Bayesian inference in particle physics

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February 11, 2025

What is a probability?

Kolmogorov's probability axioms

1. $p(\Omega) = 1$, where Ω is the sample space.
2. $p(x) \geq 0$ for any event $x \subseteq \Omega$.
3. For any sequence of disjoint events $x_1, x_2, \ldots,$

$$p\left(\bigcup_{i=1}^{\infty} x_i\right) = \sum_{i=1}^{\infty} p(x_i)$$

Conditional probability

Is **defined** as the probability of an event x if we know that an event y is true

$$p(x|y) = \frac{p(x \cup y)}{p(y)}$$

Probability interpretations

The probability axioms and probability rules

- allow you to calculate new probabilities from old ones.
- do not tell you how to assign probabilities to begin with. For this we need probability interpretations.

The interpretations share the same mathematical framework, but the meaning of $p(x)$ is different.

Frequentist interpretation

Assign a probability as relative frequency

$$p(x) = \lim_{n \to \infty} \frac{n_x}{n}$$

- Can only be assigned to repeatable experiments
- Not everything is repeatable...
- No probabilities of single events

Bayesian interpretation

Assign a probability $p(x)$ as *degree of belief*.

- Probability depends on the experimenters' knowledge.
- Inference results are subjective.
- Everything is a random variable.

Bayesian inference

The Bayesian posterior is

$$p(\text{theory}|\text{data}) = \frac{p(\text{data}|\text{theory})p(\text{theory})}{p(\text{data})}$$

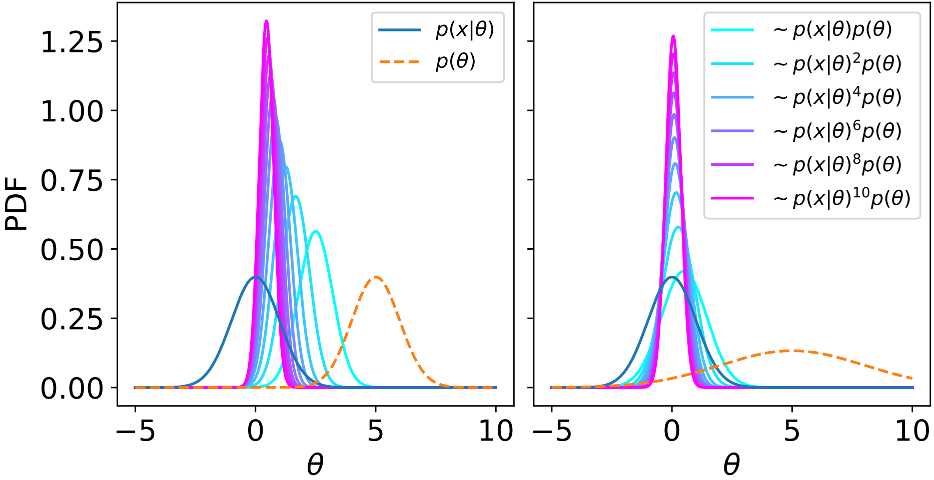
- **Likelihood** $p(\text{data}|\text{theory})$
- **Prior** $p(\text{theory})$
- **Evidence** $p(\text{data}) = \int p(\text{data}|\text{theory})p(\text{theory}$

Bayesian updating

Parameter values θ under which data x_1, x_2 is more probable on average get weighted up, other values get weighted down.

$$p(\theta|x_1, x_2) = \frac{p(x_2|\theta)}{p(x_2)} \frac{p(x_1|\theta)}{p(x_1)} p(\theta)$$

Bayesian updating



The common ground

Frequentist inference is based on

- the model of the observable data

$$\boldsymbol{p(x|\theta)}$$

Bayesian inference is based on

- the model of the observable data

$$\boldsymbol{p(x|\theta)}$$

- your prior belief

$$p(\theta)$$

Physics does not care...

... about our interpretation

For many inference problems, the frequentist and Bayesian approaches give similar numerical values, even though they answer different questions and are based on fundamentally different interpretations of probability.

Pour all energy into constructing the best possible $\boldsymbol{p(x|\theta)}$.

Nuisance parameters and priors

Frequentist nuisance parameters

Models are not perfect ➜ **systematic bias**
More general models include additional **nuisance** parameters, ν,

$$p(x|\theta, \nu)$$

Leads to increased statistical uncertainties on POIs (due to correlation)
Want to constrain nuisance parameters, but in the frequentist language **everything is data**.

... everything is data

"*The great advantage of the Bayesian approach is that it allows you to incorporate subjective beliefs, while the Frequentist approach pretends that you don´t have any.*"

– associated with Jim Berger by ChatGPT

... everything is data

Are we being honest here?

Prior knowledge in a typical frequientist analysis

- theory predictions
- model parameters (masses, couplings, ...)
- missing higher-order corrections
- MC normalizations
- ...

Frequentist "priors"

Constrain nuisance parameters using "auxiliary data" a,

$$L(\theta, \nu) = p(x|\theta, \nu)p(a|\nu)$$

$p(a, \nu)$ represents our "degree of belief" in ν.

Often "auxiliary data" is *created* to match our desired constraint term.

Bayesian nuisance parameters

If one has auxiliary data, the prior is

$$p(\nu|a) \propto p(a|\nu)p_0(\nu)$$

If $p_0(\nu)$ is chosen to have minimal impact, this overlaps with the frequentist treatment.
In the Bayesian case, other prior choices are also allowed, e.g.

$$p(\nu) = \text{Gauss}(\nu|\nu_0, \sigma_\nu)$$

Bayesian approach also requires priors for POIs.

Parameter inference

Parameter inference

Point estimates

Identify the most probable parameter point.

Interval estimation

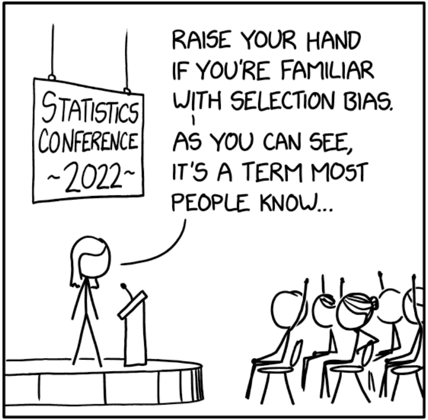
Identify extended regions in parameter space based on compatibility with the data.

Frequentist point estimates: estimators

Estimator is a *statistic* $\hat{\theta}(x)$, i.e. a well chosen function of the data.
Desired properties

- *consistency* $\lim_{N_x \to \infty} E(\hat{\theta}) = \theta_{true}$
- *unbiasedness* $b = E(\hat{\theta}) - \theta_{true}$
- *efficiency* (minimum variance)
- ...

A good data set is the key to success ...



Method of maximum likelihood

We find maximum likelihood estimators $\hat{\theta}$ by solving

$$\frac{\partial \ln L(x|\theta)}{\partial\theta}\Big|_{\theta=\hat{\theta}} = 0$$

With the property

$$\lim_{N\to\infty} p\left(\sqrt{N}(\hat{\theta} - \theta_{true})\right) = \mathcal{N}(0, I^{-1}(\theta))$$

This implies consistency, asymptotic unbiasedness and efficiency

$$\lim_{N\to\infty} V(\hat{\theta}) = I(\theta)^{-1} = E\left[\frac{\partial \ln L(x|\theta)}{\partial\theta}\right]^{-1}$$

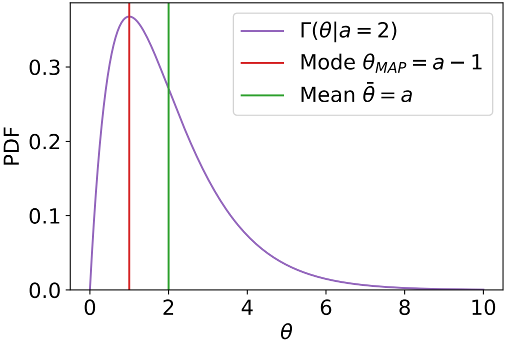
Bayesian point estimates

Mode / MAP
Value of θ with maximum a-posteriori probability

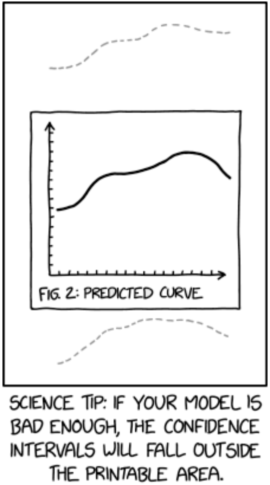
$$\theta_{MAP} = \text{argmax}_{\theta}\, p(\theta|x)$$

Mean
Expected value of θ under the posterior

$$\bar{\theta} = E_{p(\theta|x)}[\theta]$$

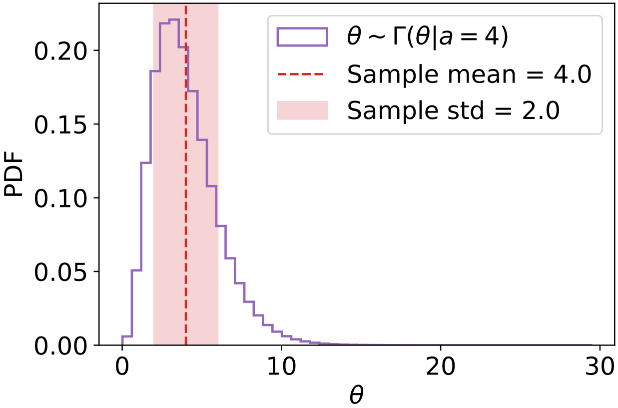


Intervals and limits



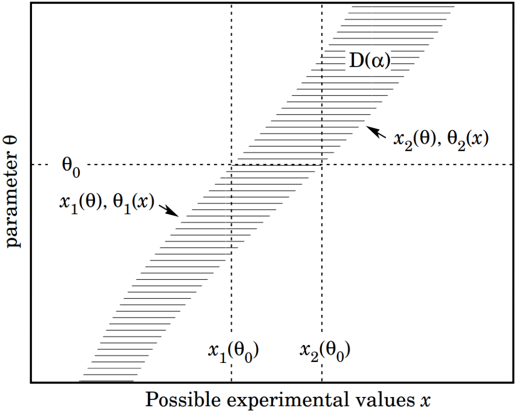
Intervals and limits

If an estimator PDF is not Normal, $\hat{\theta} \pm \sigma_\theta$ is meaningless.



Neyman confidence belt

$$\int_{x_1}^{x_2} dx\, p(x|\theta) \geq 1 - \alpha$$



Bayesian intervals

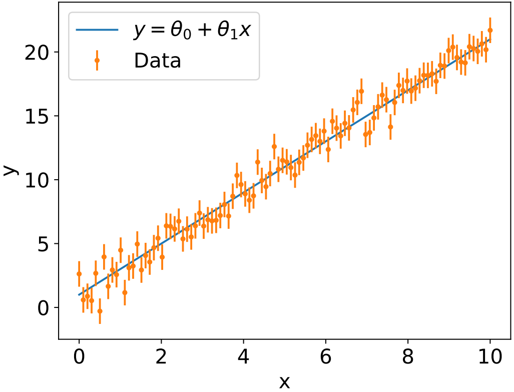
Credible intervals $[\theta_l, \theta_u]$ cover $1 - \alpha$ of the posterior

$$1 - \alpha = \int_{\theta_l}^{\theta_u} d\theta \, p(\theta, x)$$

- For upper/lower limits: set θ_l or θ_u to boundary
- Highest (posterior) density intervals (HDI): smallest possible interval

A simple linear model

- Our independent data : x_i, y_i, σ_i



A simple linear model

- Our independent data: x_i, y_i, σ_i
- Our model:

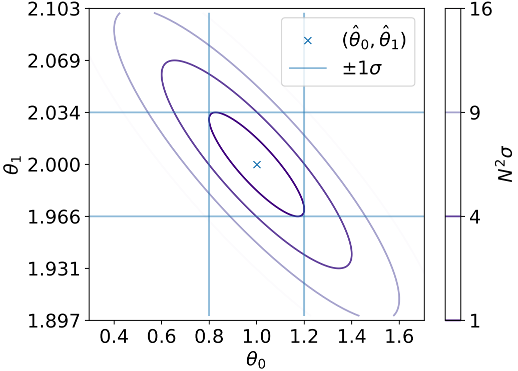
$$p(\mathbf{x}|\theta_0, \theta_1) = \prod_{x_i \in \mathbf{x}} \mathrm{Gauss}(x_i|\mu(x_i|\theta_0, \theta_1), \sigma_i)$$

$$\mu(x_i|\theta_0, \theta_1) = \theta_0 + \theta_1 x_i$$

➜ We want to know about θ_0, do not care about θ_1.

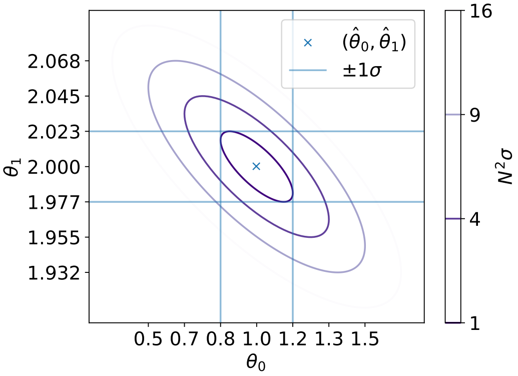
Unconstrained likelihood

$$-2\log p(\mathbf{x}|\theta_0,\theta_1) = \sum_{x_i\in\mathbf{x}} \frac{(x_i-\mu(x_i|\theta_0,\theta_1))^2}{\sigma_i^2}$$



Including a measurement t_1 of θ_1

$$-2\log p(\mathbf{x}|\theta_0,\theta_1) = \sum_{x_i\in\mathbf{x}} \frac{(x_i - \mu(x_i|\theta_0,\theta_1))^2}{\sigma_i^2} + \frac{(\theta_1 - t_1)^2}{\sigma_{t_1}^2}$$



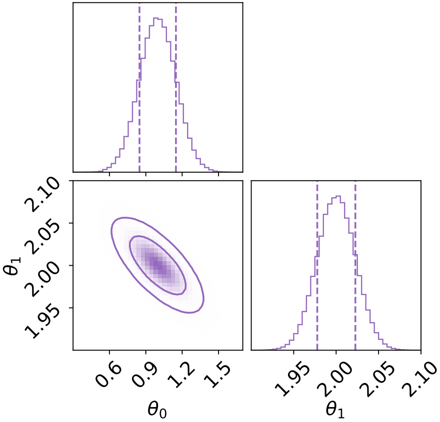
Posterior

$$p(\theta_0, \theta_1 | \mathbf{x}) \propto p(\mathbf{x} | \theta_0, \theta_1) \pi(\theta_0) \pi(\theta_1)$$

$$\pi(\theta_0) = \text{Uniform}(0, 2)$$

$$\pi(\theta_1) = \text{Gauss}(\theta_1 | t_1, \sigma_{t_1})$$

Corner plots are nice for visualization.



Marginal posterior

$$p(\theta_0|\mathbf{x}) = \int d\theta_1\, p(\theta_0, \theta_1|\mathbf{x}) = \text{Gauss}(\theta_0|\hat{\theta}_0, \sigma_{\theta_0})$$

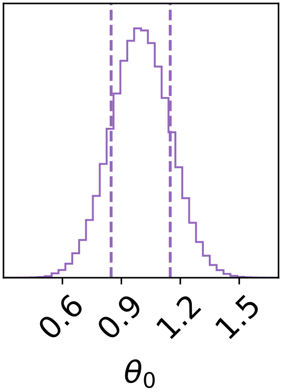
In this case, we get:

- Same $\hat{\theta}_0$ as for ML

$$\hat{\theta}_0 =$$

- Same σ_{θ_0} as for ML

$$\sigma_{\theta_0}^2 = \sum_{x_i,\sigma_i \in \mathbf{x},\sigma} \sigma_{t_1} x_i^2 + \sigma_i^2$$



MCMC

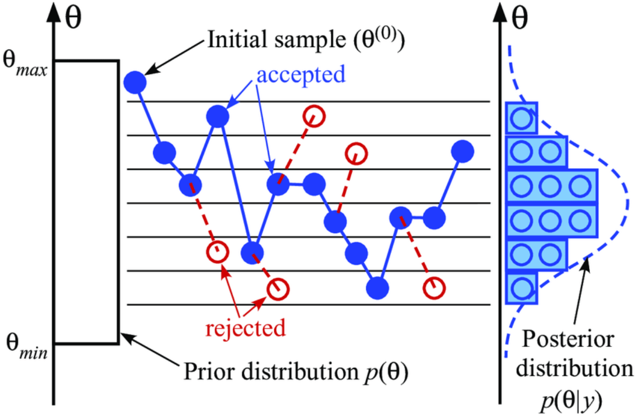
The hard part ...

- Usually, we are not interested in the nuisance parameters ν.
- One can obtain the posterior p.d.f. for θ alone by integrating over ν.
- The *marginal posterior* is

$$p(\theta|x) = \int d\nu \, p(\theta, \nu|x)$$

- Commonly a high dimensional integral
➜ compute with Monte Carlo methods.

Markov Chain Monte Carlo (MCMC)



Markov Process

The next element in the sequence (the Markov Chain) is proposed as a random variate y_{i+1} of a PDF g that is conditioned on a location parameter, set to the current location θ_i,

$$\ldots \rightarrow \theta_i \sim g(\theta_i|\theta_{i-1}) \rightarrow \theta_{i+1} \sim g(\theta_{i+1}|\theta_i) \rightarrow \ldots$$

Metropolis-Hastings

1. Generate $\theta \sim g(\theta|\theta_0)$
2. Set θ_1,

$$\theta_1 = \begin{cases} \theta & u \leq \min\left(1, \frac{p(\theta)g(\theta|\theta_0)}{p(\theta_0)g(\theta_0|\theta)}\right) \\ \theta_0 & \text{otherwise} \end{cases}$$

   where $u \sim \text{Uniform}(0, 1)$
3. Set $\theta_0 = \theta_1$ and return to step 1.

Note: We need to define a proposal distribution $g(\theta|\theta_0)$.

Chains

In MCMC we generate a sequence

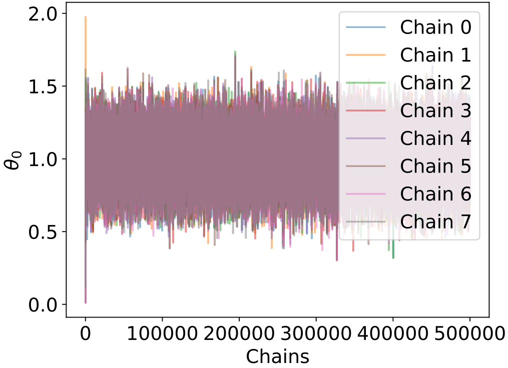
$$\theta_0 \to \theta_1 \to \theta_2 \to \dots$$

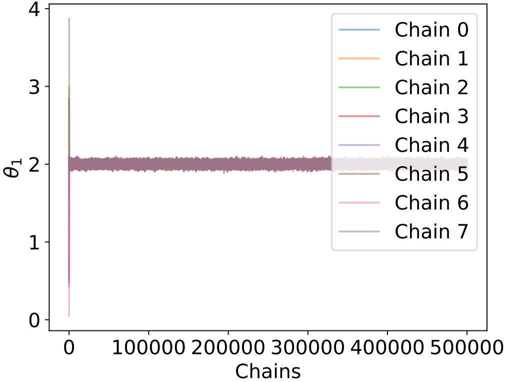
Only starting at one point can land you in local minima, hence often we sample

$$\begin{gathered}
\theta_0^0 \to \theta_1^0 \to \theta_2^0 \to \dots \\
\theta_0^1 \to \theta_1^1 \to \theta_2^1 \to \dots \\
\theta_0^2 \to \theta_1^2 \to \theta_2^2 \to \dots \\
\dots
\end{gathered}$$

Convergence

Trace plots are a useful convergence diagnostic





... but one can become more fancy.

Tools to try

PyMC

ArviZ