Data Analysis and Bayesian Methods Lecture 3

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DARN, NOT SIGNIFICANT. WE NEED MORE DATA. HAVE THEM EACH TRY YELLING INTO THE MIC A FEW MORE TIMES.

Hypothesis Testing

๏*You could exclude a signal hypothesis, given the observation*

๏*H0: BKG-only*

๏*H1: SIG+BKG*

๏*limit setting:check if the data exclude H1 in favour of H0*

๏*Establishing a signal: given the observation, reject H0 in favour of H1 with some level of confidence*

๏*in HEP, the famous "5*σ*"*

Hypothesis Testing

- ๏*The test statistics is any quantity with some discriminating power between H0 and H1*
	- ๏*The larger the separation between the two distributions, the better the test*
- ๏*You need a model of your test statistics* Λ(*D*|*θ*, *α*)
	- ๏*An analytical description*
	- ๏*A simulation-based template (e.g., a histogram)*
- ๏*There will be nuisance parameters ν morphing this model in various ways*
- ๏*The model might depend on some parameter of interest* θ *(e.g., resonance mass in a resonance search)*

The test statistics

๏*In your counting experiment you could use*

๏*The distribution of the recorded energy, described with multiple-bin histogram (product of Poisson)*

๏*The likelihood for a Poisson count above threshold*

๏*…*

 $\mathscr{L} = P(n | \lambda_B + \lambda_S) G(\bar{\lambda}_S | \lambda_S, \sigma_{\lambda_S})$ $\big)G(\bar{\lambda})$ $B \mid \lambda_B, \sigma_{\lambda_B}$

๏*We will see what is usually adopted and why*

The test statistics

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๏*In your counting experiment, the expected signal depends on the mass of the particle and its cross section*

๏*Assume a mass value*

๏*For each mass value, assume a cross section and build the two distributions for your test statistic*

๏*Your problem might be more complicated, requiring end-toend simulations to build your model numerically. But the principle stays the same*

Trying to exclude a signal

Your observation

Observed CLs+b

Dividends Λobs

Dividends Λobs

I Amedian Λmedian

Expected "1 sigma" CLs

๏*At fixed mass value, and for a fixed cross section, compute*

๏*observed CLs*

๏*expected CLs @ median*

๏*expected CLs ±1*σ

๏*expected CLs ±2*σ

๏*Then repeat, for the same mass value and changing the cross section*

Build the CLs exclusion

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Cross section

Cross section

๏*Doing so, you associate each mass value to a band/line of expected/ observed CLs as a function of the cross section*

๏*For a 95% CL result, you would intersect the band/line with a horizontal line at 0.05*

Build the CLs exclusion

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Cross section

0.4 1.8

๏*The intercepted values determine the observed and expected limits for that mass value*

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Cross section

๏*The intercepted values determine the observed and expected limits for that mass value*

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Cross section

๏*The intercepted values determine the observed and expected limits for that mass value*

๏*Repeating the procedure for every mass value, one derives the exclusion plot that you typically see on papers*

Build the CLs exclusion

- ๏*Sometimes observed line goes outside the band. This is the sign that something is going on*
	- ๏*A weak limit implies that the outcome is signal-like, so the signal can't be excluded*
	- ๏*A strong limit implies the opposite: data fluctuated below the expectation*

๏*People read this as evidence of a signal. But this is not a correct quantitative statement. A different procedure is needed in that case*

How to read these plots wrongly

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๏*To claim a discovery, one needs to exclude the possibility that background could mimic a signal*

๏*To do so, one measures (with toy experiments? by hand?) the probability that a bkg-only sample gives a result as signallike as what was seen on data*

๏*If a conventional threshold (decided a-priori, e.g., the 5*σ *threshold in HEP) is passed, a discovery is claimed*

Number of Sigmas

Background p-value

Background p-value

๏*The power of your test depends on how well separating the chosen* Λ *quantity is (the Energy distribution in our example)*

๏*What's the best* Λ*? In absence of systematic uncertainties (aka, simple hypotheses, more about this later), we have an*

$$
L(\mathbf{X}) = \frac{f_0(\mathbf{X})}{f_1(\mathbf{X})}
$$

Theorem 6.1 (Neyman-Pearson lemma). Let H_0 and H_1 be simple hypotheses (in which the data distributions are either both discrete or both continuous). For a constant $c > 0$, suppose that the likelihood ratio test which rejects H_0 when $L(\mathbf{x}) < c$ has significance level α . Then for any other test of H_0 with significance level at most α , its power against H_1 is at most

answer

type I error per unit increase of power". Another interpretation is that these are the points providing the strongest evidence in favor of H_1 over H_0 . The statistic

is called the likelihood ratio statistic, and the test that rejects for small values of $L(X)$ is called the likelihood ratio test. The Neyman-Pearson lemma shows that the likelihood ratio test is the most powerful test of H_0 against H_1 :

the power of this likelihood ratio test.

Which test statistics?

๏*Given a statistical model (e.g., our Poisson of known* λ *and unknown k), we can assess probabilities. Pr is a function of k*

๏*Given a class of statistical models for k, function of unknown* λ*, we have a likelihood model*

๏*A likelihood is a function of* λ*, given the observed k*

[Reminder] Likelihood

- ๏*Let's imagine a histogram of a quantity x and a curve b(x) predicting the amount of expected background*
	- ๏*for each bin centre xi we can compute bi=b(xi)*
	- ๏*the bi values will depend on a set of parameters that describe the curve* $y = b(x)$
- ๏*In each bin, we observe some counting ni*
- ๏*The likelihood of the model is given by*

 $\mathscr{L}(\vec{n} \mid \vec{\alpha}) = \prod P(n_i | b_i(\vec{\alpha}))$ *i* $)) = \prod$

[Reminder] Likelihood

$$
\prod_i P(n_i | b(x_i | \overrightarrow{\alpha})) = \prod_i \frac{e^{-b(x_i | \overrightarrow{\alpha})} b(x_i | \overrightarrow{\alpha})}{n_i!}
$$

๏*A simple hypothesis is one in which the statistical model is fully specified (no nuisance parameters)*

๏*In our example, we do know the* α *values for a BKG-only and and SIG+BKG model*

๏*Whenever this is not the case, the likelihood ratio is not the strongest test statistics*

๏*This is always the case, since there are always nuisance parameters determining systematic effects*

๏*This doesn't mean that the LR test statistics should not be used*

๏*In real life, many (all?) the a parameters might be unknown but we might have some*

๏*Experimental parameters (e.g., muon reconstruction efficiency) might be known from a*

๏*Frequentist:* ᾱ *is a measured value of* α *and the product of* P *and the likelihood is still a likelihood* ∏ *i e*−*b*(*xi* $|\vec{\alpha})$ $b(x_i | \overrightarrow{a})$ n_i *ni*! \rightarrow \prod *i* $e^{-b(x_i|\vec{\alpha})}b(x_i|\vec{\alpha})^{n_i}$ $n_i!$ $\boxed{1\ 1}$ *j* $(\bar{\alpha}_j | \alpha_j)$

$$
\prod_{i} \frac{e^{-b(x_i|\vec{\alpha})}b(x_i|\vec{\alpha})^{n_i}}{n_i!}.
$$

- *information on them*
	- ๏*Theory parameters might be predicted by a calculation*
	- *control sample*
- *diverge*

๏*In this case, the model is extended multiplying the likelihood by the function that constraints* α *around some measured value* ᾶ*. This is where statistical interpretations*

๏*Bayesian:* P*(*ᾱ*) is a prior function of* α *and the product of* P *and the likelihood is a*

posterior probability function

(Reminder) Non-simple hypotheses

∏

$$
\frac{e^{-b(x_i|\vec{\alpha})}b(x_i|\vec{\alpha})^{n_i}}{n_i!} \to \prod_i \frac{e^{-b(x_i|\vec{\alpha})}b(x_i|\vec{\alpha})^{n_i}}{n_i!} \prod_j \mathcal{P}(\alpha_j|\vec{\alpha}_j)
$$

๏*One would then try to go back to a simple-hypothesis case, removing the dependence on the nuisance parameters*

a Profiled likelihood: $\mathscr{L}(D|\alpha)\mathscr{P}(\bar{\alpha}|\alpha) \rightarrow \mathscr{L}(D|\hat{\alpha}) = \max_{\alpha}$ ̂ *α* $\mathscr{L}(D|\alpha)\mathscr{P}(\bar{\alpha}|\alpha)$

๏*Marginalized posterior:*

๏*In any case, when is Gaussian and narrow, the difference becomes small: even in Bayesian statistics one tends to use the maximum a-posteriori (MAP) approximation*

$$
\mathscr{L}(D|\alpha)\mathscr{P}(\bar{\alpha}|\alpha) \to \int d\alpha \mathscr{L}(D|\alpha)\mathscr{P}(\alpha|\bar{\alpha})
$$

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hypotheses. The likelihood ratio is then

- ๏*The NP Lemma does not guarantees that this is the optimal choice*
- ๏*It is also very demanding computationally*
- ๏*When using a max-like approximation, one goes back to simple*
	- **Signal yield (and shape) fixed to specific signal under test**
	- **Signal yield =0, i.e., BKG-only hypothesis**

- ๏*For hypothesis testing, one needs to generate "toy samples"* and profile the likelihood at each toy to build the test
- ๏*This might be a 1000-dim minimisation to be repeated N times*

statistics distribution

Back to simple hypothesis

$$
\frac{\hat{\mathscr{L}}(D|H_1)}{\hat{\mathscr{L}}(D|H_0)} = \frac{\hat{\mathscr{L}}(D|\mu = \bar{\mu})}{\hat{\mathscr{L}}(D|\mu = 0)}
$$

๏*At the LHC, one typically uses a different test statistics*

The LHC Test Statistics

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U

- *statistics assumes a specific nuisance (Wilks' theorem)*
	- *seconds, w/o running any toy-MC minimisation*
- **(*) [It's more complicated than that when the max on](https://s3.cern.ch/inspire-prod-files-f/fe85dc6bd026c535cb3ebb734cb90cd0) μ is outside the fit range. [See "Practical Statistics for the LHC" by K. Cranmer for more details](https://s3.cern.ch/inspire-prod-files-f/fe85dc6bd026c535cb3ebb734cb90cd0)**

๏*You are not expected to be doing this by hand*

-
- ๏*ROOT has specific packages (RooFit+RooStat) for this*
	- *implement most of the routine statistical applications*

๏*Experiments have software tools built on it that that you need to survive:*

๏*ATLAS [PyHf](https://iris-hep.org/projects/pyhf.html)*

๏*CMS [Combine](https://cms-analysis.github.io/HiggsAnalysis-CombinedLimit/)*

๏*But it is important to have clear in mind what is going on in these softwares (particularly when you have to debug the outcome)*

Hypothesis testing in practice

Bayesian Inference

WELL OK THEN WAIT A MNUTE -TAKING ALL THESE IS THAT YOUR THINGS INTO BIASED COIN? CONSIDERATION ... HEADS. AHA! PRIOR CONSTRUCTION! BAYES WINS AGAIN! **HMM TRICKY** DAMN **FREQUENTIST BAYESIAN FREQUENTIST** REVBAYES #005

๏*Bayesian applications use this rule of probability to make statements on the true values of the parameters on which a likelihood model depends on* $(D | \theta)$ *π*(*θ*)

 $\theta p(D | \theta) \pi(\theta)$

 \odot $p(D|\theta)$ is the probability model (the likelihood) of the data, function of *a parameter of interest θ*

 \odot $p(\theta|D)$ *is the posterior probability for* θ *given the data D*

 $\Theta \pi(\theta)$ *is the prior on* θ

๏*Bayes' rule starts from the probability of two dependent events* $P(A \cap B) = P(A | B)P(B) = P(B | A)P(A)$ $P(B|A) =$ *P*(*A*|*B*)*P*(*B*) *P*(*A*)

= *P*(*A*|*B*)*P*(*B*) $\sum_{B} P(A | B) P(B)$

Bayesian Statistics

$$
p(\theta | D) = \frac{p}{\int dt}
$$

Example: a global fit in HEP

- ๏*The CKM matrix determines how flavor mixing happens in charged current transitions*
	- ๏*A 3x3 complex matrix with 4 degrees of freedom*
	- ๏*One is a phase (weak phase) that cannot be removed and determines CP violation*
- ๏*All flavor-mixing processes these four parameters*
	- ๏*One can combine them and extract the CKM parameter values*
	- ๏*One can use the redundancy (more observables than parameters) to test the consistency of the SM*

๏*The CKM matrix is unitary, which imposes relations between its complex values*

$$
\sum_i V_{ij} V_{ik}^* = \delta_{jk}
$$

๏*In particular, if one looks at 3rd to 1st generation transitions, all terms have the same order in* λ

$$
V_{ud} V_{ub}^* + V_{cd} V_{cb}^* + V_{td} V_{tb}^* =
$$

๏*They identify a triangle with measurable angles (i.e., large CP violating effects)*

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$(1,0)$

๏*The apex of the UT has to be within a circle centred at (0,0)*

๏*It's a CP-conserving quantity: the boundary has* to cross $\bar{\eta} = 0$ because one *cannot establish CP violation just with this measurement*

CP conserving observables: Vub and Vcb

๏*The ratio of the semileptonic decays of the B meson give access to a combination of* $\bar{\rho}$, $\bar{\eta}$, and λ

๏*two circles of different size, entered at (1,0)*

๏*The oscillation frequencies also depend on form factors, derived from theory (latticeQCD, typically)*

$$
\Delta m_d \,\,=\,\,\frac{G_F^2}{6\pi^2} m_W^2 \,\,\eta_c S(x_t) \,\,A^2 \lambda^6 \,\,[(1
$$

$$
\frac{\Delta m_d}{\Delta m_s}~=~\frac{m_{B_d}f_{B_d}^2\hat{B}_{B_d}}{m_{B_s}f_{B_s}^2\hat{B}_{B_s}}~\left(\frac{\lambda}{1-\frac{\lambda^2}{2}}\right)^2
$$

CP conserving observables: Meson Oscillations

๏*Meson oscillation frequencies (also CP conserving) probe a different function* $of \bar{p}$, $\bar{\eta}$, and λ

๏*Working in an over constrained global analysis, one can learn a lot by looking at subset of the observables*

๏*One can predict the top mass from B physics*

๏*One can establish CP violation with CP conserving process*

๏*..*

๏*Global analyses are a powerful tool test standard models*

๏*of particle physics (UT analysis, EW precision, Higgs couplings)*

๏*of cosmology (*Λ*CDM)*

The power of a global analysis

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CP violating observables: α, β, γ

๏*At B factories, one can measure the three angles of the UT with different processes*

๏*Some of these processes are tree-level (-> New Physics should not enter). Some are loop-mediated (could have virtual effects from NP*

๏*The four unknowns are determined using a MCbased Bayesian application*

 O Values of (A, λ, $\bar{\rho}$, $\bar{\eta}$) *are sampled from 1D flat priors in a range*

๏*Experimental quantities are computed from them*

๏*The experimental likelihood is evaluated*

๏*The likelihood value is used to wait the entry when filling a histogram*

A global fit

obability density

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A global fit

$$
\mathcal{L}(\vec{x}_{exp} | A, \lambda, \bar{\rho}, \bar{\eta}) = \prod_{i} G_i(x_i(A, \lambda, \bar{\rho}, \bar{\eta}) | x_{exp,i}, \sigma
$$

A, $\lambda, \bar{\rho}, \bar{\eta} | \vec{x}_{exp}) = \mathcal{L}(\vec{x}_{exp} | A, \lambda, \bar{\rho}, \bar{\eta}) \Pi(A) \Pi(\lambda) \Pi(\bar{\rho}, \bar{\eta})$

๏*In our case, the math is even simpler, since the*

 $P(\lambda) \propto e^{-\frac{(\lambda_{exp})}{2\sigma}}$

likelihood is formally symmetric for probability exchange (i.e., the exchange of the measurement and the observable)

๏*First iteration: Flat prior and Gaussian likelihood*

๏*Second iteration: use a Gaussian prior and forget about*

the first measurement in the likelihood

 $\Pi(\lambda)$

$$
\frac{(2\pi\sigma^2)^2}{2\sigma^2}\prod(\lambda) = e^{-\frac{(\lambda_{exp}-\lambda)^2}{2\sigma^2}}
$$

$$
\propto e^{-\frac{(\lambda_{exp} - \lambda)^2}{2\sigma^2}}
$$

Example of prior update

• no prior information on counting expectation $x \in [0,1] \rightarrow$ use a flat prior

• a measurement of n counts, described by a Poisson likelihood $\mathscr{L}(n \mid x) =$

• The posterior is a function of x $P(x | n) \propto x^n e^{-x} \propto Gamma(x | n + 1,1)$

• At the next measurement one can

• use a flat prior and as a likelihood the product of the two likelihoods • use the first posterior as an updated prior and a likelihood only the second

 $\Gamma(z) = \int$ ∞ 0

- ๏*Sometimes sampling from flat prior can be inefficient*
	- ๏*e.g.,* λ *is known to a high precision* $(\lambda = 0.22534 \pm 0.00089)$
	- ๏*its determination factories from the rest*

๏*So one can directly*

sample from the

experimental

Gaussian

- -
-

 $Gamma(x | k, \theta) =$

๏*This is an example of prior update*

Efficient MC generation

๏*Sometimes a loose prior can result in inefficient sampling when the likelihood is narrow*

๏*Example:* ε*^K*

๏*Experimentally well known*

๏*But the theoretical expression depends on parameters from Lattice QCD, which have broader theoretical prior*

๏*Solution: invert the role of the observable and the input*

๏*Use the lattice QCD determination in the likelihood*

๏*Use prior update to write the prior on* ε*K in the global fit as the posterior of its standalone determination*

๏*Optimizing the strategy is part of your judgment call*

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MC efficiency: observable vs unknown

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Which Prior?

๏*The choice of a prior is a crucial aspect of a Bayesian analysis. There are two classes of issues*

๏*Modeling knowledge: when something is known about a quantity, one needs to find a prior that models that knowledge*

๏*Modeling ignorance: this is where troubles start. Even an innocent assumption on a quantity x (e.g., a flat prior) can become a strong statement on some function of x (mind the Jacobian)*

Which prior?

In HEP, this is the issue of modeling TH uncertainties

๏*The choice of a prior is a crucial aspect of a Bayesian analysis. There are two classes of issues*

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Which prior?

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- ๏*We said that a prior is the modeling on a-priori knowledge (subjective prior)*
- ๏*When modeling ignorance, it was suggested to instead fix the prior by a formal rule (objective prior)*
	- ๏*We are trading the instability of a "democratic" flat function with a desired property, e.g., invariance under specific reparameterization*
- ๏*Often called non-informative priors. Misleading name, since they carry a lot of information (they prefer certain values over others)*

Objective priors

- ๏*The principle of indifference states that in the absence of any relevant evidence, agents should distribute their credence (or 'degrees of belief') equally among all the possible outcomes under consideration.*
	- ๏*Starting point for the first writers on probability (Laplace, Bernoulli, etc.)*
	- ๏*The simplest example of noninformative priors*
	- ๏*Obvious application in case of discrete outcomes (dice, etc.)*
-
- ๏*Doesn't work for continuous variables: flat on what?*

[https://en.wikipedia.org/wiki/Principle_of_indi](https://en.wikipedia.org/wiki/Principle_of_indifference)fference

Principle of Indifference

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- Suppose there is a cube hidden in a box. A label on the box says the cube has a side length between 3 and 5 cm.
- We don't know the actual side length, but we might assume that all values are equally likely and simply pick the mid-value of 4 cm.
- The information on the label allows us to calculate that the volume of the cube is between 27 and 125 cm3. We don't know the actual volume, but we might assume that all values are equally likely and simply pick the mid-value of 76 cm3.
- However, **we have now reached the impossible conclusion that the cube has a side length of 4 cm and a volume of 76 cm3**

๏*Generalization of principle of indifference, by E. T. Jaynes*

- ๏*One should have an indifferent choice between equivalent problems (i.e., equivalent quantities of interest) rather than between different outcomes*
- ๏*In practice, given two quantities x and y, one looks for a prior f such that solving for f(x) or f(y) gives the same result*
- ๏*Reduces to principle of indifference for a discrete problem (which has to be permutation invariant)*

๏*The prior to choose depends on what one is ignorant about*

Principle of Transformation Group

Reparameterization invariance: consider two possible parameterisations θ and ϕ of a given model. Assume that one is a smooth function of the other.

A reparameterization invariant prior is a prior that transforms under the usual rule of the change-of-variables theorem

$$
p_{\phi}(\phi) = p_{\theta}(\theta) \left| \frac{d\theta}{d\phi} \right|
$$

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๏*The prior to choose depends on what one is ignorant about* 53 **Translation invariance:** consider a likelihood of x of the form

Principle of Transformation Group

The likelihood is invariant under this transformation

$$
\mathscr{L}(x|\mu) = f(x - \mu)
$$

where μ is a parameter. Consider a transformation

$$
x \to x + b = \hat{x}
$$

$$
\mu \to \mu + b = \hat{\mu}
$$

$$
\mathcal{L}(\hat{x} | \mu) = \left| \frac{dx}{d\hat{x}} \right| f(x - \mu) = f((x + b) - (\mu + b)) = \mathcal{L}(\hat{x})
$$

Solving for μ or for $\hat{\mu}$ give two equivalent problems. One would then look for a prior Π such that

$$
\Pi(\mu + b) = \Pi(\hat{\mu}) = \left| \frac{d\mu}{d\hat{\mu}} \right| \Pi(\mu) = \Pi(\mu) \ \forall b
$$

which holds for a constant $\Pi(\mu)$

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 $\textbf{Scale invariance: }$ a parameter σ is a scale parameter when the $|$ likelihood has the form

Solving the problem for σ or for $\hat{\sigma}$ should be equivalent. We then look for a function such that

๏*The prior to choose depends on what one is ignorant about*

Principle of Transformation Group

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which holds for $\Pi(\sigma)$ $\boldsymbol{\propto}$ 1 *σ*

Consider a translation

The likelihood is invariant under the rescaling of the parameter

Notice that the normalization factors will be different (because each prior will be normalized to 1 in its definition domain)

$$
\mathscr{L}(x \mid \sigma) = \frac{f(x \mid \sigma)}{\sigma}
$$

$$
x \to ax = \hat{x}
$$

$$
\sigma \to a\sigma = \hat{\sigma}
$$

$$
\mathcal{L}(\hat{x} | \sigma) = \left| \frac{dx}{d\hat{x}} \right| \mathcal{L}(x | \sigma) = \frac{f(x | \sigma)}{a\sigma} = \mathcal{L}(\hat{x} | \hat{\sigma})
$$

$$
\Pi(a\sigma) = \Pi(\hat{\sigma}) = \left| \frac{d\sigma}{d\hat{\sigma}} \right| \Pi(\sigma) = \frac{1}{a} \Pi(\sigma)
$$

Back to the box problem

We are looking for a function $\Pi(x)$ such that

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A function of the kind $\Pi(L^n) = \frac{N^n}{L^n}$ would provide a solution to this equation. For instance for n=3 we obtain *Kn Ln*

 K_1 can be fixed normalizing the prior for $L \in [3,5]$

$$
\Pi(L) =
$$

which implies
$$
\Pi(L) = \frac{1}{\log(5/3)L}
$$
 and $\Pi(V) = \frac{1}{3 \log(5/3)V}$

One can now verify that the two priors would result in the same result, when solving the problem for L or L^3 . For instance

$$
\frac{dL^n}{dL}\bigg|\,\Pi(L^n)=nL^{n-1}\Pi(L^n)
$$

$$
\frac{K_1}{L} = 3L^2 \frac{K_3}{L^3}
$$

$$
1 = \int_3^5 dL \frac{K_1}{L} = K_1 \log(\frac{5}{3})
$$

$$
\frac{1}{\log(5/3)V}
$$

)

$$
P(L < 4) = \int_3^4 \frac{dL}{L \log(5/3)} = \frac{\log(4/3)}{\log(5/3)}
$$

$$
P(V < 64) = \int_{27}^{64} \frac{dV}{3V \log(5/3)} = \frac{3 \log(4/3)}{3 \log(5/3)} = \frac{\log(4/3)}{\log(5/3)}
$$

๏*We described LHC-style hypothesis testing* ๏*We discussed Bayesian inference with a physics example (the extraction of the CKM matrix from flavor measurements)*

๏*We discussed the choice of the prior*

