A Good Measure for Bayesian Inference

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Abstract

The Gaussian theory of errors has been generalized to situations, where the Gaussian distribution and, hence, the Gaussian rules of error propagation are inadequate. The generalizations are based on Bayes’ theorem and a suitable measure. The following text sketches some chapters of a monograph \footnote{1} that is presently prepared. We concentrate on the material that is — to the best of our knowledge — not yet in the statistical literature. See especially the extension of form invariance to discrete data in section 4, the criterion on the compatibility between a proposed distribution and sparse data in section 7 and the “discovery” of probability amplitudes in section 9.

1 The Prior Distribution

Bayes’ theorem \footnote{1} allows one to deduce the distribution $P(\xi|x)$ of the parameter $\xi$ conditioned by the data $x$. The distribution $p(x|\xi)$ of the data conditioned by the parameter $\xi$ must be given. The theorem reads

\begin{equation}
P(\xi|x)m(x) = p(x|\xi)\mu(\xi)
\end{equation}

\begin{equation}
m(x) = \int d\xi p(x|\xi)\mu(\xi).
\end{equation}

See e.g. \footnote{1}. Here, $\mu(\xi)$ is called the prior and $P$ the posterior distribution of $\xi$. The posterior can be used to deduce an interval $I$ of error: We define it as the smallest interval in which $\xi$ is with probability $K$. This is called

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the Bayesian interval \( I = I(K) \). In order to make it independent of any reparametrisation \( \eta = T(\xi) \), one has to judge the size \( A \) of an interval \( I \) by help of a measure \( \mu(\xi) \), i.e.

\[
A = \int_I d\xi \, \mu(\xi) .
\]

We identify this measure with the prior distribution of \( \mu \).

## 2 Form Invariance

Ideally the conditional distribution \( p(x|\xi) \) possesses a symmetry called form invariance. This family of distributions then emerges by a mathematical group of transformations \( G_{\xi} x \) from one and the same basic distribution \( w \), i.e.

\[
p(x|\xi)dx = w(G_{\xi} x)dG_{\xi} x. \tag{4}
\]

It is not required that every acceptable \( p \) has this symmetry. But the symmetry guarantees an unbiased inference in the sense of section 3. If there is no form invariance, unbiased inference can be achieved only approximately.

The prior distribution is defined as the invariant measure of the group of transformations. Symmetry arguments were first discussed in \[3, 4, 5, 6\]. They were not generally accepted because not all reasonable distributions possess the symmetry \[4\]. It cannot exist at all if \( x \) is discrete. Since \( \xi \) is assumed to be continuous, it can be changed infinitesimally. However, no infinitesimal transformation of a discrete variable is possible. In section 4, we generalize form invariance to this case.

Form invariance is a property of ideal, well behaved distributions. However, its existence is not a prerequisite of statistical inference, see section 6.

The invariant measure can be found from \( p \) — without analysis of the group — by evaluating the expression

\[
\mu(\xi) \propto \det \left( \int dx \, p(x|\xi) \partial_\xi L \partial^T_\xi L \right)^{1/2}. \tag{5}
\]

Here, the function \( L \) is

\[
L(\xi) = \ln p(x|\xi) \tag{6}
\]

and \( \partial_\xi L \partial^T_\xi L \) means the dyadic product of the vector \( \partial_\xi L \) of partial derivatives with itself. Eq.\((5)\) is known as Jeffreys’ rule \[4\].

One shall see in section 6 that this expression defines \( \mu \) in any case that is to say in the absence of form invariance, too.
3 Invariance of the Entropy of the Posterior Distribution

The posterior distribution \( P(\xi|x) \) has the same symmetry as the conditional distribution \( p(x|\xi) \) if form invariance exists. The entropy

\[
H(x) = -\int dx \, P(\xi|x) \ln \frac{P(\xi|x)}{\mu(\xi)}
\]

is then independent of the true value \( \hat{\xi} \) of the parameter \( \xi \) because one has

\[
H(x) = H(G_\rho x)
\]

for every transformation \( G_\rho \) of the symmetry group. This entails that \( H(x) \) does not depend on \( \hat{\xi} \) but only on the number \( N \) of the data \( x_1 \ldots x_N \). One can say that all values of the parameter \( \xi \) are equally difficult to measure. In this sense, form invariance guarantees unbiased estimation of \( \xi \) and by the same token the invariant measure \( \mu \) is the parametrization of ignorance about \( \xi \).

4 Form Invariance for Discrete \( x \)

If the variable \( x \) is discrete — e.g. a number of counts — then form invariance cannot exist in the sense of eq.(4) since an infinitesimal shift of \( \xi \) cannot be compensated by an infinitesimal transformation of \( x \). One then has to define a vector \( a(\xi) \) the components of which are labelled by \( x \). The probability \( p(x|\xi) \) must be a unique function of \( a_x(\xi) \). Form invariance then means that

\[
a(\xi) = G_\xi a(\xi = 0)
\]

Again \( \mu \) is the invariant measure of the group. The transformation \( G_\xi \) shall be linear so that it is the linear representation of the symmetry group of form invariance. It is necessarily unitary.

The choice \( a_x(\xi) = p(x|\xi) \) is precluded because a group of transformations cannot — for all of its elements — map a vector with positive elements onto one with the same property. With the choice

\[
a_x(\xi) = \sqrt{p(x|\xi)}
\]

one succeeds. That means: Important discrete distributions — such as the Poisson and the binomial distributions — possess form invariance. Furthermore the property (3) can be recast into a relation corresponding to eq.(9).
i.e. it can be written as a linear transformation of the space of functions \((p(x|\xi))^{1/2}\). Hence, (4) is not different from (4); it is a generalization.

Note that (10) is a probability amplitude as it is used in quantum mechanics. However, it is real up to this point. The generalization to complex probability amplitudes is sketched in section 8.

5 The Poisson Distribution

Form invariance in the sense of section 4 does not seem to have been treated in the literature on statistics. As an example let us consider the Poisson distribution

\[
p(x|\xi) = \frac{\lambda^x}{x!} \exp(-\lambda)
\]

\(x = 0, 1, 2 \ldots \) \hspace{1cm} (11)

With

\[\xi = \lambda^{1/2}\]

one obtains the amplitudes

\[a_x(\xi) = \frac{\xi^x}{\sqrt{x!}} \exp(-\xi^2/2).\] \hspace{1cm} (13)

The derivative of \(a\) is found to be

\[\frac{\partial}{\partial \xi} a(\xi) = (A^+ - A)a(\xi),\]

(14)

where \(A, A^+\) are linear operators independent of \(\xi\). They have the commutator

\[[A, A^+] = 1.\]

Hence, \(A, A^+\) are destruction and creation operators of numbers of counts or events. Integrating the differential equation (14) one finds

\[a(\xi) = \exp (\xi (A^+ - A)) |0\rangle.\]

(16)

Here, the vacuum \(|0\rangle\) is the vector that provides zero counts with probability 1. Equation (16) means that the linear transformation \(G_\xi\) is

\[G_\xi = \exp (\xi (A^+ - A)).\]

(17)

The measure \(\mu\) of this group of transformations is

\[\mu(\xi) \equiv \text{const.}\]

(18)
It can also be obtained by straightforward application of Jeffreys’ rule (3) without analysis of the symmetry group.

This can be generalized to the joint Poisson distribution

$$p(x_1 \ldots x_M|\xi_1 \ldots \xi_M) = \prod_{k=1}^M \frac{\xi_k^{2x_k}}{x_k!} \exp(-\xi_k^2)$$

(19)

of the numbers $x_k$ of counts in a histogram with $M$ bins. One finds the amplitude vector

$$a(\xi_1 \ldots \xi_M) = \exp \left( \sum_k^M \xi_k(A_k^+ - A_k) \right) |0\rangle$$

(20)

and again the uniform measure $\mu(\xi) \equiv \text{const}$.

As a further generalization, one can introduce destruction and creation operators $B_\nu, B_\nu^+$ of quasi-events $\nu = 1 \ldots n$ via

$$B_\nu = \sum_{k=1}^M c_{k\nu} A_k.$$

(21)

If the vectors $|c_\nu\rangle$ for $\nu = 1 \ldots n$ are orthonormal then

$$[B_\nu, B_\nu^+] = \delta_{\nu\nu'},$$

(22)

whence $B_\nu, B_\nu^+$ are destruction and creation operators. One finds the amplitude vector

$$a(\xi) = \exp \left( \sum_{\nu=1}^n \xi_\nu (B_\nu^+ - B_\nu) \right) |0\rangle$$

(23)

The amplitude $a_x$ to find the event $x$ is given by

$$a_x(\xi) = \prod_{k=1}^M \frac{1}{\sqrt{x_k}} (\Xi_k)^{x_k} \exp \left( -\frac{1}{2} \sum_{\nu}^n \xi_{\nu}^2 \right).$$

(24)

Here, the amplitude

$$\Xi_k = \sum_{\nu=1}^n \xi_{\nu} c_{k\nu}$$

(25)

to find events in the $k$-th bin is given by an expansion into the orthogonal system of amplitude vectors $|c_\nu\rangle$. More precisely: By working with the creation operators $B_\nu^+$, one infers an expansion of the vector $|\Xi\rangle$ in terms of
the orthogonal system $|c_\nu\rangle$. The prior distribution of the amplitudes $\xi_\nu$ is again uniform,

$$\mu(\xi_1 \ldots \xi_\nu) \equiv \text{const.} \quad (26)$$

On Summary: The problem of finding the expansion coefficients $\xi_\nu$ from the counting rates $x_k$ is form invariant and thus guarantees unbiased inference. One should therefore expand probability amplitudes and not probabilities in terms of an orthogonal system if one performs e.g. a Fourier analysis.

6 The Prior Probability in the Absence of Form Invariance

Jeffreys’ rule (5) can be rewritten in the form

$$\mu(\xi) \propto \det \left( \int dx \partial_\xi a \partial_\xi^T a \right)^{1/2}. \quad (27)$$

The integral means a summation if $x$ is discrete.

In differential geometry [8, 9], it is shown that (27) is the measure on the surface defined by the parametrisation $a(\xi)$. A prerequisite for this measure is the assumption that one has the same uniform measure on each coordinate axis in the space; more precisely, the metric tensor of the space must be proportional to the unit matrix. Since the coordinates $a_x$ are probability amplitudes, this is justified by the last result of section 5.

Hence, Jeffreys’ rule provides the prior distribution in any case. In the absence of form invariance, however, one cannot guarantee that all values of the parameter $\xi$ are equally difficult to measure, i.e. one cannot guarantee unbiased inference.

7 Does a Proposed Distribution Fit an Observed Histogram?

The Poisson distribution (19) yields the posterior

$$P(\xi_1 \ldots \xi_M|x_1 \ldots x_M) \propto \prod_{k=1}^{M} \xi_k^{2x_k} \exp(-\xi_k^2) \quad (28)$$

We want to decide whether — in the light of the data — the proposal $\tau_k$ is a reasonable estimate of $\xi_k$, $k = 1 \ldots M$. This is equivalent to the question whether $\tau$ is in the Bayesian Interval $I = I(K)$. The Bayesian interval is
bordered by the “contour line” $\Gamma(K)$ which is — in the case at hand — defined as the set of points with the property $P(\xi|x) = C(K)$. This means that $\tau \in I$ exactly if

$$P(\tau|x) > C(K)$$

or that $\tau$ is accepted if and only if (29) holds. The number $C(K)$ can be calculated.

If the count rates $x_k$ are large in every bin $k$, the procedure essentially yields the well-known $\chi^2$-criterion.

If, however, $M \geq N = \sum_k x_k$, i.e. if the data are sparse, then this leads to the condition

$$\frac{1}{N} \sum_{k=1}^{M} x_k \left( \frac{N}{x_k} - 1 - \ln \frac{N \tau_k^2}{x_k} \right) < \ln \left( 1 + \frac{M}{2N} \right) + N^{-1/2} \Phi^{-1}(K).$$

(30)

Here, $\Phi^{-1}$ is the inverse of the probability function. Note that the expression in brackets (…) on the l.h.s. is $\geq 0$ if

$$\sum_k \tau_k^2 = 1.$$

(31)

Hence, the inequality (30) sets an upper limit to a positive expression. This criterion is new. It is needed because the situation $M \geq N$ is surely met if $k$ is a multidimensional variable i.e. if the observable is multidimensional. See [10]. Any attempt to apply Gaussian arguments is hopeless in this case.

8 Does a Proposed Probability Density Fit Observed Data?

Suppose that the data $x_1 \ldots x_N$ have been observed. Each $x_k$ is supposed to follow, say, an exponential distribution

$$p(x|\xi) = \xi^{-1} \exp(-x/\xi).$$

(32)

They shall all be conditioned by one and the same hypothesis parameter $\xi$. If this is true, the posterior $P(\xi|x_1 \ldots x_N)$ yields the distribution of $\xi$ and, hence, the Bayesian interval for $\xi$. It is intuitively clear that — at least for large $N$ — one can learn from the data not only the best fitting values of $\xi$ but one can even decide whether the exponential (32) is justified at all. I.e.
one can find out whether the model is satisfactory. How does this work? We do not want to produce a histogram by binning the data. This would reduce the problem to the one solved in section 7 but it would introduce an arbitrary element into the decision: The definition of the bins.

The basic idea is to determine \( \xi \) from every data point, i.e. \( N \) times, and to decide whether this result is compatible with \( \xi \) having the same value everywhere.

One defines the distribution \( q \) of the \( N \)-dimensional event \( (x_1 \ldots x_N) \) conditioned by the \( N \)-dimensional hypothesis \( (\xi_1 \ldots \xi_N) \) as the product

\[
q(x_1 \ldots x_N | \xi_1 \ldots \xi_N) = \prod_{k=1}^{N} p(x_k | \xi_k). \tag{33}
\]

One writes down the posterior distribution \( Q(\xi_1 \ldots \xi_N | x_1 \ldots x_N) \) of the \( N \)-dimensional hypothesis \( (\xi_1 \ldots \xi_N) \). One studies its Bayesian interval \( I(\mathcal{K}) \).

A proposed hypothesis \( (\tau_1 \ldots \tau_N) \) is acceptable exactly if it is an element of \( I \). In the case at hand, one determines the best value \( \alpha \) of the hypothesis \( \xi \) from the model that assigns one and the same hypothesis to all the data. One then asks whether the \( N \)-dimensional \( \tau \) with \( \tau_k = \alpha \) for all \( k \) is in \( I \).

The criterion (30) has been derived by help of this argument.

Note, however, that the argument fails, when one wants to know whether the data \( (x_1 \ldots x_N) \) follow the proposed distribution \( t(x) \). There is no hypothesis \( \xi \). The family of distributions is not defined from which \( t(x) \) is taken. Indeed the above argument does not judge the distribution \( p(x | \alpha) \) all by itself. It actually judges whether the family of distributions, i.e. the whole model \( p(x | \xi) \), is compatible with the data. The question whether \( t(x) \) fits the data, is too general to be answered. One must specify which features of the distribution are important — its form in a region, where one finds most events or in a region where there are very few events? The relevant features are expressed by the parametric dependence on \( \xi \) and the measure derived from it.

9 The Logic of Quantum Mechanics

The results of section 5 show that probability amplitudes rather than probabilities can be inferred in an unbiased way from counting events. Alternatives \( \nu, \nu' \) are defined by two vectors \( |c_\nu\rangle \) and \( |c_{\nu'}\rangle \). Each vector characterizes a distribution over the bins \( k = 1 \ldots M \) of a histogram. A decision between \( \nu \) and \( \nu' \) amounts to assess the amplitudes \( \xi_\nu \) and \( \xi_{\nu'} \). They determine the strength with which the distributions \( \nu \) and \( \nu' \) are present in the data.
However, the amplitudes can interfere — the probabilities cannot. The real amplitudes introduced so far can be generalized to complex ones: We arrive at the quantum mechanical way to treat alternatives.

The parameters $\xi$ deduced from counting events are then completely analogous with quantum mechanical probability amplitudes. It may be better to turn this statement around and to say: The logic of quantum mechanics is the logic of unbiased inference from random events; it is not a collection of the rules according to which the microworld “exists”.

The generalization of real amplitudes to complex ones is achieved by generalizing the amplitude vector (23) to

$$a(\xi, \zeta, \phi) = \exp \left( i \sum_{\nu=1}^{n} D_{\nu} \right) |0\rangle,$$

where the operator $D_{\nu}$ is

$$D_{\nu} = \zeta_{\nu} (B_{\nu} + B_{\nu}^{+}) + i \xi_{\nu} (B_{\nu} - B_{\nu}^{+}) + \phi_{\nu}.$$

Here, the three generators do generate a group since one has the commutator

$$[B_{\nu} - B_{\nu}^{+}, B_{\nu} + B_{\nu}^{+}] = 2.$$

The invariant measure is

$$\mu(\xi, \zeta, \phi) \equiv \text{const.}$$

By explicit evaluation of eq.(34) one finds

$$a_{x} = \prod_{k=1}^{M} \frac{1}{\sqrt{x_{k}}} \left( \sum_{\nu=1}^{n} \Xi_{k} \right)^{x_{k}} \exp \left( -\frac{1}{2} \sum_{\nu} (\xi_{\nu}^{2} + \zeta_{\nu}^{2} - 2i\phi_{\nu}) \right)$$

This is a generalization of expression (24). It is again a Poisson distribution, but now the amplitude $\Xi_{k}$ to find events in the k-th bin is

$$\Xi_{k} = \sum_{\nu=1}^{n} (\xi_{\nu} + i\zeta_{\nu}) c_{k\nu}^{*}.$$

This is an expansion of the probability amplitude in terms of the system of mutually orthogonal vectors $|c_{\nu}^{*}\rangle$ which may be complex. The expansion coefficients $\xi_{\nu} + i\zeta_{\nu}$ may be complex, too.
The phase $\sum_\nu \phi_\nu$ that appears in (38) cannot be measured since only the modulus of (38) is accessible.

The Poisson distribution possesses form invariance with respect to the probability amplitudes even if these are complex. Put differently, one should expand the square root of a distribution into a system of orthonormal vectors. They may be complex. The expansion coefficients deduced from the data may also be complex. Inference on the real and imaginary parts of the expansion coefficients is unbiased. The Fourier expansion is an example; however, it must be the square root of the probability distribution that is expanded.

10 Alternatives that cannot Interfere

In quantum physics alternatives can interfere. Suppose that a cross section $\sigma = \sigma(E)$ is observed as a function of energy $E$ — e.g. in neutron scattering by heavy nuclei. Suppose that this excitation function shows a resonance line plus a smooth background. The book [11] is full of examples. Look e.g at the middle part of page 691. There is a flat background with superimposed resonances. The resonance lines destructively and constructively interfere with the background.

Speaking in the language of section 5, the figure offers a simple alternative $\nu = 1, 2$. The first possibility ($\nu = 1$) is that the incoming neutron together with the target forms a compound system which decays after some time. The second possibility ($\nu = 2$) is the reaction to occur without delay. The probability amplitudes $\xi_\nu + i\zeta_\nu$ for these two possibilities interfere. The interference pattern is visible if the resolution of the detection system is better than the width of the resonance. If the resolution is much worse, the interference pattern disappears and the cross section due to the resonance is added to the cross section due to the background, i.e. one adds the probabilities $\pi_\nu = \xi_\nu^2 + \zeta_\nu^2$ instead of the amplitudes.

The situation of insufficient resolution is the situation of classical physics and classical statistics: Alternatives do not interfere. Their probabilities are added.

The typical situation of classical physics is that the detection system lumps many events together that have distinguishable properties. In our example: It does not well enough discriminate the energies of the scattered particles. The events recorded in classical physics can in principle be differentiated according to more properties than are actually used to distinguish them. The tacit assumption of classical physics was that this were always
If objects are observed that allow for a small number of distinctions only, one is lead to the logic of interfering probability amplitudes by the way sketched in sections 5 and 9.

Consider the two slit experiment as a further example. If it is performed with polarized electrons, an impressive interference pattern appears. Use of unpolarized electrons reduces the contrast of the pattern. Had the scattered particles more than two “ways to be”, the contrast of the interference would be reduced up to the point, where the probability of a particle going through the first slit would be added to the probability of the particle going through the second slit. See chapter 1 of [12].

Suppose that we know that there is interference between the two possibilities in the above neutron scattering experiment. The amplitudes $\xi_\nu + i\zeta_\nu$ for the possibilities $\nu = 1, 2$ would be inferred from the data $x_1 \ldots x_k$ as follows. The distribution of the data is

$$p(x_1 \ldots x_N|\xi_1\xi_2\zeta_2) = \prod_{k=1}^{M} \frac{\lambda_k^{x_k}}{x_k!} \exp(-\lambda_k) ,$$

(40)

where the expectation value $\lambda_k$ in the $k$-th bin is a function of $\xi_\nu, \zeta_\nu$, namely

$$\lambda_k = |(\xi_1 + i\zeta_1)\text{Line}(k) + (\xi_2 + i\zeta_2)\text{Bg}(k)|^2 .$$

(41)

Here, $\text{Line}(k)$ is the line shape and $\text{Bg}(k)$ is the shape of the background. By section 9, this is a form invariant model allowing for unbiased inference.

Suppose on the contrary that there cannot be any interference between the two possibilities in the neutron experiment. The probabilities $\pi_1$ and $\pi_2$ are inferred via the model $p(x_1 \ldots x_N|\pi_1\pi_2)$ which is again given by eq. (40). But now $\lambda_k$ is the incoherent sum

$$\lambda_k = \pi_1|\text{Line}(k)|^2 + \pi_2|\text{Bg}(k)|^2 .$$

(42)

The prior distribution for this model must be calculated by help of (5). The model is not form invariant, whence unbiased inference cannot be guaranteed. A closer inspection shows that the model “has a prejudice against” very small values of $\pi_1$ or $\pi_2$. This means: Small values are harder to establish than large ones.

11 Summary

The basis of the foregoing work is twofold: (i) All statements and relations in statistical inference must be invariant under reparametrizations and (ii) to state ignorance about $\xi$ means to claim a symmetry.
It is the symmetry of form invariance that guarantees unbiased inference of the hypothesis \( \xi \), if the invariant measure of the symmetry group is identified with the prior distribution in Bayesian inference. The invariant measure is obtained in a straightforward way — i.e. without analysis of the group — by Jeffreys’ rule. We have shown that even distributions of counted numbers possess form invariance.

A study of the Poisson distribution shows that the basic quantities in statistical inference are probability amplitudes not probabilities. The amplitudes may even be complex. This is not only an analogy to the logic of quantum mechanics. This says that the logic of quantum mechanics is the logic of unbiased inference from counted events.

These considerations do not mean that form invariance is a condition for the possibility of inference. Lack of form invariance precludes unbiased inference; it does not preclude inference. In the absence of form invariance, the prior distribution is defined as the differential geometrical measure on a suitably defined surface: The surface must lie in a space of probability amplitudes. The measure on the surface is again given by Jeffreys’ rule.

As a practically useful result, we have formulated the decision whether a proposed distribution fits an observed histogram. The decision covers the case of sparse data. This case does not allow a Gaussian approximation and, hence, no \( \chi^2 \)-test.

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