Introduction to frequentist statistics and Bayesian inference

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(HUST GW Summer School 2022, Lecture 1)

References

- Romano and Cornish, Living Reviews in Relativity article, 2017 (section 3)
- Rover, Messenger, Prix, “Bayesian versus frequentist upper limits,” PHYSTAT 2011 workshop
- Gregory, “Bayesian Logical data analysis”, 2005
- Howson and Urbach, “Scientific reasoning: the Bayesian approach”, 2006
- Helstrom, “Statistical theory of signal detection”, 1968
- Wainstein and Zubakov, “Extraction of signals from noise,” 1971

Outline

1. Probabilistic inference (broadly defined)
2. Frequentist statistics
3. Bayesian inference
4. Exercises - worked examples

Frequentist vs Bayesian "pre-test"

- An astronomer measures the mass of a NS in a binary pulsar system to be $M = (1.39 \pm 0.02) M_\odot$ with 90% confidence. How do you interpret the quoted result?
- Answer 1: You are 90% confident that the true mass of the NS lies in the interval $[1.37 M_\odot, 1.41 M_\odot]$
- Answer 2: You interpret 90% as the long-term relative frequency with which the true mass of the NS lies in the set of intervals $\{[\hat{M} - 0.02 M_\odot, \hat{M} + 0.02 M_\odot]\}$ where $\{\hat{M}\}$ is the set of measured masses.

Frequentist vs Bayesian "affiliation"

- If you chose answer 1, then you are a Bayesian
- If you chose answer 2, then you are a frequentist

Goal of science is to infer nature's state from observations

- Observations are:
  - **incomplete** (problem of induction)
  - **imprecise** (measurement noise, quantum mechanics, …)

$\Longrightarrow$ conclusions are uncertain!!

- **Probabilistic inference** (aka "plausible inference", "statistical inference") is a way of **dealing with uncertainty**

- **Different from** mathematical deduction

I. Probabilistic inference

Definitions of probability

- Frequentist definition: **Long-run relative frequency** of occurrence of an event in a set of repeatable identical experiments
- Bayesian definition: **Degree of belief** (or confidence, plausibility) in any proposition

NOTE: For the frequentist definition, probabilities can only be assigned to propositions about outcomes of repeatable identical experiments (i.e., **random variables**), not to hypotheses or parameters describing the state of nature, which have fixed but unknown values

Algebra of probability

- Possible values:

$$P(X = \text{true}) = 1$$
$$P(X = \text{false}) = 0$$
$$0 < P(X = \text{not sure}) < 1$$

- Sum rule:

$$P(X) + P(\bar{X}) = 1$$

- Product rule:

$$P(X\,|\,Y)P(Y) = P(X, Y)$$

- NOTE: $P(X\,|\,Y)$ is the probability of X conditioned on Y (assuming Y is true)
- $P(X\,|\,Y) \neq P(Y\,|\,X)$ in general. Example X="person is pregnant", Y="person is female"

Bayes' theorem (a simple consequence of the product rule!!)

likelihood

posterior

prior

$$P(H|D) = \frac{P(D|H)P(H)}{P(D)}$$

evidence

where $\quad P(D) = P(D|H)P(H) + P(D|\bar{H})P(\bar{H})$

"Learning from experience": the probability of H being true (in light of new data) increases by the ratio of the probability of obtaining the new data D when H is true to the probability of obtaining D in any case

Bayes' theorem (for parameters associated with a given hypothesis or model)

$$p(a|d,H) = \frac{p(d|a,H)p(a|H)}{p(d|H)}$$

where $$p(d|H) = \int \mathrm{d}a \, p(d|a,H)p(a|H)$$

"marginalization" over a

Comparing frequentist & Bayesian inference

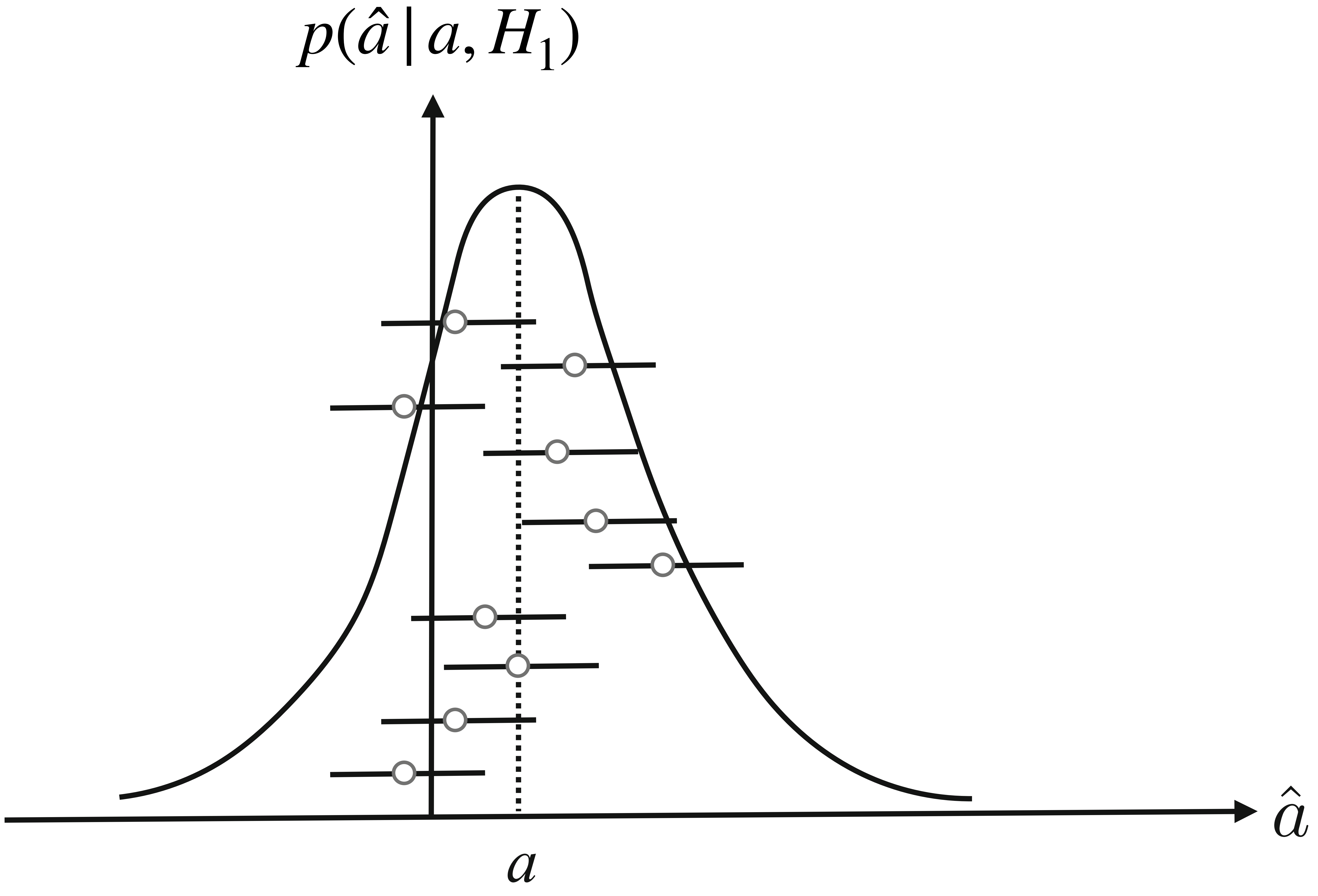
Frequentist statistics	**Bayesian infererence**
Probabilities are long-run relative occurrences of outcomes of repeatable expts —> can't be assigned to hypotheses	Probabilities are degree of belief —> can be assigned to hypotheses
Usually start with a likelihood function p(d|H)	Same as frequentist
Construct a statistic (some function of the data d) for parameter estimation or hypothesis testing	Need to specify priors for parameters and hypotheses
Calculate sampling distribution of the statistics (e.g., using time slide)	Use Bayes' theorem to update degree of belief in a parameter or hypothesis
Calculates confidence intervals (for parameter estimation) and p-values (for hypothesis testing)	Construct posteriors (for parameter estimation) and odds ratios (Bayes factors) (for hypothesis testing)

II. Frequentist statistics

Frequentist parameter estimation

- Construct a statistic (**estimator**) $\hat{a}$ for the parameter you are interested in
- Calculate the **sampling distribution** $p(\hat{a} \,|\, a, H_1)$ where $H_1 = \cup_{a>0} H_a$
- Statements like Prob$(a - \Delta < \hat{a} < a + \Delta)$ make sense since $\hat{a}$ is a random variable
- Statements like $a = \hat{a} \pm \Delta$ with 90% confidence must be interpreted as statements about the **randomness of the intervals**—i.e., 90% is the long-term relative frequency with which the true value of the parameter lies in the set of intervals $\{[\hat{a} - \Delta, \hat{a} + \Delta]\}$ where $\{\hat{a}\}$ is the set of measured parameter estimates

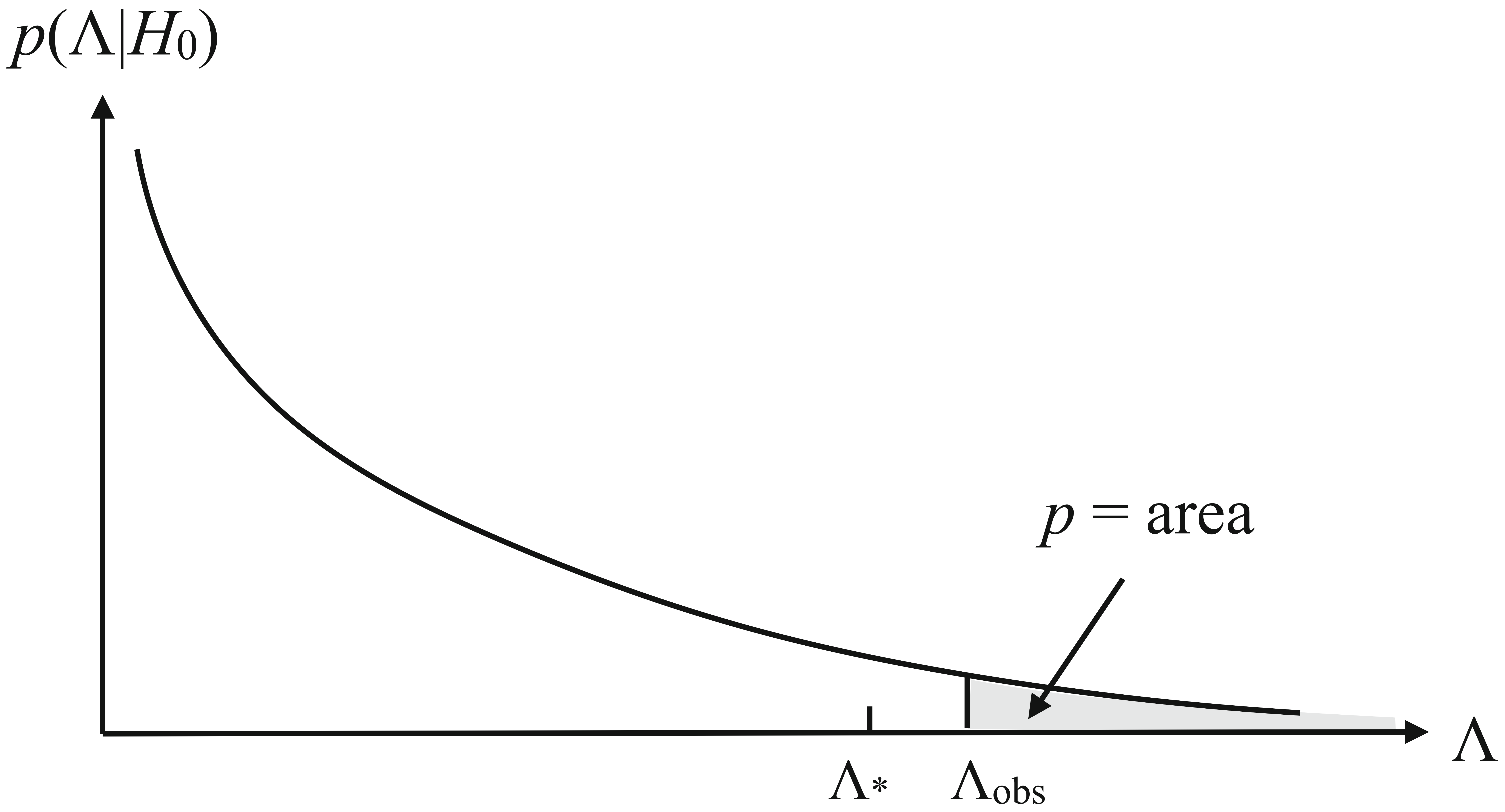
Frequentist parameter estimation



Frequentist hypothesis testing

- Suppose you want to test a hypothesis H_1 that a GW signal with some fixed but unknown amplitude $a > 0$ is present in the data ($H_1 \equiv \cup_{a>0} H_a$)
- Since you can't assign probabilities to hypotheses as a frequentist, you introduce the null hypothesis $H_0 = \bar{H}_1$ (for this example, $a = 0$), and then **argue for H_1 by arguing against H_0** (like proof by contradiction)
- So you construct a **test statistic** Λ and calculate its sampling distributions $p(\Lambda \,|\, H_0)$ and $p(\Lambda \,|\, a, H_1)$ conditioned on H_0 and H_1
- If the observed value of Λ lies far out in the tail for the null distribution, $p(\Lambda \,|\, H_0)$, you reject H_0 (accept H_1) at the $p \times 100\,\%$ level where $p = \text{Prob}(\Lambda > \Lambda_{\text{obs}} \,|\, H_0)$ is the so-called p-**value**

Frequentist p-value

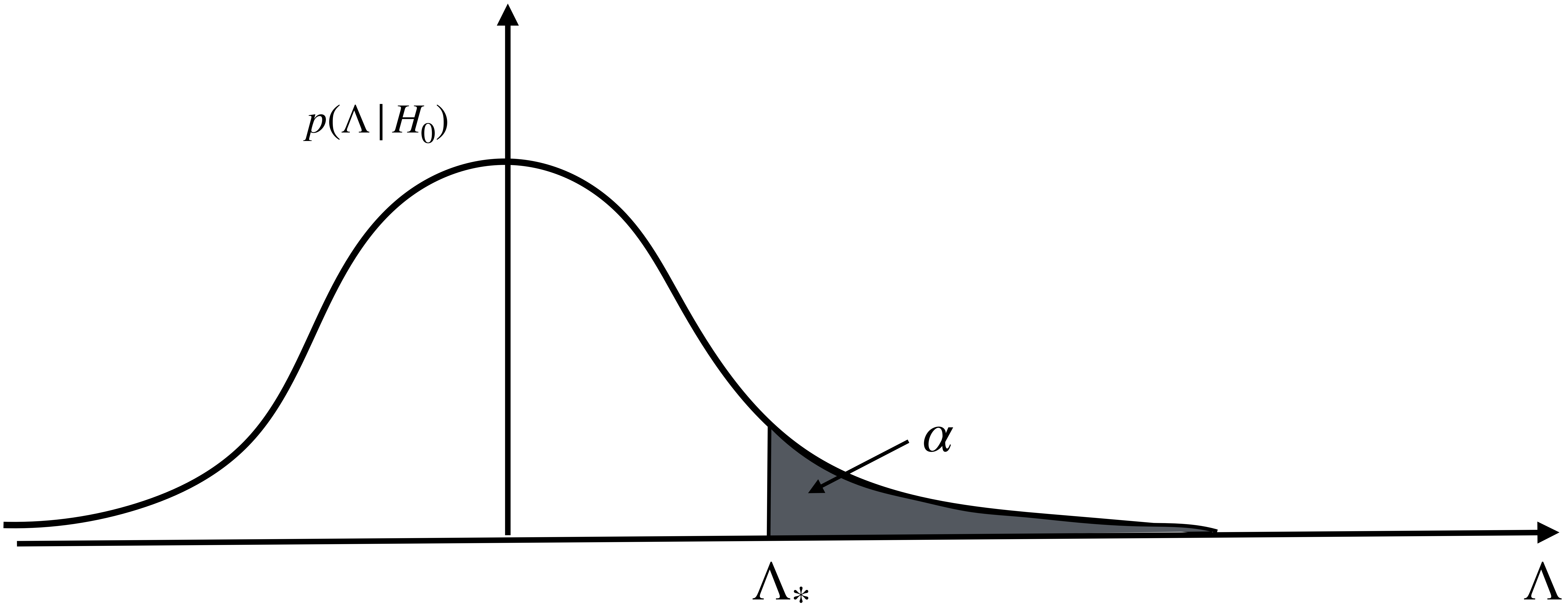


False alarm, false dismissal probabilities

- The p value needed to reject the null hypothesis defines a **threshold** Λ_*
- There are **two types of errors** when using the test statistic Λ:
  - **False alarm**: Reject the null hypothesis ($\Lambda_{\mathrm{obs}} > \Lambda_*$) when it is true
  - **False dismissal**: Accept the null hypothesis ($\Lambda_{\mathrm{obs}} \leq \Lambda_*$) when it is false
- Different test statistics are **judged according to their false alarm and false dismissal probabilities**
- In GW data analysis, one typically sets the false alarm probability to some acceptably low level (e.g., 1 in 1000), then finds the test statistic that minimizes the false dismissal probability for fixed false alarm probability (called the **Neyman-Pearson criterion**)

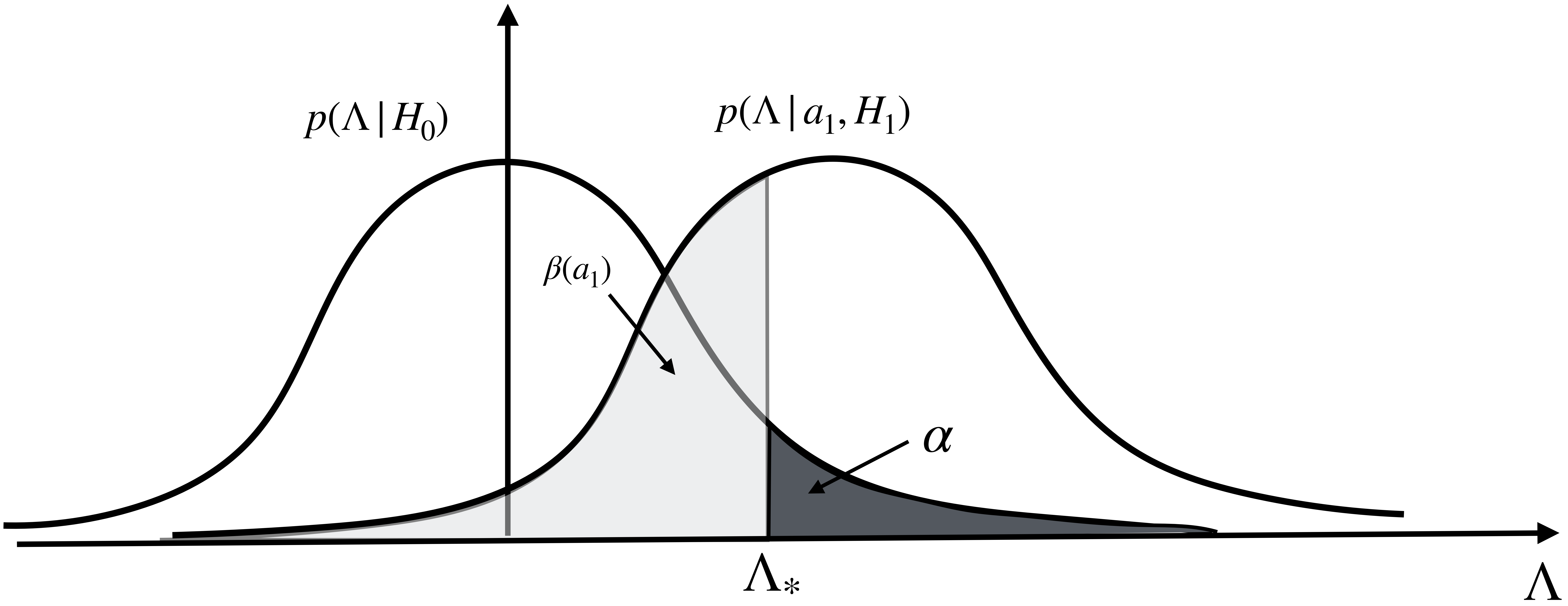
False alarm, false dismissal probabilities

- α is the false alarm probability (refers to H_0), e.g., 10%



False alarm, false dismissal probabilities

- α is the false alarm probability (refers to H_0)
- $\beta(a)$ is the false dismissal probability (refers to $H_1 \equiv \cup_{a>0} H_a$)



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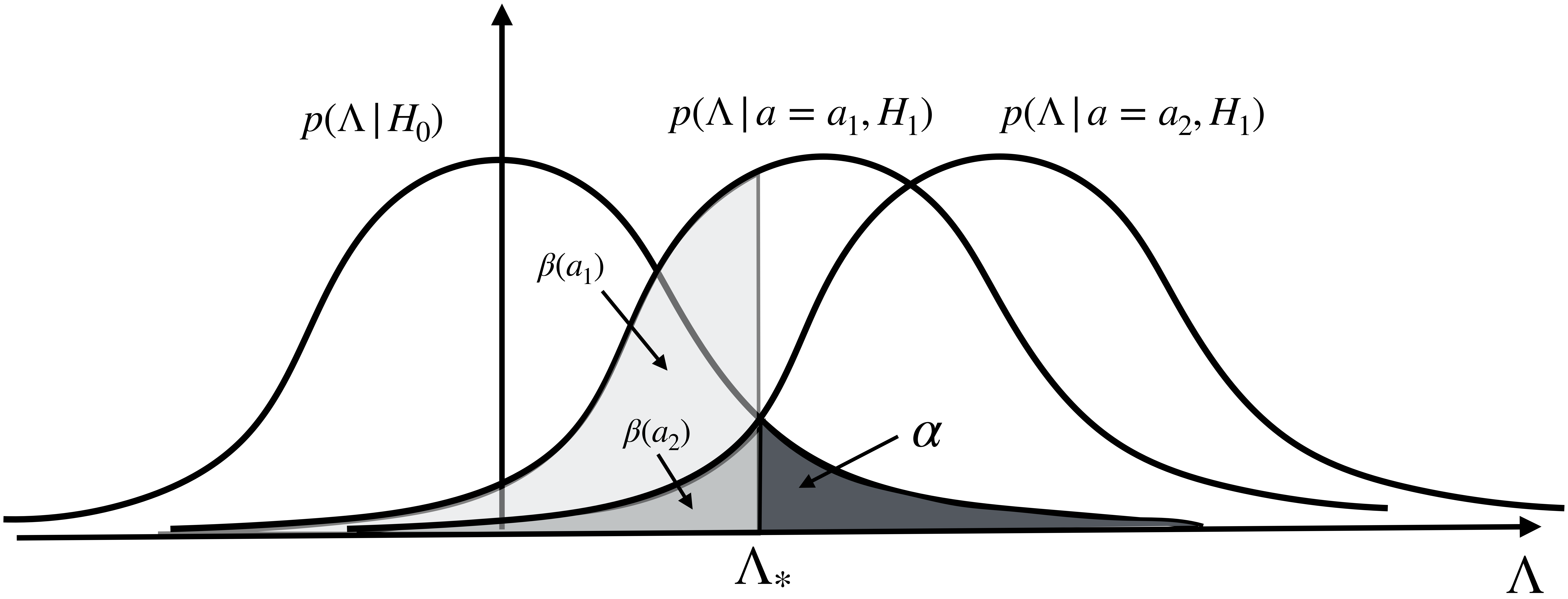
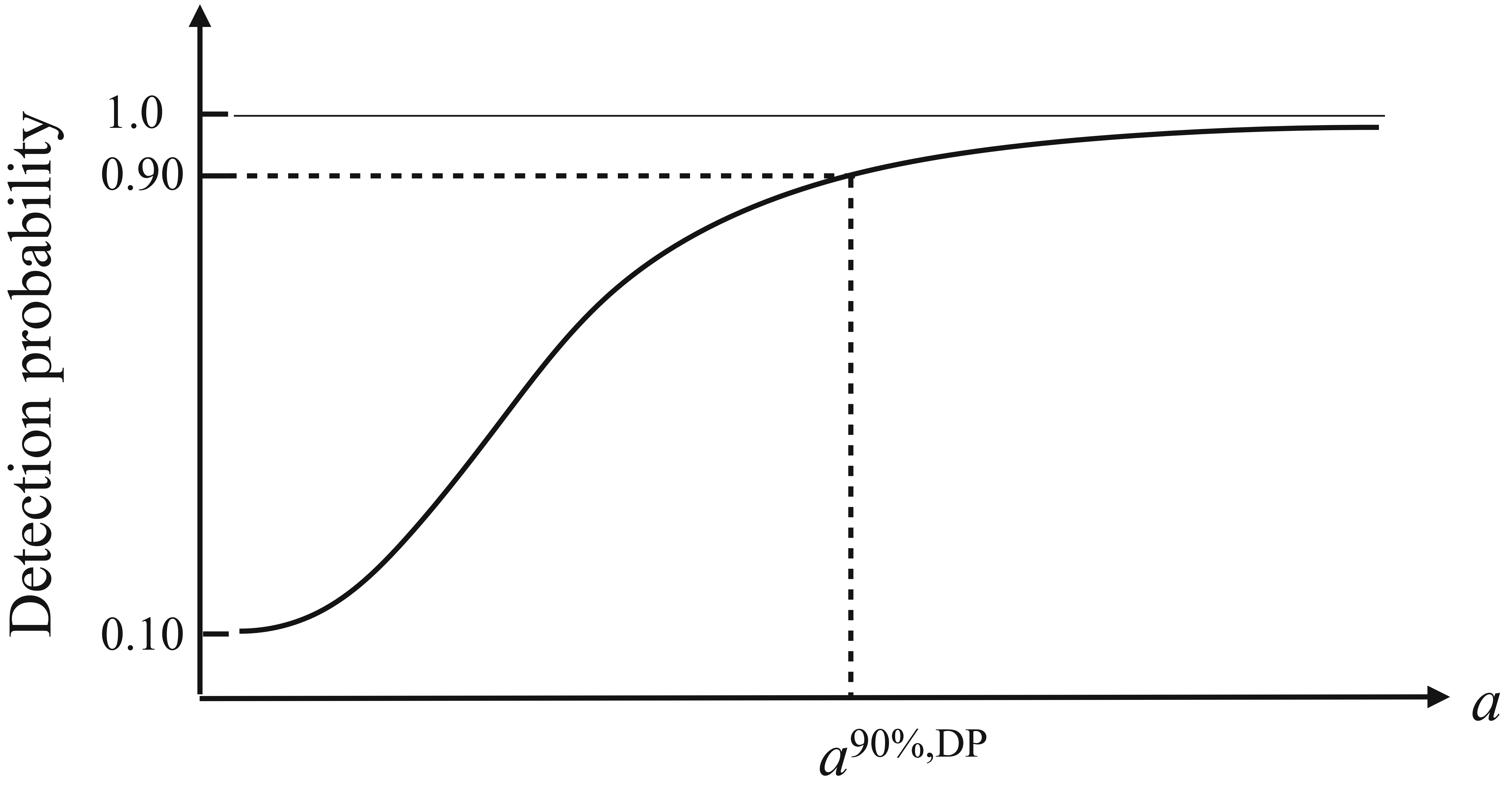


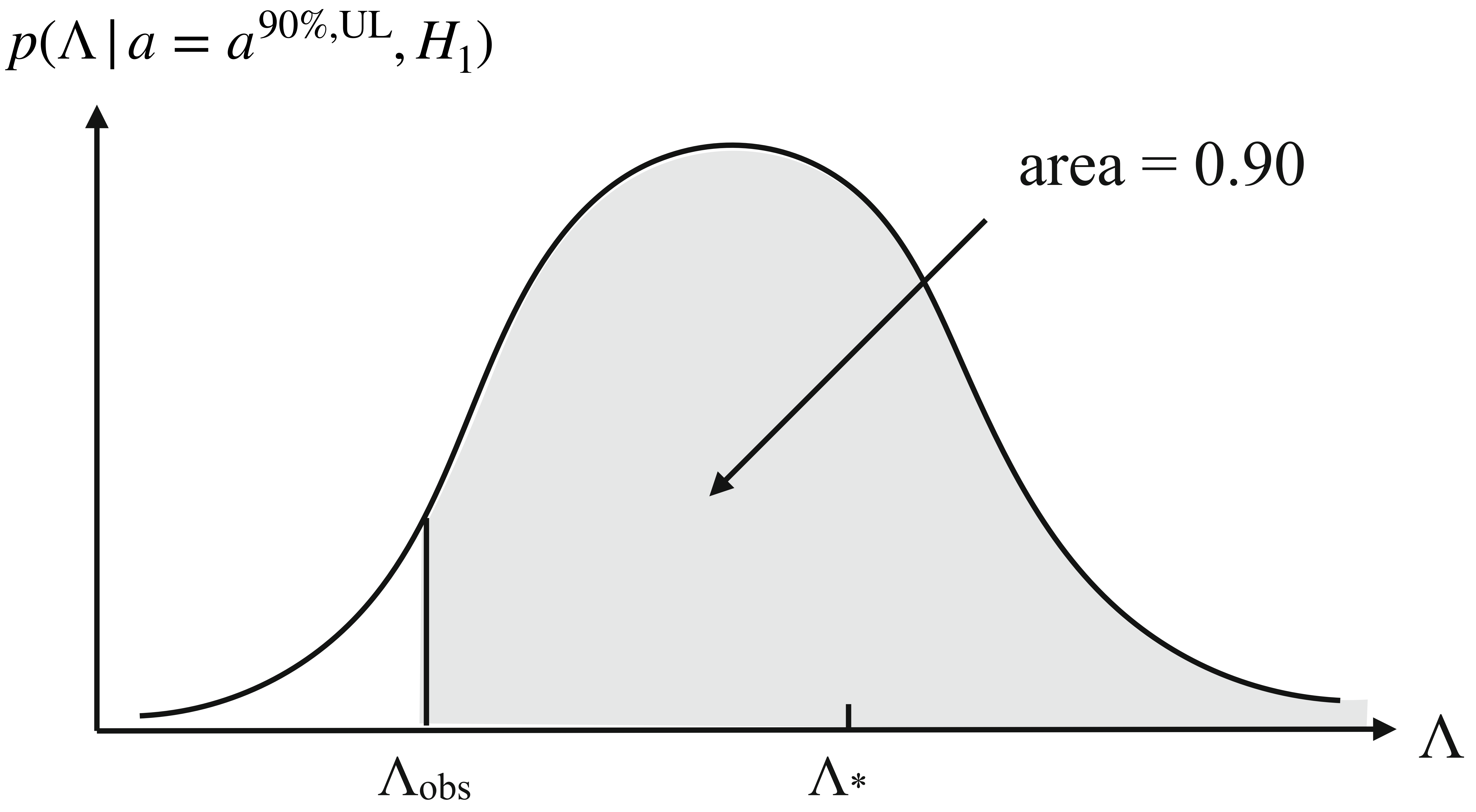
Detection probability

- $\gamma(a) \equiv 1 - \beta(a)$ is the fraction of the time that the test statistic Λ **correctly identifies the presence of a signal** with amplitude a



Frequentist upper limits

- If $\Lambda_{\rm obs} < \Lambda_*$ one often sets an UL on the amplitude a of the signal
- $a^{90\%,{\rm UL}}$ is the value of a for which ${\rm Prob}\,(\Lambda \geq \Lambda_{\rm obs}\,|\,a = a^{90\%,{\rm UL}}, H_1) = 0.90$



III. Bayesian inference

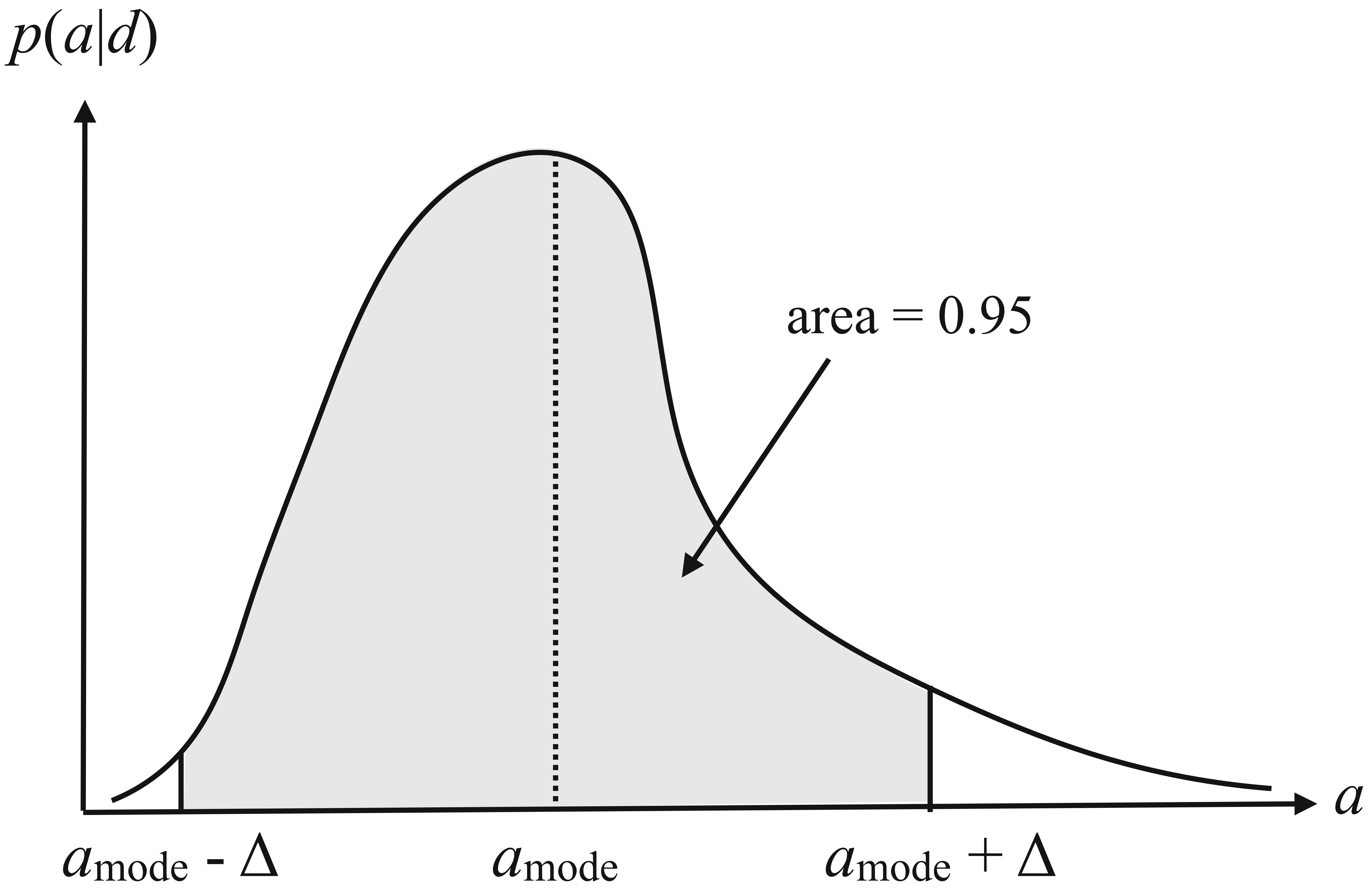
Bayesian parameter estimation

- Bayesian parameter estimation is via the **posterior** distribution $p(a\,|\,d,H)$
- The **posterior distributions contains all the information** about the parameter, but you can reduce it to a few numbers (e.g., mode, mean, stddev, …)
- If the posterior distribution depends on several parameters, you can obtain the posterior for one parameter by **marginalizing** over the others,

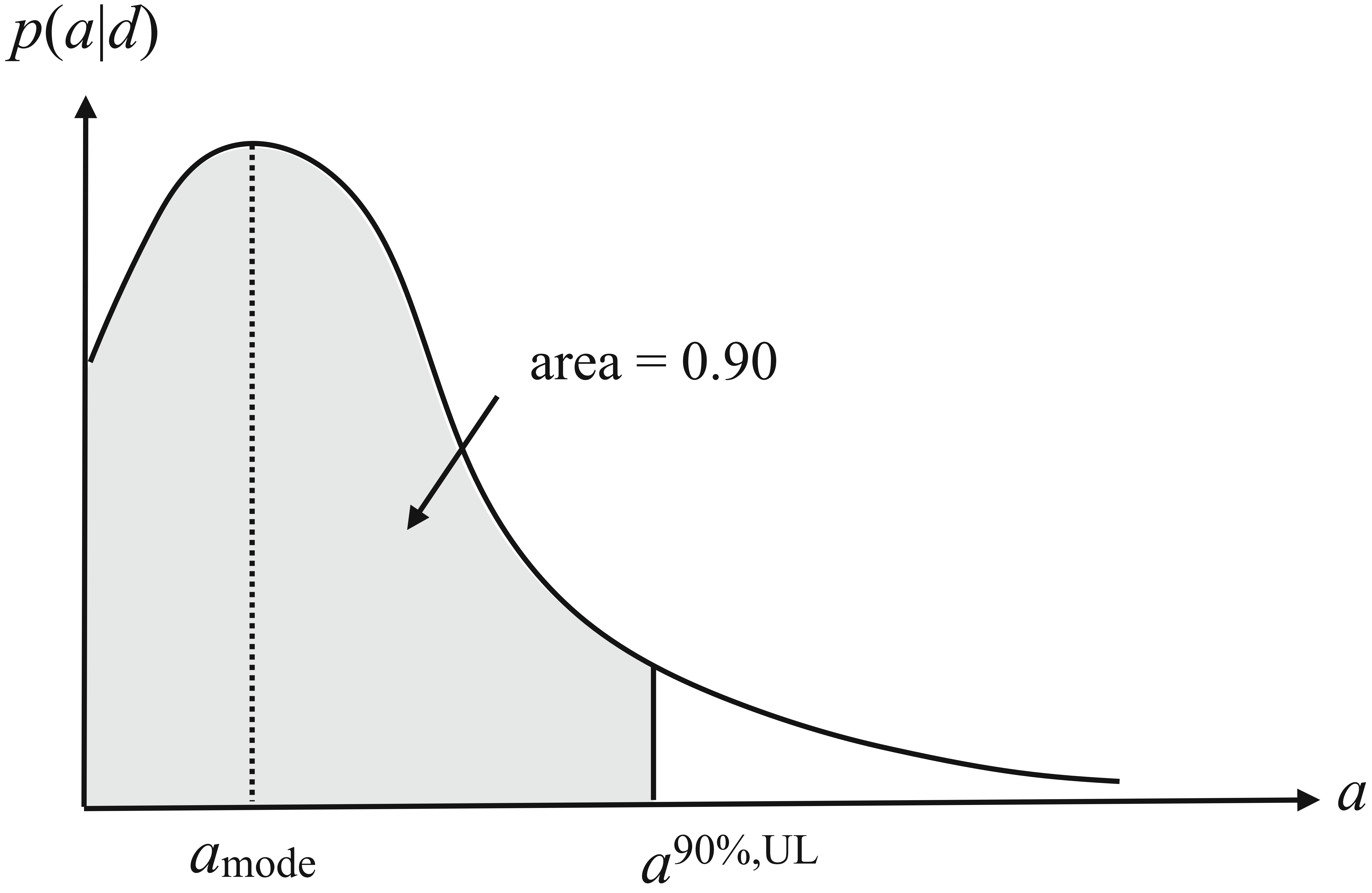
$$p(a\,|\,d,H) = \int \mathrm{d}b\, p(a,b\,|\,d,H) = \int \mathrm{d}b\, p(a\,|\,b,d,H)p(b\,|\,H)$$

- A Bayesian **credible interval** or **upper limit** defined in terms of the area under the posterior distribution

Bayesian credible interval



Bayesian credible upper limit



Bayesian hypothesis testing / model selection

- Compare two hypotheses H_1 and H_0 by taking their posterior **odds ratio**:

$$\frac{p(H_1|d)}{p(H_0|d)} = \frac{p(d|H_1)}{p(d|H_0)}\frac{p(H_1)}{p(H_0)}$$

posterior odds

Bayes factor $\mathscr{B}_{10}(d)$
(ratio of marginalized likelihoods or "evidences")

prior odds

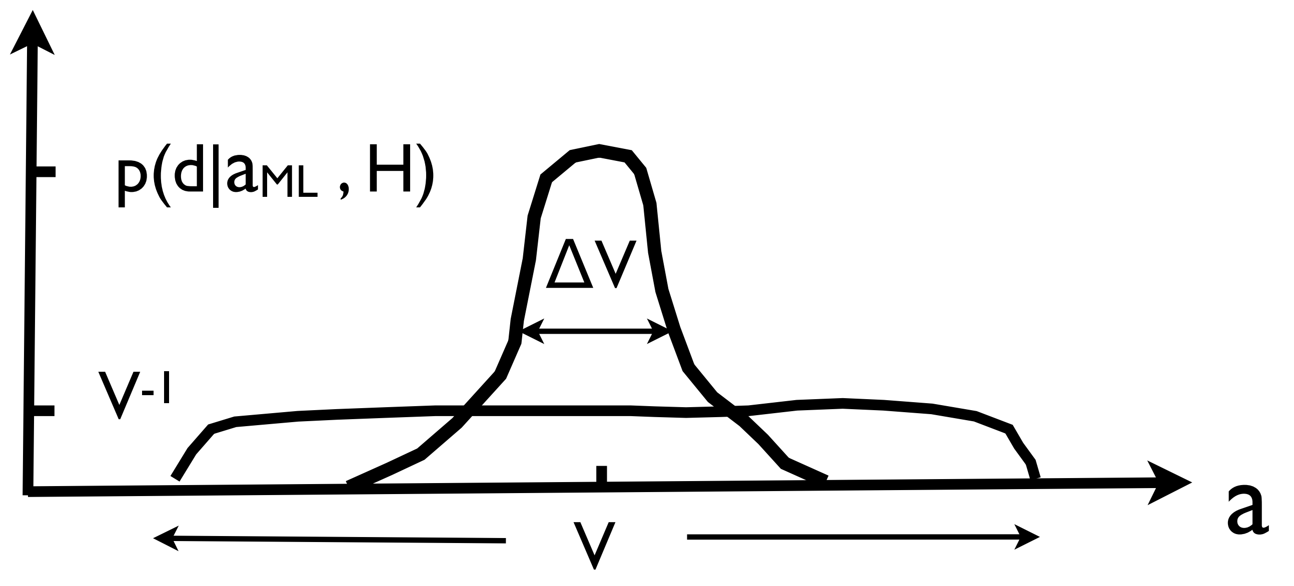
Relating Bayes factors and maximum-likelihood ratios

- Calculation of the evidence (=likelihood of an hypothesis) usually involves **marginalization over the parameters** associated with the hypothesis/model:

$$p(d|H) = \int \mathrm{d}a\, p(d|a,H)p(a|H)$$

- When the **data are informative**:

$$p(d|H) \simeq p(d|a_{\mathrm{ML}},H)p(a_{\mathrm{ML}}|H)\Delta a = \mathscr{L}_{\mathrm{ML}}(d|H)\Delta V/V$$



- Bayes factor:

$$\mathscr{B}_{10}(d) \equiv \frac{p(d|H_1)}{p(d|H_0)} = \frac{\int \mathrm{d}a_1\, p(d|a_1,H_1)p(a_1|H_1)}{\int \mathrm{d}a_0\, p(d|a_0,H_0)p(a_0|H_0)} \simeq \Lambda_{\mathrm{ML}}(d)\frac{\Delta V_1/V_1}{\Delta V_0/V_0}$$

- The $\Delta V/V$ factors penalize hypotheses that uses more parameter space volume V than necessary to fit the data ΔV (**Occam's penalty factor**)

Significance of Bayes factor values

approximately equal to the
squared SNR of the data

$\mathcal{B}_{\alpha\beta}(d)$	$2\ln\mathcal{B}_{\alpha\beta}(d)$	Evidence for model $\mathcal{M}_\alpha$ relative to $\mathcal{M}_\beta$
<1	<0	Negative (supports model $\mathcal{M}_\beta$)
1–3	0–2	Not worth more than a bare mention
3–20	2–6	Positive
20–150	6–10	Strong
>150	>10	Very strong

Adapted from Kass and Raftery (1995)

IV. Exercises / worked examples

1. Practical application of Bayes' theorem

- Suppose on your last visit to the doctor's office you took a test for some rare disease. This type of disease occurs in only 1 out of 10,000 people, as determined by a random sample of the population. The test that you took is rather effective in that it can correctly identify the presence of the disease 95% of the time, but it gives false positives 1% of the time.
- Suppose the test came up positive. What is the probability that you have the disease?

Solution to Bayes' theorem problem

- H = have the disease; + = test positive
- Information:

$$P(H) = 0.0001 \qquad P(\bar{H}) = 0.9999$$

$$P(+\,|\,H) = 0.95 \qquad P(+\,|\,\bar{H}) = 0.01$$

- Calculate:

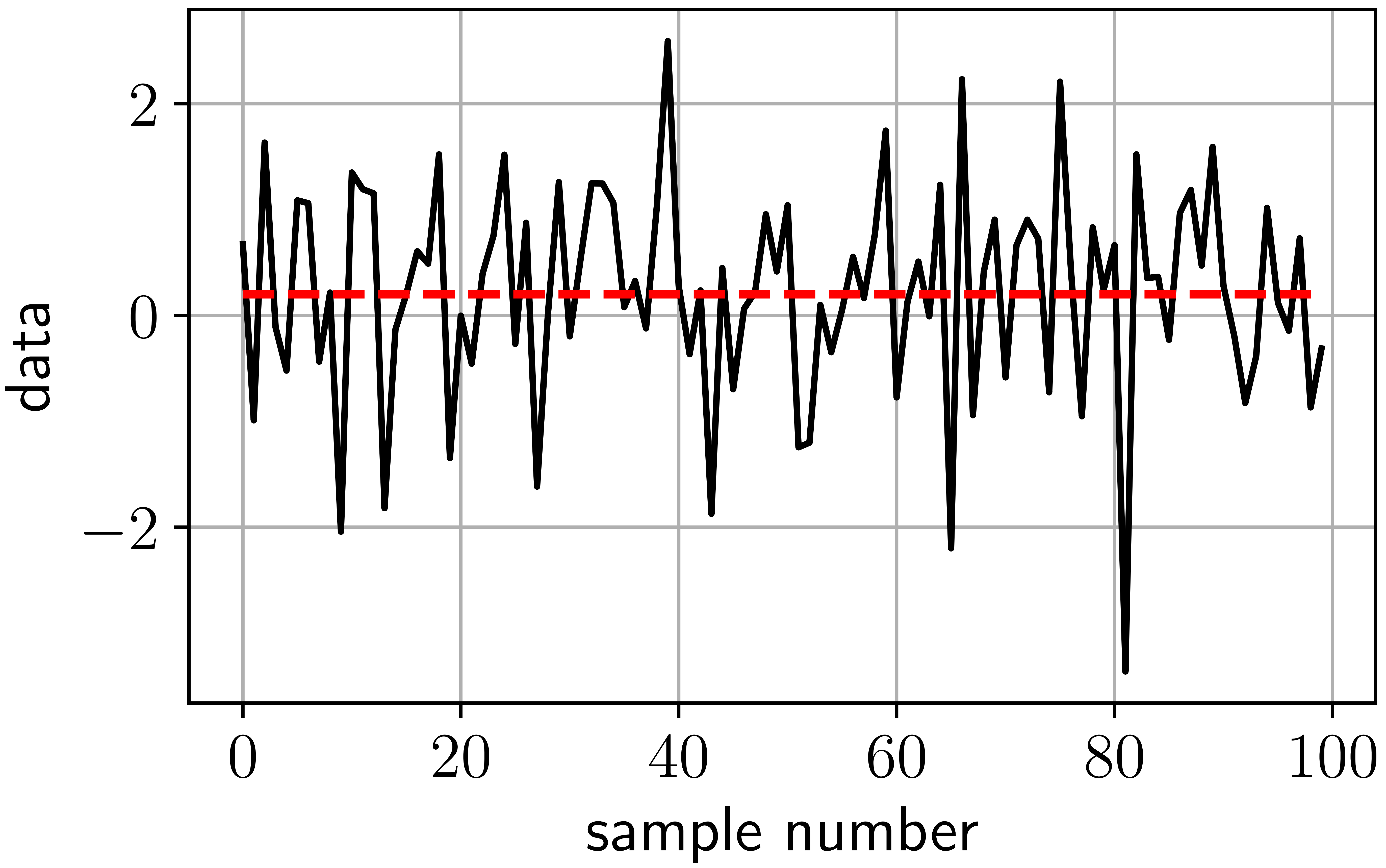
$$P(H\,|\,+) = \frac{P(+\,|\,H)P(H)}{P(+)}$$

$$\begin{aligned} P(+) &= P(+\,|\,H)P(H) + P(+\,|\,\bar{H})P(\bar{H}) \\ &= 0.95 \times 0.0001 + 0.01 \times 0.9999 \\ &\approx 0.01 \end{aligned}$$

- Final result:

$$P(H\,|\,+) \approx 0.0095 \approx 0.01$$

2. Comparing frequentist and Bayesian analyses for a constant amplitude signal in white noise



Key formulae

Likelihoods functions:

$$p(d\,|\,\mathcal{M}_0) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^N \exp\left[-\frac{1}{2\sigma^2}\sum_{i=1}^{N} d_i^2\right]$$

$$p(d\,|\,a, \mathcal{M}_1) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^N \exp\left[-\frac{1}{2\sigma^2}\sum_{i=1}^{N} (d_i - a)^2\right]$$

Prior:

$$p(a\,|\,\mathcal{M}_1) = \frac{1}{a_{\max}}$$

Parameter choices:

$N = 100\,, \quad \sigma = 1\,, \quad 0 \leq a \leq a_{\max}\,, \quad a_0 =$ true value

Key formulae

Maximum-likelihood estimator:

$$\hat{a} \equiv a_{\rm ML}(d) = \frac{1}{N}\sum_{i=1}^{N} d_i \equiv \bar{d} \qquad \sigma_{\hat{a}}^2 = \frac{\sigma^2}{N}$$

Useful identity:

$$\sum_{i=1}^{N}(d_i - a)^2 = \sum_i d_i^2 - N\hat{a}^2 + N(a-\hat{a})^2 = N\left(\mathrm{Var}[d] + (a-\hat{a})^2\right)$$

Likelihood function (in terms of ML estimator):

$$p(d\,|\,a,\mathscr{M}_1) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^N \exp\left[-\frac{\mathrm{Var}[d]}{2\sigma_{\hat{a}}^2}\right]\exp\left[-\frac{(a-\hat{a})^2}{2\sigma_{\hat{a}}^2}\right]$$

Evidence:

$$p(d\,|\,\mathscr{M}_1) = \frac{\exp\left[-\frac{\mathrm{Var}[d]}{2\sigma_{\hat{a}}^2}\right]\left[\mathrm{erf}\left(\frac{a_{\max}-\hat{a}}{\sqrt{2}\sigma_{\hat{a}}}\right) + \mathrm{erf}\left(\frac{\hat{a}}{\sqrt{2}\sigma_{\hat{a}}}\right)\right]}{2a_{\max}\left(\sqrt{2\pi}\sigma\right)^{N-1}\sqrt{N}}$$

Posterior distribution:

$$p(a\,|\,d,\mathscr{M}_1) = \frac{1}{\sqrt{2\pi}\sigma_{\hat{a}}}\exp\left[-\frac{(a-\hat{a})^2}{2\sigma_{\hat{a}}^2}\right] 2\left[\mathrm{erf}\left(\frac{a_{\max}-\hat{a}}{\sqrt{2}\sigma_{\hat{a}}}\right) + \mathrm{erf}\left(\frac{\hat{a}}{\sqrt{2}\sigma_{\hat{a}}}\right)\right]^{-1}$$

Key formulae

Bayes factor:

$$\mathscr{B}_{10}(d) = \exp\left[\frac{\hat{a}^2}{2\sigma_{\hat{a}}^2}\right]\left(\frac{\sqrt{2\pi}\sigma_{\hat{a}}}{a_{\max}}\right)\frac{1}{2}\left[\mathrm{erf}\left(\frac{a_{\max}-\hat{a}}{\sqrt{2}\sigma_{\hat{a}}}\right)+\mathrm{erf}\left(\frac{\hat{a}}{\sqrt{2}\sigma_{\hat{a}}}\right)\right] \simeq \exp\left[\frac{\hat{a}^2}{2\sigma_{\hat{a}}^2}\right]\left(\frac{\sqrt{2\pi}\sigma_{\hat{a}}}{a_{\max}}\right)$$

Maximum likelihood ratio statistic:

$$\Lambda_{\mathrm{ML}}(d) = \exp\left(\frac{\hat{a}^2}{2\sigma_{\hat{a}}^2}\right)$$

Frequentist test statistic:

$$\Lambda(d) \equiv 2\ln\Lambda_{\mathrm{ML}}(d) = \frac{\hat{a}^2}{\sigma_{\hat{a}}^2} = \left(\frac{\sqrt{N}\bar{d}}{\sigma}\right)^2 \equiv \rho^2$$

Sampling distributions of the test statistic:

$$p(\Lambda\,|\,\mathscr{M}_0) = \frac{1}{\sqrt{2\pi\Lambda}}e^{-\Lambda/2}$$

$$p(\Lambda\,|\,a,\mathscr{M}_1) = \frac{1}{\sqrt{2\pi\Lambda}}\frac{1}{2}\left[e^{-\frac{1}{2}(\sqrt{\Lambda}-\sqrt{\lambda})^2}+e^{-\frac{1}{2}(\sqrt{\Lambda}+\sqrt{\lambda})^2}\right] \qquad \lambda = \langle\rho\rangle^2 = \frac{Na^2}{\sigma^2}$$

See romano_notes1.pdf and romano_code1.ipynb for solutions