Sceptical combination of experimental results using JAGS/rjags with application to the $K^\pm$ mass determination

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Abstract

The question of how to combine experimental results that ‘appear’ to be in mutual disagreement, treated in detail years ago in a previous paper, is revisited. The first novelty of the present note is the explicit use of graphical models, in order to make the deterministic and probabilistic links between the variables of interest more evident. Then, instead of aiming for results in closed formulae, the integrals of interest are evaluated by Markov Chain Monte Carlo (MCMC) sampling, with the algorithms (typically Gibbs Sampler) implemented in the package JAGS (“Just Another Gibbs Sampler”). For convenience, the JAGS functions are called from R scripts, thus gaining the advantage given by the rich collection of mathematical, statistical and graphical functions included in the R installation. The results of the previous paper are thus easily re-obtained and the method is applied to the determination of the charged kaon mass. This note, based on lectures to PhD students and young researchers has been written with a didactic touch, and the relevant JAGS/rjags code is provided. (A curious bias arising from the sequential application of the $\sqrt{\chi^2/\nu}$ scaling prescription to ‘apparently’ discrepant results, found here, will be discussed in more detail in a separate paper.)

“...to emancipate us from the capricious ipse dixit of authority”
(J.H. Newman)

“Use enough common sense to know when ordinary common sense does not apply”
(I.J. Good’s guiding principle of all science)
| $i$ | Authors                          | pub. year | central value $[d_i]$ (MeV) | uncertainty $[s_i]$ (MeV) |
|-----|----------------------------------|-----------|----------------------------|---------------------------|
| 1   | G. Backenstoss et al. [4]        | 1973      | 493.691                    | 0.040                     |
| 2   | S.C. Cheng et al. [5]            | 1975      | 493.657                    | 0.020                     |
| 3   | L.M. Barkov et al. [6]           | 1979      | 493.670                    | 0.029                     |
| 4   | G.K. Lum et al. [7]              | 1981      | 493.640                    | 0.054                     |
| 5   | K.P. Gall et al. [8]             | 1988      | 493.636                    | 0.011 (*)                 |
| 6   | A.S. Denisov et al. [9] & Yu.M. Ivanov [10] | 1991      | 493.696                    | [0.0059]                  |

Table 1: Experimental values of the charged kaon mass, limited to those taken into account by the 2019 issue of PDG [3] (see footnote 3 for remarks).

1 Introduction

It is not rare the case in which experimental results ‘appear’ to be in mutual disagreement. The quote marks are mandatory, as a reminder that also very improbable events might by nature occur.\(^1\) The fact that they ‘appear’ to us in mutual disagreement is because we know by experience that uncertainties\(^2\) might be underestimated, systematic errors overlooked, theoretical corrections not (properly) taken into account, or even mistakes of different kinds having possibly been made in building/running the experiment or in the data handling. It is enough to browse the PDG [3] to find cases of this kind, as the one of Fig. 1 concerning the mass of the charged kaon, whose values, as selected by the PDG, are reported in Tab. 1.\(^3\)

The usual probabilistic interpretation\(^4\) of the results is that each experiment pro-

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\(^1\)Remember that all events of our life were indeed VERY improbable, if observed with enough detail, because they are just points in a high dimensional configuration space!

\(^2\)For the meaning of error and uncertainty see [1] and [2]. Hereafter ‘error’ in quote marks is to remind that the noun refers in reality to uncertainty, or, more precisely, standard uncertainty.

\(^3\)Details can be found in the 2000 edition of the PDG [11]. Moreover, comparing the two editions of the PDG and taking into account that not always the details of the experiment are publicly available, it is clear that a serious work to determine at best the charged kaon mass goes beyond the aim of this paper, being mainly methodological. Nevertheless, the uncertainty reported for the 5th result of table Tab. 1 is not a good account of the experimental result, as it will be discussed later on in this paper.

\(^4\)Note that this interpretation is valid, under hypotheses which generally hold, especially if $s_i/d_i \ll 1$ (as it happens in this case), even if the results were produced with frequentistic methods that do not contemplate the possibility of attributing probabilities to the values of physics quantities. In fact, most results obtained using standard statistics (‘frequentistic’) are based on the analysis of the so called likelihood around its maximum. And they can then be easily turned into probabilistic results (see e.g. [12], in particular section 12.2.1 and the related figure 12.1).
Figure 1: Charged kaon mass from several experiments as summarized by the PDG [3]. Note that besides the ‘error’ of 0.013 MeV, obtained by a $\times 2.4$ scaling, also an ‘error’ of 0.016 MeV is provided, obtained by a $\times 2.8$ scaling. The two results are called ‘OUR AVERAGE’ and ‘OUR FIT’, respectively.

Provides a probability density function (pdf) centered in $d_i$ with standard deviation $s_i$, as shown by the solid lines of Fig. 2. The standard way to combine the individual results consists in calculating the weighted average, with weights equal to $1/s_i^2$, that is

$$d_w = \frac{\sum_i d_i/s_i^2}{\sum_i 1/s_i^2},$$ (1)

$$s_w = \left(\sum_i 1/s_i^2\right)^{-\frac{1}{2}},$$ (2)

which, applied to the values of Tab. 1, yields $d_w = 493.6766$ MeV and $s_w = 0.0055$ MeV, i.e. a charged kaon mass of $493.6766 \pm 0.0055$ MeV, graphically shown in Fig. 2 with

\footnote{In most cases I stick here to two digits for the standard uncertainty.}
Figure 2: Graphical representation of the results on the charged kaon mass of Tab. 1 (solid lines). The dashed red Gaussian shows the result of the naive standard combination (see text).

As a matter of fact, a situation of this kind is not impossible, but nevertheless, there is a natural tendency to believe that there must be something not properly taken into account by one or more experiments. Told with a dictum attributed to a famous Italian politician, “a pensar male degli altri si fa peccato ma spesso ci si indovina”. For example, looking at Fig. 2, one is strongly tempted to lower, just as an exercise,

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6 “To think badly would be to sin, but very often one gets it right”\(^(*)\). Most Italians attribute it to Giulio Andreotti, but it seems due no less than to a pope [13].

\(^{(*)}\)https://forum.wordreference.com/threads/a-pensare-male-si-fa-peccato-ma-spesso-ci-si-azzetta.2397506/
Figure 3: Same as Fig. 2 but with one result arbitrarily shifted by $-50$ keV (dotted line).

the highest value by 50 keV,\(^7\) thus getting the excellent overall agreement shown in Fig. 3 (shifted Gaussian plotted with a dotted gray line), yielding a combined mass value of 493.6460 ± 0.0055 MeV. And the question would be settled. But this sounds at least unfair. In particular because we are aware, from the history of measurements, of a kind of ‘inertia’ of new results to different from old ones – but sometimes the new results moved ‘too far’ from the old ones and the presently accepted value lies somewhere in the middle. Figure 4 shows some of the history plots traditionally reported by the PDG [14].

In such a state of uncertainty, probability theory can help us in building up a model in which the values about which we are in doubt are allowed to vary from the

\(^7\)Value just decided by eye looking at the figure with some experienced colleagues, and not resulting from fits or optimizations of any kind.
nominal ones. Obviously, the model is not unique, as not unique are the probability distributions that can be used. Following then [15], inspired to [16], these are the criteria followed and some (hopefully shareable) desiderata:

- the quantities on which we focus our doubts are the reported uncertainties $s_i$, assumed to have the meaning of standard uncertainty [1, 2], as commented above;\(^8\)

- the ‘true’ standard deviations $\sigma_i$ are related to $s_i$ by a factor $r_i$ (one for each

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\(^8\)A possible alternative would be to allow a shift of the measured quantity. However this model seems unable to yield multimodal final pdf’s, which is, in my opinion, one of the desiderata of the model, as stated here. Perhaps the question requires further study but, given the limited aims of this paper, I prefer to stick for the moment to the models of Refs. [15, 16].
\(\sigma_i = r_i s_i\)
\[d_i \sim \mathcal{N}(\mu, \sigma_i),\]

where the last notation means that \(d_i\) is described by a Gaussian ('normal') distribution centered on the ‘true’ value of the quantity of interest, generically indicated by \(\mu\), with standard deviation \(\sigma_i\);

- all experiments are treated democratically and fairly, i.e. our prior belief of each \(r_i\) has expected value equal to 1, and its prior distribution does not depend on the experiment:
\[
f(r_1 | I) = f(r_2 | I) = f(r_3 | I) = \cdots \]
\[\mathbb{E}[r_i | I] = 1,\]

where ‘\(I\)’ stands for the background status of information (probability is always conditional probability!);

- but we are sceptical, and hence each \(r_i\) has \(a\) pri\(o\)ri a wide range of possibilities described by a suitable (easy to handle) probability distribution, the details of which will be given later – we just anticipate that we take a prior 100% standard uncertainty on \(r_i\), i.e. \(\sigma(r_i | I) / \mathbb{E}[r_i | I] = 1\);

- one of the desiderata of the model is that the posterior pdf of the physical quantity of interest should not be limited to a Gaussian and could even be multimodal if the individual results cluster in different regions; or it could be narrower than the pdf obtained by the standard weighted average, if the individual results tend to overlap ‘too much’ (see e.g. Figs. 4 and 5 of Ref. \[15\]);

- finally, once the parameters of \(f(r_i | I)\) are defined on benchmarks and checked against ‘reasonable’ variation (as done in Figs. 4 and 5 of Ref. \[15\]), fine tuning and cherry peaking of the individual results to be included in the combination should be avoided (unless we have good reasons to mistrust some results).

Once the model has been built, we can easily write down the multidimensional probability pdf \(f(d, \mu, \underline{r} | \underline{s}, I)\), of all the variables of interest (the ‘observed’ \(d_i\) and the uncertain values \(\mu\) and \(r_i\)’s – the \(s_i\) will be instead considered as fixed conditions, as it will be clear in a while; \(d\) stands for all the \(d_i\), and so on).

Once the multi-dimensional pdf has been settled, writing down the unnormalized pdf of the uncertain quantities,
\[
\tilde{f}(\mu, \underline{r} | \underline{d}, \underline{s}, I) \propto f(\mu, \underline{r} | \underline{d}, \underline{s}, I),
\]
is straightforward, as we shall see in a while. But, differently from [15], the rest of the technical work (normalization, marginalization and calculation of the moments of interest) will be done here by sampling, i.e. by Monte Carlo, and the use of a suitable software package will make the task rather easy.

But, before we build up the model of interest, let us start with a simpler one, in which we fully trust the reported standard uncertainty, i.e. we assume \( f(r_i | I) = \delta(1) \), and hence \( \sigma_i = s_i \). We also take for the prior, following Gauss [17, 18], a flat distribution of \( \mu \) in the region of interest.\(^9\)

## 2 Standard combination from a probabilistic perspective

Let us start with just two experimental outcomes,\(^{10}\) \( x_1 \) and \( x_2 \), resulting from the uncertain ‘true’ value \( \mu \) (what we are interested in) when measured in two independent experiments having Gaussian error functions with standard deviations \( \sigma_1 \) and \( \sigma_2 \), as sketched in the left hand graph of Fig. 5. That is

\[
x_1 \sim \mathcal{N}(\mu, \sigma_1) \\
x_2 \sim \mathcal{N}(\mu, \sigma_2).
\]

The general case, with many measurements of the same \( \mu \), is shown on the right hand graph of the same figure. From a probabilistic point of view our aim will be to assess, with a probability distribution, the intervals where we believe \( \mu \) lies with different

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\(^9\)For the Gauss’ use of what we would nowadays call a Bayesian reasoning, starting form the concept of probabilities of the true value, see Section 6.12 of Ref. [12] based on Section III of Book II of Ref. [17] [see Ref. [19] for details on the missing steps between Eq.(6.53) and Eq.(6.54)]. Here I just want to comment on the meaning of a ‘flat’ prior, which does not imply that it has to be interpreted as strictly constant all over the real axis. With this respect it is interesting the comment that Gauss adds after he derived the ‘Gaussian’ as the error function characterized by good mathematical behavior and such that the posterior gets its maximum in correspondence of the arithmetic average, in the case of independent measurements characterized by the same error probability distribution:

“The function just found [the ‘Gaussian’] cannot, it is true, express rigorously the probabilities of the errors: for since the possible errors are in all cases confined within certain limits, the probability of errors exceeding those limits ought always be zero, while our formula always gives some value. However, this defect, which every analytical function must, from its nature, labor under, is of no importance in practice, because the value of function decreases so rapidly, when \( h \Delta [\langle x_i - \mu \rangle / \sigma' \rangle \), in modern notation] has acquired a considerable magnitude, that it can safely be considered as vanishing. Besides, the nature of the subject never admits of assigning with absolute rigor the limits of error.” [18]

\(^{10}\)In this introductory section we use \( x_i \) to indicate an individual observation, while in general the \( d_i \) of Tab. 1 are results of ‘statistical analyses’ based on many direct ‘observations’.
probabilities, that is to arrive to
\[ f(\mu \mid x_1, x_2, \ldots, \sigma_1, \sigma_2, \ldots, I) \equiv f(\mu \mid \underline{x}, \underline{\sigma}, \ldots, I). \]

The pdf of interest can be (in principle) obtained easily if we knew the joint pdf of all the quantities of interest, that is \( f(\mu, \underline{x} \mid \underline{\sigma}, I) \). In fact, we just need to apply a well know general rule of probability theory (remember that in this first example the \( \sigma_i \) are just fixed conditions, although in general they might become subject to inference too, as we shall see later):
\[
\frac{f(\mu \mid x, \sigma, I)}{f(x \mid \sigma, I)} = \frac{f(\mu, x \mid \sigma, I)}{f(x \mid \sigma, I)}.
\]

At this point the reader might be scared by two reasons: the first is how to build up the joint pdf \( f(\mu, \underline{x} \mid \underline{\sigma}, I) \); the second is how to perform the integral over \( \mu \) (‘marginalization’) in order to get the denominator.\(^{11}\)

The first good news is that, given the model (those of Fig. 5 or the more complicate ones we shall see later), the denominator is just a number, in general difficult to calculate, but just a number. This means that we can rewrite the previous equation as
\[
f(\mu \mid \underline{x}, \underline{\sigma}, I) \propto f(\mu, \underline{x} \mid \underline{\sigma}, I).
\]

As next step, we can follow two strategies:

\(^{11}\)Let us remind that, in general, \( f(x \mid \sigma, I) = \int_{-\infty}^{+\infty} f(\mu, x \mid \sigma, I) \, d\mu \).
• calculate the normalization factor at the end, either analytically or numerically;
• sample the unnormalized distribution by Monte Carlo techniques, in order to get the shape of \( f(\mu | \underline{x}, \sigma, I) \) and to calculate all moments of interest.

The second good news is that the multidimensional joint pdf can be easily written down using the well known probability theory theorem known as chain rule. Indeed, sticking to the model with just two variables, we can apply the chain rule in different ways. For example, beginning from the most pedantic one, we have

\[
f(\mu, x_1, x_2 | \sigma_1, \sigma_2, I) = f(\mu | x_1, x_2, \sigma_1, \sigma_2, I) \cdot f(x_1 | x_2, \sigma_1, \sigma_2, I) \cdot f(x_2 | \sigma_1, \sigma_2, I).
\]

But this writing does not help us, since it requires \( f(\mu | x_1, x_2, \sigma_1, \sigma_2, I) \), which it is precisely what we aim for. It is indeed much better, with an eye to Fig. 5, a bottom up approach (in the following equation the order of the arguments in the left side term has been changed to make the correspondence between the two writings easier), that is

\[
f(x_1, x_2, \mu, | \sigma_1, \sigma_2 I) = f(x_1 | x_2, \mu, \sigma_1, \sigma_2, I) \cdot f(x_2 | \mu, \sigma_1, \sigma_2, I) \cdot f(\mu | \sigma_1, \sigma_2, I).
\]

This equation can be further simplified if we note that each \( x_i \) depends directly only on \( \mu \) and \( \sigma_i \), while \( \mu \) does not depend (at least in usual measurements) on \( \sigma_1 \) and \( \sigma_2 \). We get then

\[
f(x_1, x_2, \mu, | \sigma_1, \sigma_2 I) = f(x_1 | \mu, \sigma_1, I) \cdot f(x_2 | \mu, \sigma_2, I) \cdot f(\mu | I).
\]

We can easily generalize this equation, in the case of many observations described in the right hand graph of Fig. 5, rewriting it as

\[
f(\underline{x}, \mu, | \underline{\sigma}) = \prod_i f(x_i | \mu, \sigma_i) \cdot f_0(\mu)
\]

where the index \( i \) runs through all the observations and the symbol ‘\( I \)’ indicating the background state of information has been dropped, using ‘\( f_0(\mu) \)’ for the initial distribution (‘prior’) of \( \mu \). Finally, taking (for the moment) for \( f_0(\mu) \) a practically flat distribution in the region of interest (see footnote 9), making use of Eq. (3) and of the symbol \( f_N \) to indicate normal (i.e. Gaussian) error functions, we get

\[
f(\mu | \underline{x}, \underline{\sigma}, f_0(\mu) = k) \propto f(\underline{x}, \mu, | \underline{\sigma}) \propto \prod_i f_N(x_i | \mu, \sigma_i).
\]

Using the explicit expression of the Gaussian and neglecting all multiplicative factors that do not depend on \( \mu \), we get
\[ f(\mu | \mathbf{x}, \sigma, f_0(\mu) = k) \propto \prod_i \exp \left[ -\frac{(x_i - \mu)^2}{2 \sigma_i^2} \right] \]
\[ \propto \exp \left[ -\sum_i \frac{(x_i - \mu)^2}{2 \sigma_i^2} \right] \]
\[ \propto \exp \left[ -\frac{1}{2} \sum_i \frac{x_i^2 - 2x_i\mu + \mu^2}{\sigma_i^2} \right] \]
\[ \propto \exp \left[ -\frac{1}{2} \sum_i \left( \frac{x_i^2}{\sigma_i^2} - 2 \frac{x_i}{\sigma_i^2} \mu + \mu^2 \right) \right] \]
\[ \propto \exp \left[ -\frac{1}{2} \sum_i \frac{1}{\sigma_i^2} \cdot \left( \sum_i x_i^2 \sigma_i^{-2} - 2 \left( \sum_i \frac{x_i}{\sigma_i^2} \right) \mu + \left( \sum_i \frac{1}{\sigma_i^2} \right) \mu^2 \right) \right] \]
\[ \propto \exp \left[ -\frac{1}{2} \cdot \left( \sum_i 1/\sigma_i^2 \right) \cdot \left( \overline{x^2} - 2 \overline{x} \mu + \mu^2 \right) \right] \]
\[ \propto \exp \left[ -\frac{\overline{x^2} - 2 \overline{x} \mu + \mu^2}{2/(\sum_i 1/\sigma_i^2)} \right] \]
\[ \propto \exp \left[ -\frac{-2 \overline{x} \mu + \mu^2}{2 \sigma_C^2} \right] , \quad (8) \]

where

\[ \overline{x} = \frac{\sum_i x_i/\sigma_i^2}{\sum_i 1/\sigma_i^2} \]
\[ \overline{x^2} = \frac{\sum_i x_i^2/\sigma_i^2}{\sum_i 1/\sigma_i^2} \]
\[ \sigma_C^2 = \frac{1}{\sum_i 1/\sigma_i^2} . \quad (11) \]

Note that the mean of the squares \( \overline{x^2} \) has been taken out of the exponent [step from Eq. (8) to Eq. (9)] because \( \exp[-\overline{x^2}/(2\sigma_C^2)] \) does not depend on \( \mu \) and therefore it can be absorbed in the normalization constant. For the same reason we can multiply Eq. (9) by \( \exp[-\overline{x^2}/(2\sigma_C^2)] \), thus getting, by complementing the exponential,

\[ f(\mu | \mathbf{x}, \sigma, f_0(\mu) = k) \propto \exp \left[ -\frac{\overline{x^2} - 2 \overline{x} \mu + \mu^2}{2 \sigma_C^2} \right] \]
\[ f(\mu | \bar{x}, \sigma, f_0(\mu) = k) = \frac{1}{\sqrt{2\pi \sigma_C}} \exp \left[ -\frac{(\mu - \bar{x})^2}{2 \sigma_C^2} \right] \]  

(12)

with expected value \( \bar{x} \) and standard deviation \( \sigma_C \).

Someone might be worried about the dependence of the inference on the flat prior of \( \mu \), written explicitly in Eq. (12), but what really matters is that \( f_0(\mu) \) does not vary much in the region of a few \( \sigma_C \)'s around \( \bar{x} \). Since in the software package that we are going to use, starting from next section, an explicit prior is required, let us try to understand the influence of a vague but not flat prior in the resulting inference. Let us model \( f_0(\mu) \) with a Gaussian distribution having a rather large \( \sigma_0 \) (e.g. \( \sigma_0 \gg \sigma_i \)) and centered in \( x_0 \approx \mathcal{O}(x_i) \). The result is that Eq. (7) becomes

\[ f(\mu | \bar{x}, \sigma) \propto \prod_i \exp \left[ -\frac{(x_i - \mu)^2}{2 \sigma_i^2} \right] \cdot \exp \left[ -\frac{(\mu - x_0)^2}{2 \sigma_0^2} \right]. \]  

(13)

This is equivalent to add the extra term \( x_0 \) with standard uncertainty \( \sigma_0 \), which has then to be included in the calculation of \( \bar{x} \) and \( \sigma_C \) [technically the index \( i \) in the sums in Eqs. (10) and (11) run from 0 to \( n \), instead than from 1 to \( n \), being \( n \) the number of measurements]. But if \( \sigma_0 \gg \sigma_i \) (more precisely \( \frac{1}{\sigma_0^2} \ll \sum_{i=1}^{n} \frac{1}{\sigma_i^2} \)) and \( x_0 \) is ‘reasonable’, then the extra contribution is irrelevant.

### 3 Probabilistic combination achieved by Monte Carlo sampling using JAGS and rjags

The case just analyzed is so simple that, even without getting the solution in closed form, it is enough to plot the unnormalized pdf (7) to understand what is going on and to get ‘somehow’ mean value and standard deviation. The problem becomes more serious in the case we want to make a multidimensional inference, taking into account also the correlations between the quantities of interest, as for example in the fit model of Fig. 6, taken from Ref. [20].

Nowadays the most general way to handle problems of this kind is by sampling the unnormalized posterior distribution by a Markov Chain Monte Carlo (MCMC), using a suitable algorithm (see Ref. [21] for an introduction – given the imaginable interest
of the subject in many fields, much more can be found searching on the web; in particular, particle physicists might be interested in BAT [22], the Bayesian Analysis Toolkit. Perhaps (said by a non expert) the most powerful MCMC algorithm is the so called Metropolis (with variants), but for the kind of problem in which we are interested in this paper the most convenient one is the so called Gibbs Sampler,\textsuperscript{12} although it has some limitations on the conditional distributions it can handle (see [21] and [25] for details).

Instead of writing our own code, which would be anyway rather easy for our simple problem, we are going to use the program JAGS [24], born as an open source, multi-platform clone of BUGS. JAGS does not come with a graphical interface, so it is convenient to use it within a more general framework like R [27] via the package rjags [28] (those who are familiar with Python might want to use pyjags [29]).

\textsuperscript{12}Talking about the Gibbs sampler algorithm applied in probabilistic inference (and forecasting) it is impossible not to to mention the BUGS project [23], the acronym staying for Bayesian inference using Gibbs Sampler, that has been a kind of revolution in Bayesian analysis, decades ago limited to simple cases because of computational problems (see also Section 1 of [24]). In the project web site [25] it is possible to find packages with excellent Graphical User Interface, tutorials and many examples [26], which, although far from the typical interests of physicists, might help to understand the underlying reasoning and the model language, practically the same used by JAGS.

Figure 6: Graphical model for a non trivial fit with errors on both axes [20].
3.1 Gibbs sampling in the spaces \((\mu, \sigma)\) and \((\mu, \tau)\)

Before we write down the model to solve our little problem described by the graphical model of Fig. 5, some words on the Gibbs sampling are needed, also to understand why this kind of programs do not use \(\sigma\) as second parameter of the Gaussian, but rather \(1/\sigma^2\), traditionally indicated by \(\tau\).

We have seen that if we have a problem with Gaussian error functions and a flat prior on \(\mu\), then the posterior of \(\mu\) is still a Gaussian, and it remains Gaussian also if we assign to \(\mu\) a Gaussian prior characterized by \(x_0\) and \(\sigma_0\), a flat prior being recovered for \(\sigma_0 \to \infty\) (and allow me to draw again your attention on footnote 9).

Let us see what happens if we are also in condition of uncertainty concerning \(\sigma\), assumed to be the same in all \(n\) measurements (typical problem of when we collect a sample and measurements under apparently the same conditions and we are interested in inferring both \(\mu\) and \(\sigma\)). The graphical model is still the one on the right hand side of Fig. 5, but with \(\sigma_i = \sigma\) for all \(i\). The analogue of Eq. (3) is now

\[
f(\mu, \sigma | \bar{x}, I) \propto f(\mu, \sigma, x | I).
\]  

Applying the chain rule only to \(x_1\) and \(x_2\), to begin, and noting that \(\mu\) and \(\sigma\) do not depend on each other, as it is usually the case,\(^{13}\) we have, instead of Eq. (4),

\[
f(x_1, x_2, \mu, \sigma | I) = f(x_1 | \mu, \sigma, I) \cdot f(x_2 | \mu, \sigma, I) \cdot f(\mu | I) \cdot f(\sigma | I).
\]  

Equations (5) becomes then, also extending Eq. (15) to all \(x_i\),

\[
f(\bar{x}, \mu, \sigma | I) = \left[ \prod_i f(x_i | \mu, \sigma, I) \right] \cdot f(\mu | I) \cdot f(\sigma | I)
\]  

\[
= \left[ \prod_i f_N(x_i | \mu, \sigma) \right] \cdot f_0(\mu) \cdot f_0(\sigma).
\]

Now, if for some reasons we fix \(\sigma\) to the hypothetical value \(\sigma^*\) (and for simplicity we use a flat prior for \(\mu\)) then we recover, without any calculation, something similar to Eq. (12):

\[
f(\mu | \bar{x}, \sigma^*, f_0(\mu) = k) = \frac{1}{\sqrt{2\pi} \sigma_C} \exp \left[ -\frac{(\mu - \bar{x})^2}{2\sigma_C^2} \right]
\]  

where now \(\bar{x}\) is simply the arithmetic average and \(\sigma_C = \sigma^*/\sqrt{n}\). If we had taken into account a prior \(f_0(\mu)\) modeled by a Gaussian, then \(f(\mu | \bar{x}, \sigma^*)\) would still be a

\(^{13}\)But in frontier research it is not difficult to imagine cases in which this is not true.
Gaussian, as we have seen above. In particular, it easy to sample by Monte Carlo the ‘random’ variable μ described by Eq. (16), because it is rather easy to write a Gaussian ‘random’ number generator, or to use one of those available in the mathematical libraries of programming languages.

Let us now do the opposite exercise, the utility of which will be clear in a while: imagine we are interested in \( f(\sigma \mid \mu^*, f_0(\sigma) = k) \), having imposed the condition \( \mu = \mu^* \). Equations (6) and (7) are now turned into (note the factor \( 1/\sigma \) in front of each exponent, since it cannot be any longer absorbed in the normalization constant!)

\[
f(\sigma \mid \mu^*, f_0(\sigma) = k) \propto f(\mu, \mu^*, \sigma) \propto \prod_i f_N(x_i \mid \mu^*, \sigma) \propto \prod_i \frac{1}{\sigma} \exp \left[ -\frac{(x_i - \mu^*)^2}{2 \sigma^2} \right]
\]

where \( K^2(x, \mu^*) \) is a constant, given \( x \) and \( \mu^* \), written in a way to remind that it is by definition non negative. Unfortunately, opposite to the case of \( f(\mu \mid \mu^*, f_0) \), this is an unusual form in probability theory. But a simple change of variable rescues us. In fact, if instead of \( \sigma \) we use \( \tau = 1/\sigma^2 \), then the last equation becomes

\[
f(\tau \mid \mu^*, f_0(\sigma) = k) \propto \tau^{\alpha} \exp \left[ -K^2(x, \mu^*) \cdot \tau \right]
\]

in which probability and statistics experts recognize a Gamma distribution, usually written for the generic variable \( z \) as

\[
f(z \mid \alpha, \beta) = \frac{\beta^\alpha}{\Gamma(\alpha)} z^{\alpha-1} e^{-\beta z},
\]

where \( \Gamma() \) is the Gamma function (and hence the name of the distribution). Therefore

\[
f(\tau \mid \mu^*, f_0(\sigma) = k) = \frac{\beta^\alpha}{\Gamma(\alpha)} \tau^{\alpha-1} e^{-\beta \tau}
\]

with \( \alpha = 1 + n/2 \) and \( \beta = K^2(x, \mu^*) = \sum_i (x_i - \mu^*)^2/2 \). Being this a well known probability distribution, there are formulae available for the summaries of interest.\(^{14}\) For example, expected value and variance are given by \( \alpha/\beta \) and \( \alpha/\beta^2 \), respectively.

\(^{14}\)My preferred vademecum of Probability Distributions is the homonymous app [30].
But, moreover, there are Gamma random generators available, which is what we need for sampling.

We are then finally ready to describe the *Gibbs sampler* algorithm, applied to our two-dimensional case (but it can be applied in higher dimensionality problems too):

- start choosing an *arbitrary* initial point \((\mu_0, \tau_0)\) in the \((\mu, \tau)\) plane;
- extract ‘at random’ a new value of \(\mu\), let it be \(\mu_1\), given \(\tau_0\), from \(f(\mu | \bar{x}, \tau_0)\);
- extract then ‘at random’ a new value of \(\tau\), let it be \(\tau_1\), given \(\mu_1\), from \(f(\tau | \bar{x}, \mu_1)\);
- extract then ‘at random’ a new value of \(\mu\), let it be \(\mu_2\), from \(f(\mu | \bar{x}, \tau_1)\);
- continue on, through the steps \(\tau_1 \rightarrow \mu_2 \rightarrow \tau_2 \rightarrow \mu_3 \rightarrow \tau_3 \rightarrow \cdots \rightarrow \mu_N \rightarrow \tau_N\).

(And, obviously, for each \(\tau_i\) there is a related \(\sigma_i\).) Now, amazing enough (but there are mathematical theorems ensuring the ‘correct’ behavior [21]), the points so obtained *sample* the bi-dimensional distribution \((\mu, \tau)\), and then \((\mu, \sigma)\), in the sense that the expected frequency to visit a given region is proportional to the probability of that region (just *Bernoulli* theorem, not to be confused with the frequentist ‘definition’ of probability! – see e.g. Ref. [31]). Moreover, for the way it has been described, it is clear that the probability of the move \((\mu_i, \tau_i) \rightarrow (\mu_{i+1}, \tau_i)\) depends only \((\mu_i, \tau_i)\) and *not* on the previous *states*. This is what defines a *Markov Chain Monte Carlo*, of which the Gibbs sample is one of the possible algorithms.

There is still the question of \(f_0(\tau)\), less trivial then \(f_0(\mu)\), because \(\tau\) has to be positive.\(^{15}\) In this case a convenient prior would be a Gamma, with \(\alpha_0\) and \(\beta_0\) properly chosen, because it easy to see that, when multiplied by Eq. (19), the result is still a Gamma:

\[
\begin{align*}
\tau^\alpha_0 e^{\beta_0 \tau} \\
\tau^\alpha e^{-\beta \tau} \\
\tau^\alpha \tau^\alpha_0 e^{\beta_0 \tau} \\
sim \tau^{\alpha + \alpha_0 - 2} e^{-(\beta + \beta_0) \tau}.
\end{align*}
\]

We can easily see that a flat prior for \(\tau\) is recovered in the limit \(\alpha_0 \rightarrow 1\) and \(\beta_0 \rightarrow 0\).

A last comment concerning the initial point for the sampling is in order. Obviously, the initial steps of the *history* (the sequence) depend on our choice, and therefore they can be somehow not ‘representative’. The usual procedure to overcome this problem consists in discarding the ‘first points’ of the sequence, better

\(^{15}\)Also a mass, as many other physics quantities, is positively defined, and in principle one has to pay attention, either in the sampling steps or when the resulting *chain* is analyzed, that it does not get negative. But this problem does not occur in practice if the the average value \(\bar{x}\) is many standard \(\sigma_c\) above zero. Anyway, packages like *JAGS* allow also sharp constrains on the priors. (This is a general problem when we use Gaussians to describe positively defined quantities, already realized by Gauss and reminded in footnote 9.)
if after a visual inspection, or using criteria based on past experience (notoriously, *this kind of techniques are between science and art*, even when they are grounded on mathematical theorems, which however only speak of ‘asymptotic behavior’). But, as a matter of fact, the convergence of the Gibbs sampler for low dimensional problems is very fast and modern computers are so powerful that, in the case of doubt, we can simply throw away several thousands initial points ‘just for security’.

### 3.2 Implementation in JAGS/rjags

As a first example, here is the model to make the simple weighted average of the charged kaon mass values of Tab. 1 (we are indeed “breaking a nut with a mallet”):

```r
model {
  for (i in 1:length(d)) {
    d[i] ~ dnorm(m, 1/s[i]^2);
  }
  m ~ dnorm(0.0, 1.0E-8);
}
```

The loop is just the implementation of the graphical model on the right side of Fig. 5, with \(x_i\) here called \(d[i]\) in order to maintain the notation used in Eqs. (1) and (2). \(\text{dnorm()}\) stands for normal distribution density function, whose parameters are the kaon mass \(m\) (equal for all measurements, because we believe they were measuring the same thing) and \(1/s[i]^2\), that is \(\tau_i\), as discussed in the previous subsection. The last line of code defines the prior of the mass value: formally a normal distribution, but in fact a flat one in the domain of interest, being \(\sigma_0 = 10^4\) MeV. The model is saved in the file `weighted_average.bug` and we move now to the R code.

First we assign the experimental values to the vector \(d\) and \(s\) (no declarations are required in R) and then we evaluate and print the weighed average and the combined standard deviation calculated from Eqs. (1) and (2):

```r
d <- c(493.691, 493.657, 493.670, 493.640, 493.636, 493.696)
s <- c( 0.040,  0.020,  0.029,  0.054,  0.011,  0.007)
d.av <- sum(d/s^2)/sum(1/s^2)
s.av <- 1/sqrt(sum(1/s^2))
cat(sprintf("combined value: %f +- %f\n", d.av, s.av))
```

Executing the script\(^{16}\) containing these five lines, we get

```r
combined value: 493.676599 +- 0.005478
```

that for the moment is just a check.

\(^{16}\)If these lines are saved in a file, e.g. `kaon_mass_naive.R`, then the script can be run with the command `source('kaon_mass_naive.R')`. 
Let us now move to the **rjags** stuff in the **R** script:

```r
library(rjags) # load rjags
data <- NULL # declare an empty list
data$d <- d # first element of the list
data$s <- s # second element of the list
model <- "weighted_average.bug"

jm <- jags.model(model, data) # define the model
update(jm, 100) # burn in
chain <- coda.samples(jm, c("m"), n.iter=10000) # sampling
```

So, first the package **rjags** is loaded calling the function `library()`, then we fill the data in the `list` data (arbitrary name) and we put the model file name into the string variable `model` (again arbitrary name). Finally we interact with **JAGS** in three steps:

1. the function `jags.model(model, data)` passes model and the data to JAGS; the model is compiled and, if everything is ok, a summary message is reported, like in this case

   Compiling model graph
   Resolving undeclared variables
   Allocating nodes
   Graph information:
   Observed stochastic nodes: 6
   Unobserved stochastic nodes: 1
   Total graph size: 29

2. then, `update(jm, 100)` lets the Markov chain do 100 moves in the parameter space, but without recording the values, so that the initial points are not taken into account when the chain if analyzed;

3. finally, `coda.samples(jm, c("m"), n.iter=10000)` does the real work, following the evolution of the chain for `n.iter` steps, the model variable `m` is monitored and the resulting history is returned and stored in the object `chain` (arbitrary name).

At this point **JAGS** has done its work and we only need to analyze its outcome. For this task the high level functions of **R** are very helpful. For example we can make a summary plot just calling `plot(chain)`, whose result is shown in Fig. 7: the left

---

17 A ‘list’ is a very interesting object of **R**, which can contain other objects, also of different kinds and different lengths; the element of a ‘list’ can be accessed either by name, as we do here, or by indices.
Figure 7: Summary plot of the chain returned by JAGS.

Hand plot shows the history of $m$ during the 10000 recorded iterations; the right hand one is a smoothed representation of the histogram of the sampled values of $m$.

R provides also a summary of the result, using the function `summary(chain)` [or, better, `print(summary(chain))` if we want to include it into a script], with many statistical informations like average, standard deviation and quantiles for each sampled variable. Or we can do it in more detail using the high level R functions. Here is, for example, how to calculate mean and standard deviation (also to show a way to extract the history of a single variable from the object returned by `coda.samples()`):

```r
m.mean <- mean(chain[[1]][,'m'])
m.sd <- sd(chain[[1]][,'m'])
cat(sprintf("JAGS result: %f +- %f\n", m.mean, m.sd))
```

resulting (with this particular sampling) in

JAGS result: 493.676632 +- 0.005451

practically identical to the weighted average obtained using exact formulae.
4 Sceptical combination with JAGS – Preliminaries

It is now time to improve our model in order to implement what has been discussed in the introduction, where it was said that our skepticism would act on the variable $r_i = \sigma_i/s_i$. However, following Ref. [16], in the previous paper on the subject [15] a different variable was indeed considered, namely $\omega_i = s_i^2/\sigma_i^2$. The relations between the variables which enter the game are conveniently shown in the graphical model of Fig. 8, where the following convention has been used:

- arrows with solid lines represent – this is the usual convention – probabilistic links between parent(s) and child(ren), in our case $d_i$ depending from $\mu$ and $\tau_i$;
- arrows with dashed lines represent deterministic links, that is $\tau_i = \omega_i/s_i^2$;
- finally the arrow with dotted line is unusual, in the sense that it is not used in the literature. It is in fact still a deterministic link, being $r_i = 1/\sqrt{\omega_i}$, but it is irrelevant for the model itself and it could be also (and perhaps better, as
far as the efficiency of the program is concerned) calculated at the end of the sampling.

In the graphical model there are three kind parents having no ‘ancestors’: \( \mu, \omega_i, \) and \( s_i \). Therefore they need priors, that is \( f(\mu \mid I) = f_0(\mu) \), and so on. But \( s_i \) are simply constant and do not require priors (or, if you like, they are just Dirac delta’s). For \( f_0(\mu) \) we choose, as before, a practically flat prior obtained by a Gaussian distribution with very large \( \sigma_0 \). The mathematically convenient prior of \( \omega_i \) is instead a Gamma distribution, implying that the distribution of \( r_i \) is instead not an elementary one, as it can be seen comparing Eq. (11) and (12) of Ref. [15].

For the parameters of the Gamma pdf of \( \omega_i \) we stick to those chosen in Ref. [15],\(^{18}\) i.e. \( \delta = 1.3 \) and \( \lambda = 0.6 \), in order to get \( E[r_i] = \sigma(r_i) = 1 \). Figure 9, taken from Fig. 4 of Ref. [15], shows how the model performs in some situations which represent kind of extreme cases with respect to the usual ‘disagreements’ within a set of results.

Particularly interesting are the cases in which the individual results cluster in two regions, or when they overlap ‘too much’. In the first case, while the simple weighted average prefers mass values in a region where there is no experimental support, the sceptical combination exhibits a bimodal distribution, because we tend to believe with equal probability that the true value is in either side (but it could also be in the middle, although with low probability). In the second case, instead, in which the results overlap too much, the method has the nice feature of producing a pdf narrower than that obtained by the simple weighted average, reflecting our natural suspicion that the quoted uncertainties might have been overestimated. In Ref. [15] (Fig. 5 there) it was also studied how the results varied if the initial \( \sigma(r_i) \) was allowed to move by \( \pm 50\% \). This leads us to be rather confident that the choice of \( \delta = 1.3 \) and \( \lambda = 0.6 \) is not critical.

Here is, finally, the JAGS model, easy to understand if we compare it with the graphical model of Fig. 8:

```r
var tau[N], r[N], omega[N];
model {
  for (i in 1:N) {
    d[i] ~ dnorm(mu, tau[i]);
    tau[i] <- omega[i]/s[i]^2;
    omega[i] ~ dgamma(delta, lambda);
    r[i] <- 1.0/sqrt(omega[i]);
  }

  mu ~ dnorm(0.0, 1.0E-8);
}
```

\(^{18}\)For easier comparison with the results of Ref. [15] for the Gamma parameters we use hereafter \( \delta \) and \( \lambda \) instead of the standard \( \alpha \) and \( \beta \).
Figure 9: Examples of sceptical combinations taken from [15]. The plots on the left-hand side show the individual results. The plots on the right-hand side show the combined result obtained using a sceptical combination (continuous lines), compared with the standard combination (dashed lines).

Before running it, let us make a very trivial model in which JAGS is used as a simple random generator, without any inferential purpose, just to get confidence with the prior distribution of $r_i$. Moreover, consisting the core of the model of just two lines of code, we write it directly from the R script into a temporary file. Here is the complete script, in which it also shown an alternative way (indeed the simplest one in R) to prepare the ‘list’ data to be passed to JAGS via jags.model() – note the missing update(), because we deal here with direct sampling and there are no burn-in issues:
library(rjags)
data = list(delta=1.3, lambda=0.6)
model = "tmp_model.bug"
write("model{
    omega ~ dgamma(delta, lambda);
    r <- 1.0/sqrt(omega);
}
", model)

jm <- jags.model(model, data)
chain <- coda.samples(jm, c("omega","r"), n.iter=10000)
plot(chain)
print(summary(chain))

This is the result of the last command:

1. Empirical mean and standard deviation for each variable,
   plus standard error of the mean:

   | Variable | Mean    | SD      | Naive SE | Time-series SE |
   |----------|---------|---------|----------|---------------|
   | omega    | 2.1979  | 1.9127  | 0.019127 | 0.019065      |
   | r        | 0.9948  | 0.9096  | 0.009096 | 0.009096      |

2. Quantiles for each variable:

   | Variable | 2.5%    | 25%     | 50%      | 75%    | 97.5%   |
   |----------|---------|---------|----------|--------|---------|
   | omega    | 0.1162  | 0.8045  | 1.6582   | 3.035  | 7.329   |
   | r        | 0.3694  | 0.5741  | 0.7766   | 1.115  | 2.934   |

We see that the (indirectly) sampled \( r \) has (with good approximation) the expected unitary mean and standard deviation. As a further check, let us use directly the Gamma random generator \( \text{rgamma()} \) of R,

\[
r <- 1/\sqrt{\text{rgamma}(10000, 1.3, 0.6)}
\]

cat(sprintf("mean(r) = %f, sd(r) = %f\n", mean(r), sd(r)))

whose (aleatory) result is left as exercise to the reader.

5 Sceptical combination with JAGS – Results

The core of the R script is very similar to the one of section 3.2, besides the model used, the number of iterations and the variables to be monitored. Note that we pass the Gamma parameter \( \text{delta} \) and \( \text{lambda} \) to the model via the list \( \text{data} \) (a different choice could have been to define them directly inside the model). Here is the entire script, including statistics and plot summaries (plots not shown here).
library(rjags)
data <- NULL # 'data' to be passed to the model
data$d <- c(493.691, 493.657, 493.670, 493.640, 493.636, 493.696)
data$s <- c( 0.040, 0.020, 0.029, 0.054, 0.007, 0.007)
data$N <- length(data$d)
data$delta = 1.3 # parameters of Gamma(omega): delta <-- 'alpha'
data$lambda = 0.6 # lambda <-- 'beta'

jm <- jags.model(model, data) # define the model
update(jm, 1000)# burn in
chain <- coda.samples(jm, c("mu", "r"), n.iter=100000) # sampling
print(summary(chain))
plot(chain)

This is what we get from summary(chain):

1. Empirical mean and standard deviation for each variable,
   plus standard error of the mean:

   |     | Mean   | SD    | Naive SE | Time-series SE |
   |-----|--------|-------|----------|----------------|
   | mu  | 493.6678 | 0.01608 | 1.608e-05 | 0.0000515      |
   | r[1]| 0.8790   | 0.53138 | 5.314e-04 | 0.0006477      |
   | r[2]| 0.9671   | 0.63559 | 6.356e-04 | 0.0010050      |
   | r[3]| 0.8330   | 0.49631 | 4.963e-04 | 0.0005264      |
   | r[4]| 0.8450   | 0.50271 | 5.027e-04 | 0.0005771      |
   | r[5]| 2.1528   | 1.62050 | 1.621e-03 | 0.0034153      |
   | r[6]| 2.9148   | 2.35537 | 2.356e-03 | 0.0052502      |

2. Quantiles for each variable:

   |     | 2.5%  | 25%  | 50%  | 75%  | 97.5% |
   |-----|-------|------|------|------|-------|
   | mu  | 493.6394 | 493.6555 | 493.6666 | 493.6807 | 493.696 |
   | r[1]| 0.3763   | 0.5173   | 0.7457   | 1.0179   | 2.177   |
   | r[2]| 0.3803   | 0.5965   | 0.8054   | 1.1338   | 2.515   |
   | r[3]| 0.3656   | 0.5467   | 0.7090   | 0.9619   | 2.045   |
   | r[4]| 0.3703   | 0.5550   | 0.7194   | 0.9753   | 2.077   |
   | r[5]| 0.5391   | 1.1500   | 1.7672   | 2.6621   | 6.101   |
   | r[6]| 0.5073   | 1.3988   | 2.4184   | 3.7211   | 8.600   |

The result is then a mass of 493.668 ± 0.016 MeV, where the ‘error’ is provided by the standard uncertainty [1, 2]. However, this does not imply that the value of the mass is normally distributed around the average.\(^{19}\) This can be checked on the quantiles of ‘mu’ (see above output), and better on the histogram of the sampled values, shown in the upper plot of Fig. 10, whose smoothed profile is reported in the bottom plot of

\(^{19}\)An example in which the sceptical combination produces a result narrower that the weighted average is shown in the Appendix.
Figure 10: Above: histogram of charged kaon mass by MCMC sampling. Below: profile of the above histogram compared with the individual results, the naive weighted average (dashed) and the Gaussian based on the average and the PDG prescription to scale the ‘error’ (see text).
the same figure, together with the individual measurements, the standard weighted average (red dashed) and the combination got following the PDG prescriptions (gray) with the $\times 2.4$ (narrower curve) and $\times 2.8$ scaling (wider curve)\[3\].

Here is a summary of the results:

| method                          | $m_{K^\pm}$ (MeV) |
|---------------------------------|-------------------|
| simple weighted average         | 493.677 ± 0.006   |
| PDG (‘OUR AVERAGE’, $\times 2.4$ scaling) | 493.677 ± 0.013 |
| PDG (‘OUR FIT’, $\times 2.8$ scaling)     | 493.677 ± 0.016 |
| sceptical                       | 493.668 ± 0.016   |

As far as the rescaling factor $r_i$ are concerned, we see from the output of the summary that only those relative to the items 5 and the 6 are preferred to be higher than the initial ones, with mean values 2.2 and 2.9, respectively. Therefore with this data set the most ‘suspicious’ one is nr. 6, as we had judged by eye in the introduction. But since the $r_i$ were inferred simultaneously, and together with the mass, it is interested to give a look to the correlation matrix. Here is directly the R output:

\[
\begin{bmatrix}
\text{mu} & r[1] & r[2] & r[3] & r[4] & r[5] & r[6] \\
\text{mu} & 1.00 & -0.21 & 0.31 & -0.03 & 0.16 & 0.55 & -0.59 \\
r[1] & -0.21 & 1.00 & -0.05 & 0.02 & -0.03 & -0.11 & 0.13 \\
r[2] & 0.31 & -0.05 & 1.00 & 0.03 & 0.06 & 0.18 & -0.17 \\
r[3] & -0.03 & 0.02 & 0.03 & 1.00 & 0.00 & -0.01 & 0.02 \\
r[4] & 0.16 & -0.03 & 0.06 & 0.00 & 1.00 & 0.09 & -0.09 \\
r[5] & 0.55 & -0.11 & 0.18 & -0.01 & 0.09 & 1.00 & -0.32 \\
r[6] & -0.59 & 0.13 & -0.17 & 0.02 & -0.09 & -0.32 & 1.00
\end{bmatrix}
\]

We see, for example, that the highest correlation of the mass (‘mu’) is with $r[5]$ and $r[6]$, related to the two most precise measurements: the first is positive, meaning that a larger $\sigma_5$ would allow mu to rise towards $d_6$; the second is negative, meaning that a larger $\sigma_6$ would allow mu to descend towards $d_5$. For this reason, among the several $r_i$, $r[5]$ and $r[6]$ get the highest (in absolute value) correlation coefficient, having a negative sign. But it is only $-32\%$, indicating that $\sigma_5$ and $\sigma_6$ could possibly be both larger than the stated standard uncertainty.

Going back to the mass value, we see that our result does not differ much from the PDG one, if we are only interested in average and standard uncertainty (just $-9\text{keV}$ lower, with similar uncertainty). What differs mostly is the shape of the probability

\[20\text{The histogram with the over-imposed profile was produced by} \]

\[
\text{chain.df} <- \text{as.data.frame( as.mcmc(chain) )} \\
\text{hist(chain.df$mu,nc=100,prob=TRUE,xlab='K mass (MeV)\',ylab='f(m)\', col='cyan',main='') } \\
\text{lines(density(chain.df$mu, adjust=1.0), lwd=3)}
\]
distribution, which is has nothing to do with a Gaussian. Instead, in the the weighted average, with the resulting ‘error’ as it comes straight from Eq. (2) or scaled with $\sqrt{\chi^2/\nu}$, the interpretation is tacitly Gaussian, or it is assumed as such in further analyses [35]. For example, if one is interested, for some deep physical reasons, in the chance that the mass is larger than 493.70 MeV, it is clear from the bottom plot of Fig. 10 that the results would be quite different.

One might argue if, for such a purpose, we could use the bi-modal curve of the PDG ideogram (see Fig. 1), in alternative to the pdf resulting from the sceptical analysis performed here. But what is the meaning of the bi-modal curve of Fig. 1? If one compares it with the individual Gaussians reported in Fig. 2 we see that it follows somehow the profile of highest points of the curves. Therefore the first guess is that it is just an unnormalized sum, that is $\sum_i f_N(m | d_i, \sigma_i)$. But checking it, it does not seem to be the case. The second guess was a kind of weighted average, with weights equal to $1/s_i^2$, i.e. $\sum_i f_N(m | d_i, \sigma_i)/s_i^2$, but it did not work either. The third attempt was to set the weights to $1/s_i$, i.e. $\sum_i f_N(m | d_i, \sigma_i)/s_i$, and this seems to be the case. The three attempts are reported in Fig. 11, but just as a curiosity, as they have no probabilistic meaning.

Let us end this section showing how to re-obtain the standard combination with the same general model used in the sceptical combination. We just need to choose values suitable $\delta$ and $\lambda$ to get $E[r_i] = 1$ and $\sigma(r_i) \to 0$. Inverting Eqs. (13) and (14) of [15] seems complicate, but in the limit of zero variance, this is the same as requiring $E[\omega_i] = 1$ and $\sigma(\omega_i) \to 0$, a condition easier to apply in practice. Being in fact $E[\omega_i] = \delta/\lambda$ and var[$\omega_i] = \delta/\lambda^2 = (\delta/\lambda)/\lambda$, the requirement simply translates into $\delta = \lambda$ with both parameters ‘very large’. In practice is is enough to set e.g. $\delta = \lambda = 10000$ to recover the result of the weighed average of 493.6766 ± 0.0055 MeV.

6 Further scepticism

If the purpose of this paper would have been just to search around for a case of ‘apparent’ discordant results, as a real life example to which apply to the model of Ref.[15] implemented in JAGS, then the game would be at the end. But since I am presently interested in the charged kaon mass, I tried to understand the results a bit more. I expected in fact to find in the publications extensive discussions on the details of the analysis, with explanations of what the results really meant and detailed accounts for the sources of uncertainties, as it has presently become a good practice by most experimental teams. But this was not the case. Already trying to understand the (apparently, as we shall see) most precise value, I was quite surprised when I realized that Ref. [9] gives no detailed information on how they got their numbers and on what their ‘error’ really means. Furthermore the PDG uses an
Figure 11: Attempts to re-obtain the bi-modal curve shown in the PDG ideogram of Fig. 1. They are not normalized but just equalized to the value of their maximum. Solid line: $\propto \sum_i f_X(m \mid d_i, s_i)/s_i$; dotted line: $\propto \sum_i f_X(m \mid d_i, s_i)$; dashed line: $\propto \sum_i f_X(m \mid d_i, s_i)/s_i^2$.

The 'error' of 0.007 MeV, instead of the 0.0059 MeV reported by [9], on the basis of a PhD thesis [10] which it is impossible to find (not even in Russian!). Fortunately this is more a methodological paper than a real attempt to get a deep understanding of the charged kaon mass, for which a thorough analysis of all relevant published matter on the subject would be required.  \(^{21}\)

Nevertheless, there is a point I would like to touch, related to the second most

\(^{21}\) Presently the value of the charged kaon mass, with relative uncertainty of around 26 ppm, is not critical for fundamental issues. For example its contribution to $|V_{us}|$ of the Standard Model is of the order of 66 ppm, to be combined in quadrature with the relative uncertainties of the other quantities from which $|V_{us}|$ depends (the branching ratios of interest depend on $M_{K^\pm}^2 \cdot |V_{us}|^2$ and hence the relative uncertainty on $M_{K^\pm}$ is propagated with a factor $5/2$ into the relative uncertainty on $|V_{us}|$).
TABLE II. Experimental mass measurements from each transition in megaelectronvolts. If the $\chi^2$ per degree of freedom was greater than 1.0, the error listed with the weighted average is the statistical error scaled up by a factor of $(\chi^2/\nu)^{1/2}$.

| Transition       | $M_{K^{-}}$     | Transition       | $M_{\Sigma^{-}}$ |
|------------------|-----------------|------------------|------------------|
| $K^{-}\text{Pb}(11 \rightarrow 10)$ | $493.675 \pm 0.026$ | $\Sigma^{-}\text{Pb}(14 \rightarrow 13)$ | $1197.731 \pm 0.192$ |
| $K^{-}\text{Pb}(9 \rightarrow 8)$   | $493.631 \pm 0.007$ | $\Sigma^{-}\text{Pb}(13 \rightarrow 12)$ | $1197.492 \pm 0.098$ |
| $K^{-}\text{W}(11 \rightarrow 10)$  | $493.806 \pm 0.095$ | $\Sigma^{-}\text{W}(14 \rightarrow 13)$  | $1197.412 \pm 0.186$ |
| $K^{-}\text{W}(9 \rightarrow 8)$   | $493.709 \pm 0.073$ | $\Sigma^{-}\text{W}(13 \rightarrow 12)$  | $1197.397 \pm 0.396$ |
| $\Sigma^{-}\text{W}(12 \rightarrow 11)$ | $1197.788 \pm 0.127$ | $\Sigma^{-}\text{W}(12 \rightarrow 11)$  | $1197.677 \pm 0.109$ |
| **Average**      | $493.636 \pm 0.011$ | **Average**      | $1197.532 \pm 0.057$ |
| $\chi^2/\nu=2.31$ |                 | $\chi^2/\nu=0.968$ |                 |

Figure 12: Details of Ref. [8].

The precise result of the list [8] whose conservative uncertainty is uncritically accepted by the PDG. The paper provides in fact four mass values, reported for the reader’s convenience in Fig. 12. The weighted average is $493.6355 \pm 0.0067$, rescaled (and rounded) to $493.636 \pm 0.011$ based on a ‘high $\chi^2$’, which is in reality not so bad, being 7.0 with 3 degrees of freedom,\footnote{Providing just ‘$\chi^2/\nu$’ is, as now well understood, rather misleading, because the $\chi^2$ does not scale with $\nu$. Therefore, though a ratio of 2.31 would be a clear alarm bell for $\nu = 100$, it is quite ‘in the norm’ for $\nu = 3$.} and thus yielding a $p$-value of 0.072, above even the (in-)famous threshold of 0.05 [32]. For this reason I could not resist to make a couple of exercises: first to see what a sceptical analysis would suggest if we stick to the simple weighted average, without the $\sqrt{2.31} (= 1.52)$ scaling; second to see what we get if we make an overall sceptical analysis in which individual results are used.

### 6.1 Sceptical analysis using the unscaled result of Ref. [8]

Once the $\times 1.52$ scaling factor on the lowest value is removed, the weighted average is shifted down and falls right in the middle of the two most measurements, as shown by the dashed line of Fig. 13, yielding $m_{K^{-}} = 493.666 \pm 0.005$ MeV. But a sceptical analysis yields a broader distribution, overlapping the two precise measurements on the sides, thus taking into serious account also the results in between. Having to report the result as average and standard deviation of the distribution we get then $493.662 \pm 0.017$ MeV (but remember that the complete result is provided by the
Looking into the details of the inference, we see that, as imaginable, high values for $r_5$ and $r_6$ are preferred ($2.8 \pm 2.4$ and $3.4 \pm 2.7$, respectively), while the others remain more or less around the prior values of $\approx 1.0$.

### 6.2 Sceptical analysis using the individual values of Ref. [8]

Let us know go into the details of the results which contribute to 5-th entry of Tab. 1, reported in Fig. 12 [8] and in the entries 5-8 of Tab. 2. There is one high precision value favoring a small mass value ($493.631 \pm 0.007\text{ MeV}$), and three values of minor precision preferring higher mass values. The simple weighted average of $493.6355 \pm 0.0067\text{ MeV}$ is then practically equal to the highest precision value. But then a $\times 1.52$ scaling is applied by the authors. The combined uncertainty grows up, which is something desirable, but it does it symmetrically around the mean, not taking into account the fact that the other results would pull the mass value up.

It is then interesting to make a sceptical combination of these four points. The
| i | Authors | pub. year | $|d_i|$ (MeV) | $|s_i|$ (MeV) |
|---|---------|-----------|------------|------------|
| 1 | G. Backenstoss et al. [4] | 1973 | 493.691 | 0.040 |
| 2 | S.C. Cheng et al. [5] | 1975 | 493.657 | 0.020 |
| 3 | L.M. Barkov et al. [6] | 1979 | 493.670 | 0.029 |
| 4 | G.K. Lum et al. [7] | 1981 | 493.640 | 0.054 |
| 5 | K.P. Gall et al. [8] | 1988 | 493.675 | 0.026 |
| 6 | | | 493.631 | 0.007 |
| 7 | | | 493.806 | 0.095 |
| 8 | | | 493.709 | 0.073 |
| 9 | A.S. Denisov et al. & Yu.M. Ivanov [9, 10] | 1991 | 493.696 | 0.007 |

Table 2: Details of the individual result used in the overall analysis.

Figure 14: Standard and sceptical combination of the four data points of Ref. [8]. The dashed line is the simple weighted average; the gray line having the same center and larger width is the same with the standard deviation scaled by $\sqrt{\chi^2/\nu}$ as done in Ref. [8]. The thick, asymmetric curve represent the result of the sceptical combination.
result is shown in Fig. 14. The sceptical analysis takes into account also the results favoring higher mass values, although the peak of the distribution (the ‘mode’) remains very close to the most precise result, and there is a substantial overlap with it. The distribution is now skewed on the right side, assigning higher probability that the mass value is, for example, above 493.65 MeV with respect to what we could think judging from mean and standard deviation alone. The resulting mass is 493.642 ± 0.016 MeV shifted up by about 6 keV, with a standard uncertainty about 50% larger than that provided by the $\sqrt{\chi^2/\nu}$ scaling prescription. But what is more interesting is that the latter (gray line in the figure, just below the red dashed one) does not give a correct account of the possible values of $m_{K^\pm}$, because: i) it is extended to the low mass values sizable more than the measured points would allow it; ii) it gives practically no chance to mass values above e.g. 493.657 MeV.

Finally there is the question of combining this result with the other five ones of other experiments. What should we use as input for the global analysis? Honestly, at this point we cannot pretend to have not seen the outcome shown in Fig. 14 and to use just the resulting average and standard uncertainty. We also cannot feed into the model the complicated posterior we have got. Therefore the only solution is to make a new combined analysis, but using all individual results of Ref. [8]. For sake of clarity all points are repeated in Tab. 2. The result of the analysis, plotted in Fig 15, is quite surprising on a first sight: while the standard weighted average is practically the same of Fig. 13 (small differences might be attributed to rounding$^{23}$), the sceptical combination moves up, disfavoring the low mass solution and yielding 493.677 ± 0.013 MeV.

“The same as the PDG result”, one would promptly shout at this point, “and after so much work!” Well, yes and no... Indeed, the PDG numbers were obtained considering an arbitrarily enlarged uncertainty for the combined result of Ref. [8]. Applying, instead, the scaling prescription to the nine individual points of Tab. 2 a value of 493.664 ± 0.011 MeV would have been obtained, 13 keV below the result of the sceptical analysis (see Fig.15). Certainly this $\approx -1\sigma$ bias will not harm our understating of fundamental physics, but it is better to avoid this kind of biases because they could perhaps be important in other measurements.

$^{23}$Indeed, if we just calculate weighted averages and related standard deviations, with no arbitrary scaling, the result does not change if we use the individual results or we group them in steps. This is related to the important concept of ‘statistical sufficiency’, that will be treated in detail, for the Gaussian case, in the forthcoming Ref. [35].
Figure 15: Combined analysis obtained considering the individual points of [8]. The non-trivial final pdf of the sceptical analysis (thick continuous black line) can be summarized as $493.677 \pm 0.013$ MeV. The weighed average (dashed red) leads instead $493.6644 \pm 0.0046$, which becomes $493.664 \pm 0.011$ (solid gray Gaussian just below the dashed red one) when the standard deviation is scaled by the factor $\sqrt{\chi^2/\nu} = \sqrt{47.7/8} = 2.42$. 
6.2.1 Correlations among the values jointly inferred in the global sceptical analysis

Let us conclude showing further details concerning the MCMC sampling. Here is the output of the R command `summary(chain)` concerning the ten model parameters:

1. **Empirical mean and standard deviation for each variable,**
   plus standard error of the mean:

   |    | Mean   | SD     | Naive SE | Time-series SE |
   |----|--------|--------|----------|----------------|
   | mu | 493.6769 | 0.01285 | 1.285e-05 | 3.564e-05 |
   | r[1] | 0.8101 | 0.48421 | 4.842e-04 | 5.354e-04 |
   | r[2] | 1.0698 | 0.69051 | 6.905e-04 | 9.878e-04 |
   | r[3] | 0.8171 | 0.48464 | 4.846e-04 | 5.161e-04 |
   | r[4] | 0.8903 | 0.53044 | 5.304e-04 | 5.713e-04 |
   | r[5] | 0.8175 | 0.49282 | 4.928e-04 | 5.288e-04 |
   | r[6] | 4.5338 | 3.03359 | 3.034e-03 | 4.704e-03 |
   | r[7] | 1.1908 | 0.70179 | 7.018e-04 | 7.371e-04 |
   | r[8] | 0.8121 | 0.48643 | 4.864e-04 | 5.035e-04 |
   | r[9] | 2.0938 | 1.76421 | 1.764e-03 | 3.675e-03 |

2. **Quantiles for each variable:**

   |    | 2.5% | 25% | 50% | 75% | 97.5% |
   |----|------|-----|-----|-----|------|
   | mu | 493.6497 | 493.6680 | 493.6778 | 493.6872 | 493.697 |
   | r[1] | 0.3588 | 0.5322 | 0.6889 | 0.9332 | 1.986 |
   | r[2] | 0.4098 | 0.6661 | 0.9014 | 1.2591 | 2.736 |
   | r[3] | 0.3617 | 0.5381 | 0.6958 | 0.9420 | 1.999 |
   | r[4] | 0.3928 | 0.5865 | 0.7584 | 1.0274 | 2.175 |
   | r[5] | 0.3608 | 0.5370 | 0.6954 | 0.9426 | 2.007 |
   | r[6] | 1.3815 | 2.7852 | 3.8487 | 5.4038 | 11.809 |
   | r[7] | 0.5333 | 0.7871 | 1.0145 | 1.3696 | 2.905 |
   | r[8] | 0.3644 | 0.5374 | 0.6922 | 0.9338 | 1.979 |
   | r[9] | 0.4660 | 0.9894 | 1.6476 | 2.6319 | 6.396 |

As we can see, at this point the most suspicious measurement is the 6-th of the complete list, as we can better judge from the quantiles indicating that, for example, there is only about 2.5% probability that \( r_6 \) is below 1.38.

---

\(^{24}\)Someone would be surprised about the possibility of inferring a number of parameters superior to the number of the data points. This is not really a conceptual problem, as long as we understand that they are correlated, often in a complicate way and of which the correlation matrix is just a first order representation (and we have to be careful when using it in further analyses [36]).
Let us also give a look at the correlation matrix:

\[
\begin{array}{ccccccccccc}
  & \text{mu} & r[1] & r[2] & r[3] & r[4] & r[5] & r[6] & r[7] & r[8] & r[9] \\
\text{mu} & 1.00 & -0.15 & 0.33 & 0.07 & 0.15 & -0.01 & 0.40 & -0.11 & -0.10 & -0.61 \\
r[1] & -0.15 & 1.00 & -0.04 & 0.00 & -0.02 & 0.01 & -0.06 & 0.02 & 0.02 & 0.10 \\
r[2] & 0.33 & -0.04 & 1.00 & 0.04 & 0.05 & 0.02 & 0.14 & -0.03 & -0.03 & -0.20 \\
r[3] & 0.07 & 0.00 & 0.04 & 1.00 & 0.01 & 0.02 & 0.03 & -0.01 & 0.00 & -0.03 \\
r[4] & 0.15 & -0.02 & 0.05 & 0.01 & 1.00 & 0.00 & 0.06 & -0.02 & -0.01 & -0.09 \\
r[5] & -0.01 & 0.01 & 0.02 & 0.02 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.02 \\
r[6] & 0.40 & -0.06 & 0.14 & 0.03 & 0.06 & 0.00 & 1.00 & -0.04 & -0.04 & -0.25 \\
r[7] & -0.11 & 0.02 & -0.03 & -0.01 & -0.02 & 0.00 & -0.04 & 1.00 & 0.01 & 0.07 \\
r[8] & -0.10 & 0.02 & -0.03 & 0.00 & -0.01 & 0.00 & -0.04 & 0.01 & 1.00 & 0.06 \\
r[9] & -0.61 & 0.10 & -0.20 & -0.03 & -0.09 & 0.02 & -0.25 & 0.07 & 0.06 & 1.00 \\
\end{array}
\]

The $r_i$ with some sizable correlation with the mass are, in the order, $r_9$, $r_6$ and $r_3$, i.e. those related to the individual results that mostly differ from the barycenter of the final pdf of the mass got by the MCMC sampling (see Fig. 15 in order to get an idea of the reason for the sign of each correlation coefficient).

---

Technical remark: the correlation matrix has been obtained by the R function `cor()`, applied to the chain after a suitable transformation. For example, one can transform it into a data frame and then apply `cor()` to it:

```r
> chain.df <- as.data.frame( as.mcmc(chain) )
> round(cor(chain.df),2)
```

that includes the rounding at two decimal digits ('>' is the R prompt).

Or, more simply, we can convert the chain into a matrix, each column containing the occurrences of each variable during the sample, and calculate then the correlations between them. This is how to do it in short, with nested calls to functions (remember also `print()`, if the command hat to be included into a script):

```r
> round(cor(as.matrix(chain)),2)
```

And here are some useful commands to understand what is going on:

```r
> chain.M <- as.matrix(chain)
> str(chain.M)
> dimnames(chain.M)
> mean(chain.M[,"mu"])
> mean(chain.M[,1])
> mean(chain.M[,"r[9]" ])
> mean(chain.M[,10])
> cor(chain.M,"mu", chain.M,"r[9]" )
> cor(chain.M[,1], chain.M[,10])
```
7 Conclusions

The initial motivation of this paper was didactic, i.e. how to perform a sceptical combination of results by MCMC using a convenient program, after having got a better insight of the problem by Bayesian network (this is the name also used for the graphical models we have encountered here). The choice of the physics case was fortuitous, having been recently personally interested in the charged kaon mass and having learned thus about ‘apparent’ disagreements between the most accurate measurements. However, it is clear that this paper is far from attempting to give a definite answer, for which not only a ‘statistical’

\[ m_k = 493.677 \pm 0.013 \text{ MeV}, \]

where \( I \) stands for all the conditions referred in section 6.2 (probability is always conditional probability and hence so are also pdf’s and moments of distributions). The result seems in practical perfect agreement with the PDG one reminded in Fig. 1. But, first, the \( f(m | I) \) estimated by sampling is not trivial and definitely far from Gaussian (see solid thick line of Fig. 15), yielding e.g. the following probability intervals (not “C.L.’s!”):

\[
\begin{align*}
P(493.650 & \leq m_k / \text{MeV} \leq 493.697 | I) = 95 \% \\
P(493.668 & \leq m_k / \text{MeV} \leq 493.687 | I) = 50 \% \\
\end{align*}
\]

Second, even if the numerical results coincide, this agreement is just due to a compensation of two effects in the PDG analysis which go into opposite directions:

- a weighted average of all nine individual results (see Tab. 2), with the final ‘error’ scaled according to the \( \sqrt{\chi^2/\nu} \) prescription, would have lead to 493.664 ± 0.011 MeV, that is 13 keV lower than that reported by the PDG [3];

- however, the analysis was not performed on the nine individual results of Tab. 2, but on the six ones of Tab. 1, where the precise result 493.631 ± 0.007 MeV of Ref. [8] had been ‘weakened’ by the other three because of the \( \sqrt{\chi^2/\nu} \) scaling prescription already applied by the authors. For this reason the overall result

\[\text{For example it is important to understand how the ‘errors’ were evaluated, also because we are aware of the old custom (maintained also presently by several experimental teams) of using for ‘systematic errors’ extreme variations for sake of safety, thus providing very conservative ‘error’, instead than standard uncertainties [1, 2].}\]
went up to $493.677 \pm 0.013$ MeV, hence producing a bias of $+13$ keV, that is of the same size of the quote ‘error’.

The latter point is the surprising novelty of this work, and it deserves another paper [35] and perhaps further investigation to check if other, perhaps more important results are affected by such a bias too.

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Appendix – A case of possibly ‘too good’ agreement

Let us also see a case in which the mutual agreement among individual results ‘seems’ too good. In order to use again the kaon mass data, we take the four results published before year 1988, shown with solid blue Gaussians in Fig. 16, to which we over-impose (usual dashed red Gaussian) the outcome of the weighted average yielding $493.664 \pm 0.015 \text{ MeV}$. But in this case our suspicion is that the uncertainty could be overestimated. Indeed, if we calculate the $\chi^2$ we get 0.818, with a $\chi^2/\nu$ of 0.27 (p-value 0.85). Applying strictly the $\sqrt{\chi^2/\nu}$ scaling prescription – frequentist gurus probably might not agree, but let us go on with the exercise – we get a scaling factor of $\times 0.52$, and thus an ‘error’ of $7.7 \text{ keV}$ (dotted gray Gaussian). The posterior pdf of the sceptical analysis (solid thick black line) is this time practically Gaussian and gives $493.664 \pm 0.012 \text{ MeV}$: the curve is narrower than the simple weighted average, in agreement with our suspicions, but not as narrow as when the $\sqrt{\chi^2/\nu}$ scaling was (improperly?) used. Conclusions on this last comparisons are left to the reader.

Figure 16: Standard and sceptical analysis of the results published before year 1988.