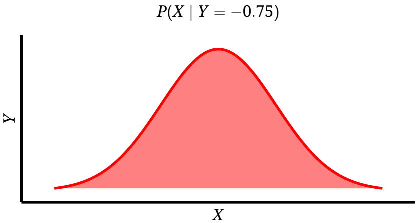
Visualization of Joint Probability versus Conditional Probability

$P(X, Y)$ versus $P(X \mid Y = -0.75)$



Visualization of Joint Probability versus Conditional Probability





Who was Thomas Bayes?

- **Thomas Bayes** (1701 - 1761) was a statistician, philosopher and Presbyterian minister who is known for formulating a specific case of the theorem that bears his name: Bayes’ theorem.
- Bayes never published what would become his most famous accomplishment; his notes were edited and published posthumously by his friend **Richard Price**.
- The theorem official name is **Bayes-Price-Laplace**, because **Bayes** was the first to discover, **Price** got his notes, transcribed into mathematical notation, and read to the Royal Society of London, and **Laplace** independently rediscovered the theorem without having previous contact in the end of the XVIII century in France while using probability for statistical inference with census data in the Napoleonic era.

Bayes Theorem

Theorem (Bayes)

Tells us how to “invert” conditional probability:

$$P(A \mid B) = \frac{P(A) \cdot P(B \mid A)}{P(B)}$$

Bayes' Theorem Proof

Remember the following probability identity:

$$P(A, B) = P(B, A)$$
$$P(A) \cdot P(B \mid A) = P(B) \cdot P(A \mid B)$$

OK, now divide everything by $P(B)$:

$$\frac{P(A) \cdot P(B \mid A)}{P(B)} = \frac{P(B) \cdot \quad P(A \mid B)}{P(B)}$$

$$\frac{P(A) \cdot P(B \mid A)}{P(B)} = P(A \mid B)$$
$$P(A \mid B) = \frac{P(A) \cdot P(B \mid A)}{P(B)}$$

Another Probability Textbook Classic[viii]

Example (Breast Cancer)

How accurate is a **breast cancer** test?

- 1% of women have **breast cancer** (Prevalence)
- 80% of mammograms detect **breast cancer** (True Positive)
- 9.6% of mammograms detect **breast cancer** when there is no incidence (False Positive)

$$P(C \mid +) = \frac{P(+ \mid C) \cdot P(C)}{P(+)}$$

$$P(C \mid +) = \frac{P(+ \mid C) \cdot P(C)}{P(+ \mid C) \cdot P(C) + P(+ \mid \neg C) \cdot P(\neg C)}$$

$$P(C \mid +) = \frac{0.8 \cdot 0.01}{0.8 \cdot 0.01 + 0.096 \cdot 0.99}$$

$$P(C \mid +) \approx 0.0776$$

[viii] Adapted from: Yudkowski - *An Intuitive Explanation of Bayes' Theorem*.

Why Bayes' Theorem is Important?

Idea (We can Invert the Conditional Probability)

$$P(hypothesis \mid data) = \frac{P(data \mid hypothesis) \cdot P(hypothesis)}{P(data)}$$

But isn't this the p-value? **NO!**

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What are p-values?

Definition (p-value)

p-value is the probability of obtaining results at least as extreme as the observed, given that the null hypothesis H_0 is true:

$$P(D \mid H_0)$$

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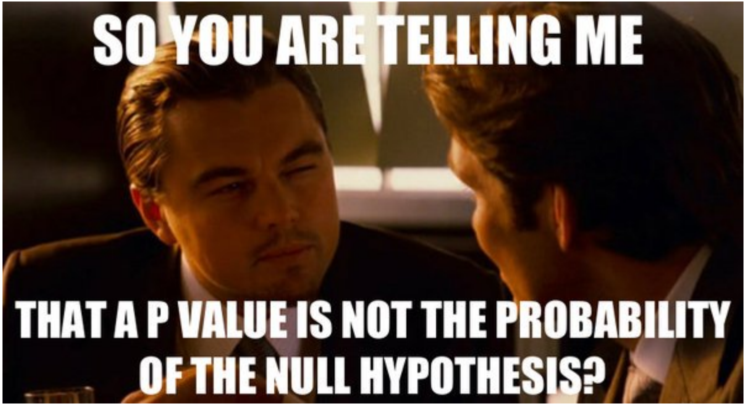
What p-value is **not**!



What p-value is **not**!

- **p-value is not the probability of the null hypothesis** - Infamous confusion between $P(D \mid H_0)$ and $P(H_0 \mid D)$. To get $P(H_0 \mid D)$ you need Bayesian statistics.

- **p-value is not the probability of data being generated at random** - No! We haven't stated nothing about randomness.

- **p-value measures the effect size of a statistical test** - Also no... p-value does not say anything about effect sizes. Just about if the observed data diverge of the expected under the null hypothesis. Besides, p-values can be hacked in several ways [12].

The relationship between p-value and H_0

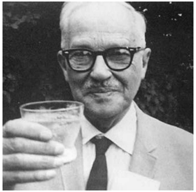
To find out about any p-value, **find out what H_0 is behind it**. It's definition will never change, since it is always $P(D \mid H_0)$:

- **t-test**: $P(D \mid \text{the difference between the groups is zero})$
- **ANOVA**: $P(D \mid \text{there is no difference between groups})$
- **Regression**: $P(D \mid \text{coefficient has a null value})$
- **Shapiro-Wilk**:
  $P(D \mid \text{population is distributed as a Normal distribution})$

What are Confidence Intervals?

Definition (Confidence Intervals)

A confidence interval of X% for a parameter is an interval (a, b) generated by a repeated sampling procedure has probability X% of containing the true value of the parameter, for all possible values of the parameter.



Neyman [13] (the "father" of confidence intervals)

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What are Confidence Intervals?

Example (Confidence Intervals of a Public Policy Analysis)

Say you performed a statistical analysis to compare the efficacy of a public policy between two groups and you obtain a difference between the mean of these groups. You can express this difference as a confidence interval. Often we choose 95% confidence. This means that **95 studies out of 100**, that uses the **same sample size and target population**, performing the **same statistical test**, will expect to find a result of the mean difference between groups inside the confidence interval.

Doesn't say anything about you **target population**, but about you **sample** in an insane process of **infinite sampling** …

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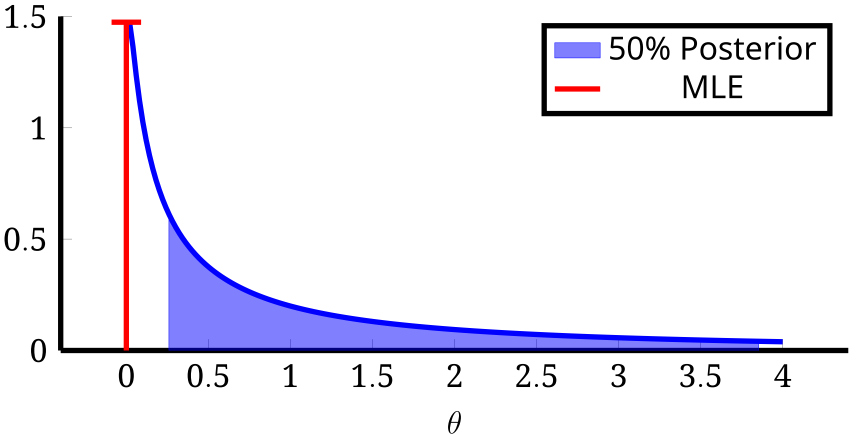
Confidence Intervals versus Posterior Intervals



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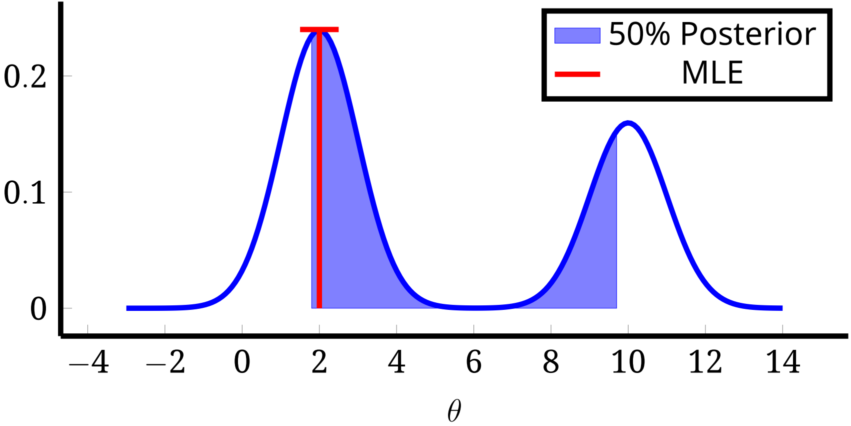
Confidence Intervals versus Posterior Intervals



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But why I never see stats without p-values?

We cannot understand p-values if we do no not comprehend its origins and historical trajectory. The first mention of p-values was made by the statistician Ronald Fischer in 1925 [14]:

> *[p-valor is a] measure of evidence against the null hypothesis*

- To quantify the strength of the evidence against the null hypothesis, Fisher defended "$p < 0.05$ as the standard level to conclude that there is evidence against the tested hypothesis"
- "We should not be off-track if we draw a conventional line at 0.05"

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$p = 0.06$

- Since p-value is a probability, it is also a continuous measure.
- There is no reason for us to differentiate $p = 0.049$ against $p = 0.051$.
- Robert Rosenthal, a psychologist said “surely, God loves the .06 nearly as much as the .05” [15].

But why I never heard about Bayesian statistics?[ix]

> *. . . it will be sufficient . . . to reaffirm my personal conviction . . . that the theory of inverse probability is founded upon an error, and must be wholly rejected.*

Fisher [14]

[ix] *inverse probability* was how Bayes' theorem was called in the beginning of the 20th century

Inside every nonBayesian, there is a Bayesian struggling to get out[x]

- In his final year of life, Fisher published a paper [16] examining the possibilities of Bayesian methods, but with the prior probabilities being determined experimentally.
- Some authors speculate [7] that if Fisher were alive today, he would probably be a Bayesian.

[x]quote from Dennis Lindley

Bayes' Theorem as an Inference Engine

Now that you know what is probability and Bayes' theorem, I will propose the following:

$$\underbrace{P(\theta \mid y)}_{\text{Posterior}} = \frac{\overbrace{P(y \mid \theta)}^{\text{Likelihood}} \cdot \overbrace{P(\theta)}^{\text{Prior}}}{\underbrace{P(y)}_{\text{Normalizing Constant}}}$$

- θ – parameter(s) of interest
- y – observed data
- **Priori**: prior probability of the parameter(s) value(s)
- **Likelihood**: probability of the observed data given the parameter(s) value(s)
- **Posterior**: posterior probability of the parameter(s) value(s) after we observed data y
- **Normalizing Constant**[xi]: $P(y)$ does not make any intuitive sense. This probability is transformed and can be interpreted as something that only exists so that the result $P(y \mid \theta)P(\theta)$ be constrained between 0 e 1 – a valid probability.

[xi] sometimes also called *evidence*.

Bayes' Theorem as an Inference Engine

Bayesian statistics allows us to **quantify directly the uncertainty** related to the value of one or more parameters of our model given the observed data. This is the **main feature** of Bayesian statistics, since we are estimating directly $P(\theta \mid y)$ using Bayes' theorem. The resulting estimate is totally intuitive: simply quantifies the uncertainty that we have about the value of one or more parameters given the data, model assumptions (likelihood) and the prior probability of these parameter's values.

Bayesian vs Frequentist Stats

	Bayesian Statistics	Frequentist Statistics
Data	Fixed — Non-random	Uncertain — Random
Parameters	Uncertain — Random	Fixed — Non-random
Inference	Uncertainty regarding the parameter value	Uncertainty regarding the sampling process from an infinite population
Probability	Subjective	Objective (but with several model assumptions)
Uncertainty	Posterior Interval — $P(\theta \mid y)$	Confidence Interval — $P(y \mid \theta)$

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Advantages of Bayesian Statistics

- Natural approach to express uncertainty
- Ability to incorporate previous information
- Higher model flexibility
- Full posterior distribution of the parameters
- Natural propagation of uncertainty

Main disadvantage: Slow model fitting procedure

The beginning of the end of Frequentist Statistics

- Know that you are in a very special moment in history of great changes in statistics
- I believe that frequentist statistics, specially the way we qualify evidence and hypotheses with p-values will transform in a "significant"[xii] way.
- 6 years ago, the *American Statistical Association* (ASA) published a declaration about p-values [17]. It states exactly what we exposed here: The main concepts of the null hypothesis significant testing and, in particular p-values, cannot provide what researchers demand of them. Despite what says several textbooks, learning materials and published content, p-values below 0.05 doesn't "prove" anything. Not, on the other way around, p-values higher than 0.05 refute anything.
- ASA statement has more than 4.700 citations with relevant impact.

[xii] pun intended ...

The beginning of the end of Frequentist Statistics

- An international symposium was promoted in 2017 which originated an open-access special edition of *The American Statistician* dedicated to practical ways to abandon $p < 0.05$ [18].
- Soon there were more attempts and claims. In September 2017, *Nature Human Behaviour* published an editorial proposing that the p-value's significance level be decreased from 0.05 to 0.005 [19]. Several authors, including highly important and influential statisticians argued that this simple step would help to tackle the replication crisis problem in science, that many believe be the main consequence of the abusive use of p-values [20].
- Furthermore, many went a step ahead and suggested that science banish once for all p-values [21, 22]. Many suggest (including myself) that the main tool of statistical inference be Bayesian statistics [23, 24, 25].

What is Pumas?

Pumas (**P**harmace**U**tical **M**odeling **A**nd **S**imulation) [26] is a suite of tools to perform quantitative analytics of various kinds across the horizontal of pharmaceutical drug development. The purpose of this framework is to bring efficient implementations of all aspects of the analytics in this domain under one cohesive package.

Pumas Features

Pumas 2.0 currently includes:

- Non-compartmental Analysis
- Specification of Nonlinear Mixed Effects (NLME) Models
- Simulation of NLME model using differential equations or analytical solutions
- Deep control over the differential equation solvers for high efficiency
- Estimation of NLME parameters via Maximum Likelihood, Expectation Maximization and Bayesian methods
- Parallelization capabilities for both simulation and estimation
- Mixed analytical and numerical problems
- Simulation and estimation diagnostics for model post-processing
- Interactive model exploration and diagnostics tools through webapps
- Automated report generation for models and non-compartmental analysis
- Global and local sensitivity analysis routines for multi-scale models
- Bioequivalence analysis
- Optimal design of experiments

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