Six textbook mistakes in data analysis

Alexandros Gezerlis\textsuperscript{1,2}, Martin Williams\textsuperscript{1,2}

\textsuperscript{1} Department of Physics, University of Guelph, Guelph, ON N1G 2W1, Canada
\textsuperscript{2} Office of Teaching and Learning, University of Guelph, Guelph, ON N1G 2W1, Canada

Received: 21 September 2022 / Accepted: 23 December 2022 © The Author(s), under exclusive licence to Società Italiana di Fisica and Springer-Verlag GmbH Germany, part of Springer Nature 2023

Abstract This article discusses a number of incorrect statements appearing in textbooks on data analysis, machine learning or computational methods; the common theme in all these cases is the relevance and application of statistics to the study of scientific or engineering data; these mistakes are also quite prevalent in the research literature. Crucially, we do not address errors made by an individual author, focusing instead on mistakes that are widespread in the introductory literature. After some background on frequentist and Bayesian linear regression, we turn to our six paradigmatic cases, providing in each instance a specific example of the textbook mistake, pointers to the specialist literature where the topic is handled properly, along with a correction that summarizes the salient points. The mistakes (and corrections) are broadly relevant to any technical setting where statistical techniques are used to draw practical conclusions, ranging from topics introduced in an elementary course on experimental measurements all the way to more involved approaches to regression.

1 Introduction

In an earlier work, we addressed the presence of many mistaken claims in computational physics textbooks.\cite{1} As noted there, while such errors are understandable in the research literature (where things are still rapidly evolving), they are more problematic (and pernicious) in the context of introductory textbooks. The present article is of a similar nature, in that it addresses a number of widespread misconceptions; this time we focus on textbook coverage of data analysis, a term typically used to describe the way that data is collected, processed, summarized, interpreted, etc. (Most of our discussion applies to linear statistical inference, but the lessons learned are of wider import.) These are topics that are taught at the undergraduate level either in a dedicated course on experimental measurements or as part of a course on numerical methods/computation.

Whether in traditional experimental analyses, or in more recent theoretical approaches, or even using tools borrowed from machine learning/data science, the theme of uncertainty quantification is increasingly important in science and engineering. The topics discussed in the present article involve applications of statistics of varying sophistication; given the broader community and applicability this entails, it should not come as a surprise that many of the mistakes discussed below are drawn from textbooks which have garnered tens of thousands of citations (each). We have selected these mistakes based on their being both widespread and important; each of the six incorrect claims elaborated on below appears in at least two standard textbooks. In other words, our focus is not on the (inevitable) typos or misunderstandings that arise when an individual author misrepresents a given topic, but on widespread errors that (while known to experts) continue to propagate through the introductory literature.

One of the authors recently finished updating an introductory computational physics textbook,\cite{2} a process preceded by an exploration of the data analysis/machine learning literature. The six themes discussed below are handled correctly in Ref.\cite{2}, but we also cite many works written by statisticians, in the spirit of providing the reader with many reliable resources. Our hope is that by bringing attention to these incorrect claims we can make sure that fewer students are exposed to them in their undergraduate education in the future; similarly, the points we raise may be of service to non-expert or novice researchers who currently treat some of these techniques as black boxes. Since many of these mistakes arise due to the use of inscrutable (or rarely scrutinized) mathematical symbols, it may be beneficial to start by discussing the notation.

2 Establishing the notation

Nearly all textbooks on numerical methods discuss the (linear algebra) problem of least-squares fitting: This is typically taken to involve as input a table of values, \((x_j, y_j)\) where \(j = 0, 1, \ldots, N - 1\) and \(N\) is the number of data points. In science, it is more
common to encounter, instead, the case of heteroskedastic errors, i.e., the scenario where each input data value \( y_j \) is itself the result of a separate experiment (and therefore associated with an input data uncertainty, \( \sigma_j \)). In other words, our input data can be thought of as \((x_j, y_j \pm \sigma_j)\). Whatever form our approximating function may take, we know that it is expected to somehow capture the behavior of the data \( y_j \), while also taking into consideration the uncertainty \( \sigma_j \) associated with each input data point. (That being said, other assumptions are typically more important than the unequal error variance) [3]. From a linear algebra perspective, this gives rise to weighted least squares; from a statistical perspective, the same results are more commonly arrived at in the context of maximum-likelihood estimation (MLE)—to which we return below.

Since the notation here can, indeed, become obscure, let us take the time to carefully distinguish between the true underlying behavior and our dataset. (Our discussion is intended merely to set the stage for Sect. 3, i.e., this is not a full pedagogical exposition.) We explicitly model the discrepancy between theory and experiment as follows:

\[
Y_j = \sum_{k=0}^{n-1} c_{*,k} \phi_k(x_j) + \mathcal{E}_j
\]

(1)

Here \( Y_j \) are the data ("dependent variable") values, the \( \phi_k \)’s are (input/frozen) basis functions, evaluated at the input ("independent variable") values \( x_j \), the \( c_{*,k} \)’s are the true/underlying parameter values, and \( \mathcal{E}_j \) is a continuous random variable. Crucially, here we are assuming that we know both the true theory (the \( \phi_k \)’s) and the true parameter values (the \( c_{*,k} \)’s); we will discuss below what to do when (as is usual in practice) you do not actually know these. The way to interpret Eq. (1) is as adding noise (the second term on the right-hand side) to the true/actual/theory value (the first term on the right-hand side), thereby producing the experimental value (on the left-hand side).

If we bundle together all the parameter values into a column vector and all the basis functions into a row vector (i.e., give \( k \) the values \( 0, 1, \ldots, n-1 \)—where, crucially, \( n \neq N \)), Eq. (1) can be compactly stated in the form \( Y_j = \Phi_j \mathbf{c}_* + \mathcal{E}_j \). (Similarly, you could bundle together all \( j \) values to summarize things as \( Y = \mathbf{8c}_* + \mathcal{E} \).) It is now time to make a specific assumption about the type of \( \mathcal{E}_j \) we are faced with: we take this to be the distribution \( \mathcal{N}(0, \sigma_j) \). Here we are employing the (standard) notation for a normal/Gaussian probability density function:

\[
\mathcal{N}(\mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left( \frac{1}{2} (\frac{x-\mu}{\sigma})^2 \right)
\]

(2)

where, as usual, the mean \( \mu \) determines the location of the peak and the standard deviation \( \sigma \) its width. (Note that, in this notation, \( \mathcal{N}(\mu, \sigma) \) lists the standard deviation, not the variance.) As a result of the central limit theorem, asymptotic normality does appear quite often in practice; even so, here we are explicitly taking the normality of \( y \) and \( \phi \). Qualitatively, Eq. (3) gives rise to the maximum-likelihood estimator (MLE); from a statistical perspective, the same results are more commonly arrived at in the context of maximum-likelihood estimation (MLE)—to which we return below.

Starting with the frequentist approach, since the data-generating distribution giving rise to \( Y_j \) in Eq. (1) was taken to be normal/Gaussian, it is reasonable to assume that something similar holds for a general parameter set \( \mathbf{c}_* \):  

\[
P(y; \mathbf{c}, \Phi, \Sigma_d) = \prod_{j=0}^{N-1} \frac{1}{\sqrt{2\pi\sigma_j}} \exp\left( \frac{-1}{2} \sum_{j=0}^{N-1} \frac{(y_j - \phi_j \mathbf{c}_*)^2}{\sigma_j} \right)
\]

(3)

where, crucially, this involves \( \mathbf{c} \) instead of \( \mathbf{c}_* \); here, \( \Sigma_d \) bundles together the input data variances (i.e., the \( \sigma_j^2 \)’s). Qualitatively, Eq. (3) is a statistical model telling us how a given \( \mathbf{c} \) gives rise to \( Y \), of which a given realization (a dataset) is \( y \); holding everything else fixed, we can then view Eq. (3) as a function of the parameters only: \( L(\mathbf{c}) = P(y; \mathbf{c}, \Phi, \Sigma_d) \). This is known as the likelihood of the parameters. Maximizing the likelihood gives rise to the maximum-likelihood estimator (MLE) \( \hat{\mathbf{c}} \):

\[
\hat{\mathbf{c}} = (\Phi^T \Sigma_d^{-1} \Phi)^{-1} \Phi^T \Sigma_d^{-1} Y, \quad \hat{\Sigma}_{kk} = (\Phi^T \Sigma_d^{-1} \Phi)^{-1}_{kk}
\]

(4)

where we took the opportunity to also show the variances in the MLE parameter estimates, \( \hat{\Sigma}_{kk} \). (As above, we make the distinction between the MLE estimator involving \( Y \) and the MLE point estimate involving \( y \).) In Fig. 1, we also show the prediction corresponding
Fig. 1 Starting from the underlying function $2 + 5 \sin x$, we add in different noise terms $\xi_j$ (left and right) to produce synthetic data. Each panel also shows the prediction corresponding to the maximum-likelihood point estimate.

to the maximum-likelihood parameter estimate $\hat{\epsilon}$ (for each dataset), i.e., $\sum_{k=0}^{n-1} \xi_k \phi_k(x)$; observe that Eqs. (3) and (4) know nothing of the underlying function (involving the true parameters $c$,), i.e., they take as input only a given dataset (each time). Take a moment to appreciate the fact that how closely the MLE prediction matches the underlying function will also depend on the noise term(s) that each panel corresponds to. Qualitatively, the motivation behind maximum-likelihood estimation is to pick that set of parameters which makes the experimentally determined dataset most probable; as we further discuss below, two major complications arise in this connection, first, $N$ might be small and, second, we typically have access to only a single dataset $y$.

The Bayesian outlook combines the statistical model of how the parameter values give rise to the dataset (i.e., the likelihood) with all prior information one has about the parameters themselves; crucially, now the parameters are a random vector, $C$. Combining the likelihood and the prior is accomplished via the application of Bayes’ rule:

$$
P(c|y; \Phi, \Sigma_d, \mu_0, \Sigma_0) = \frac{P(y|c; \Phi, \Sigma_d)P(c; \mu_0, \Sigma_0)}{P(y; \Phi, \Sigma_d, \mu_0, \Sigma_0)} = E_{\Sigma_c \sim P(c; \mu_0, \Sigma_0)} P(y|c; \Phi, \Sigma_d)P(c; \mu_0, \Sigma_0)$$

The likelihood is now written as $P(y|c; \Phi, \Sigma_d)$; note that we are limiting ourselves to the single dataset $y$. The prior distribution $P(c; \mu_0, \Sigma_0)$ is here kept general, characterized by a mean vector $\mu_0$ and a covariance matrix $\Sigma_0$. The denominator $P(y; \Phi, \Sigma_d, \mu_0, \Sigma_0)$ is the marginal likelihood (also known as the evidence) and plays an important role in model selection; here, we take it to be simply a normalization factor. Note that $P(y; \Phi, \Sigma_d, \mu_0, \Sigma_0)$ does not depend on the parameter values $c$; as clearly shown in the second equality, these are integrated out. The main entity in Bayesian regression is the posterior distribution $P(c|y; \Phi, \Sigma_d, \mu_0, \Sigma_0)$, shown on the left-hand side of Eq. (5). It encapsulates all that we know about the parameter values, combining both prior knowledge and what we learned from the dataset itself. Without getting into a detailed analysis of possible prior and likelihood forms, we note a standard textbook example, that where all three relevant entities (prior, likelihood, posterior) are Gaussian functions, leading to the posterior covariance matrix and mean vector:

$$
\Sigma_c = (\Phi^T \Sigma_d^{-1} \Phi + \Sigma_0^{-1})^{-1}, \mu_c = \Sigma_c \Phi^T \Sigma_d^{-1} y + \Sigma_0^{-1} \mu_0
$$

This can be viewed as a generalization of Eq. (4) such that the prior’s $\mu_0$ and $\Sigma_0$ are taken into account. One attractive feature of the Bayesian approach to linear regression is that, having computed the posterior distribution $P(c|y; \Phi, \Sigma_d, \mu_0, \Sigma_0)$, one may then proceed to “fold it in” to evaluate other quantities. An important example involves carrying out predictions, i.e., determining the $\hat{y}$ value corresponding to a new $\hat{x}$ value; crucially, these $\hat{x}$ and $\hat{y}$ are not part of the dataset. In the Bayesian spirit, the right approach is to write down a posterior predictive distribution:

$$
P(\hat{y}|\hat{x}; \phi, \Phi, \Sigma_d, \mu_0, \Sigma_0) = E[\hat{P}(\hat{y}|c; \phi)] = \int d^p \phi \hat{P}(\hat{y}|\phi, \Phi, \Sigma_d, \mu_0, \Sigma_0)$$

which is here seen to be an expectation of our predictive model with respect to the posterior (as spelled out in the second equality); here, $\phi$ bundles together the $\phi_k$’s evaluated at $\hat{x}$, i.e., $\phi_k(\hat{x})$ for all $k$’s.
3 Mistakes and corrections

In a spirit similar to Ref. [4], our aim in the present work is to focus on the correct understanding of data analysis, not to criticize the authors of respected textbooks; with that in mind, we now cite a superset of references, made up of many standard textbooks covering the relevant material. [5–39] (We have provided the Editor and Referees of the present manuscript with detailed bibliographic information on specific instances where these incorrect claims appear in the literature.) For each of the six themes we discuss below, our organizing principle will be to first provide some conceptual and contextual background, then give the mistake (namely, a specific quote from the literature), followed by a discussion of why the quote is substantively wrong (typically using equations and/or a figure), and conclude with a correction (namely, an improved few-sentence formulation, intended to supersede the mistake). Since this is a short article, it is inevitable that some of the more involved misconceptions are touched upon but not deeply explored; to remedy this, we provide several pointers to the specialist literature in what follows. In most of the quotes given below, we have tweaked the mathematical notation (following Sect. 2) in order to make the discussion cohere across all topics; we have not modified the original quotes in any other way (unless so marked).

3.1 Maximum-likelihood parameter estimation

In the process of introducing a new technique, an instructor/textbook author is expected to provide some motivation; a good outcome is that a newly introduced approach feels intuitive to students soon after they hear about it/see it applied. In this connection, a danger that every instructor must guard against is going so far as to make the new approach seem self-evident: If the technique is self-evident, then there is (a) no need to consider the possibility of alternative approaches and (b) a risk that students who fail to see why the technique is logically obvious end up blaming themselves. These considerations are quite relevant to the way maximum-likelihood estimation is often introduced in textbooks:

**Mistake #1** “We assume that the observed set of measurements is more likely to have come from the parent distribution [corresponding to \( c \)] than from any other similar distribution with different coefficients and, therefore, the probability [sic]

\[
P(y; c_\star, \Phi, \Sigma_d) = \prod_{j=0}^{N-1} \frac{1}{\sqrt{2\pi\sigma_j}} \exp \left[ -\frac{1}{2} \sum_{j=0}^{N-1} \left( \frac{y_j - \phi_j}{\sigma_j} \right)^2 \right]
\]

is the maximum probability [sic] attainable with Eq. (3). Thus, the maximum-likelihood estimates for \( c \) are those values that maximize the probability [sic] of Eq. (3).”

As implied above, in such expositions the attempt to justify likelihood maximization has gone too far: To make Mistake #1 is to look at Eq. (8), notice its formal similarity to Eq. (3) and thereby draw the conclusion that the value of \( c \) that maximizes the probability density in Eq. (3) gives the true parameters \( c_\star \). (Incidentally, Eq. (3) and therefore also Eq. (8), are giving probability densities, since \( Y \) is a continuous random vector.) If maximum-likelihood estimation is so self-evident, that immediately raises the question why other approaches to parametric inference (e.g., the method of moments) also exist: If finding the argument that maximizes the likelihood gives you the true parameters, then why would you not simply go ahead and just find the true parameters? A point that will keep recurring in our discussion below: when such strong assumptions are included in textbooks (especially those of a “practical” flavor) students are left either scratching their heads or pretending that they get it.

Let us elaborate a bit on why this misconception arose: If you look at Eq. (3)—keeping the \( y_j \), the \( \sigma_j \)’s and the \( \phi_j \)’s fixed—then a bit of thought will convince you that, indeed, the only way to get the answer of Eq. (8) is precisely to set \( c = c_\star \) in Eq. (3). Note, however, that this fact is unrelated to the maximization of the likelihood: Indeed, if we knew the true parameters we could plug them into the likelihood \( L(c) = P(y; c, \Phi, \Sigma_d) \) and thereby get the parent distribution, \( P(y; c_\star, \Phi, \Sigma_d) \) but this line of thinking still does not tell us how to go about approximating \( c_\star \) in the first place: just because you have a Gaussian, does not mean it is centered at the right place. The confusion seems to arise from a number of interrelated facts. First, a Gaussian distribution has a single, well-defined maximum, so it is enticing to think that the (special) location of that maximum should somehow be related to the quantity we are after. Second, it is qualitatively plausible to want to maximize the likelihood: Since the random vector \( Y \) did give rise to the specific dataset \( y \), should not we want to make it probable that the dataset that did arise would arise? Third, likelihood maximization as per Eq. (4) leads to several important properties, e.g., in the asymptotic limit (i.e., as \( N \to \infty \)) the MLE estimate is consistent (i.e., \( \hat{c} \) goes to \( c_\star \)), the MLE estimator is unbiased (i.e., \( E(\hat{c}) = c_\star \)), where this frequentist expectation is across datasets), and \( \hat{c} \) minimizes the (Kullback-Leibler) distance between the general likelihood \( P(y; c, \Phi, \Sigma_d) \) and the parent distribution \( P(y; c_\star, \Phi, \Sigma_d) \); see Refs. [40] and [41] for more details (and more properties).

The desirable properties of MLE discussed in the previous paragraph referred either to the asymptotic limit or to integrations across all possible datasets. Let us, instead, examine a single dataset with a finite number of points, \( N \); for concreteness, take the \( N = 50 \) dataset from the left panel of Fig. 1. For this example, we generated the dataset from a true/underlying function ourselves, so we can easily check whether or not the location of the maximum likelihood gives us the true parameters or not. The corresponding likelihood is plotted in Fig. 2, where you can clearly see that at the maximum \( L(\hat{c}) > L(c_\star) \) holds. [42] in direct contradiction of the quote we saw above, which assumed that \( L(\hat{c}) = L(c_\star) \). (For the sake of completeness, we note that there exist (non-Gaussian) likelihoods for which the maximum is not unique, or does not even exist; nobody would have taken it for granted in those cases.
Fig. 2 Likelihood function $L(c)$ for a given dataset $y$ and a two-dimensional parameter set $c$, normalized by the likelihood's value at the true parameters $c^\star$.

that the $c^\star$ are easy to find.) As a matter of fact, the MLE method itself is telling us how much (or whether) to trust its estimate $\hat{c}$: We discuss this more below but, for now, note that the point estimate is associated with a measure of its uncertainty in Eq. (4). To summarize the main point:

**Correction #1** Maximum-likelihood estimation is a reasonable approach to parametric inference (it is the most common one). While MLE obeys several desirable properties, you should not take it for granted that it automatically leads to the true/underlying parameter values. This will be true only if your dataset size $N$ is huge or you are interested in average properties (across datasets). For a single dataset of non-huge size $N$, you should carefully investigate the uncertainty in your estimate.

### 3.2 Chi-squared statistic and quality of fit

The approach taken in Sect. 3.1, MLE, is the statistical foundation of the more prosaic technique introduced in nearly all computational science textbooks, namely least-squares fitting. The former models the discrepancy between theory and experiment, trying to come up with systematic point estimates and uncertainties; the latter is usually provided in an ad hoc format, i.e., not really justified. When the weighted least-squares approach is justified in such works, this is typically done cursorily, precisely by bringing up maximum likelihood. The fact that the statistical background either goes unmentioned or is laconically referred to can be detrimental to students’ understanding of what is a random variable, what is not and why this matters. To make things concrete, let us turn to the next misconception (probably the most widely prevalent one):

**Mistake #2** “With this result in mind a statistical quantity named $\chi^2_{\text{red}}$ (‘reduced Chi-square’) can be defined as

$$
\chi^2_{\text{red}} = \chi^2 / (N-n) = \frac{1}{N-n} \sum_{j=0}^{N-1} \left( \frac{y_j - \phi_j c}{\sigma_j} \right)^2
$$

which evaluates to a value close to 1 for a good fit since the number of data $N$ should be considerably larger than the number of parameters of the model function $n$, i.e., $N \gg n$.”

Let us start by interpreting the $\chi^2$ statistic appearing in Eq. (9). In numerical methods textbooks, this is typically motivated, reasonably enough, by noting that it attempts to minimize the distance between the experimental value, $y_j$, and the model prediction, $\phi_j c$, weighted by the input data uncertainty each time, $\sigma_j$. While there are other choices one could have made instead of least-squares minimization (e.g., minimizing the maximum error), the above is certainly a plausible choice. Turning now to an actual justification of the form of Eq. (9): taking the natural logarithm of $L(c) = P(y; c, \Phi, \Sigma_d)$ from Eq. (3), we realize that all the prefactors are constant (since they are experimentally determined); since the exponential is monotonic, to maximize $L(c)$ we can simply minimize what’s in the exponent. But the exponent is (within a factor of 2) precisely the $\chi^2$ statistic of Eq. (9)! In other words, $\chi^2$ minimization is equivalent to maximum-likelihood parameter estimation when the errors are normally distributed. (Of course, MLE is much more general, since it also applies to cases where the errors are not normally distributed.) Similarly, the MLE solution of Eq. (4) is equivalent to the solution of the normal equations appearing in the weighted least-squares problem.

The $\chi^2$ statistic appearing in Eq. (9) is either qualitatively motivated or explicitly derived from MLE but, either way, its form is the same. This, however, is not the point of providing the above quote: Mistake #2 claims that a good fit is synonymous with $\chi^2 \approx N - n$. First, some terminology: the difference between the number of data points $N$ and the number of parameters $n$ (when $\Sigma_d$ is diagonal and the $\phi_k$’s are linearly independent) is called the number of degrees of freedom, $\nu = N - n$. In other words, the
frequently propagated advice is that $X^2_{\text{red}} = \chi^2 / \nu$ should be as close as possible (from above) to 1; some expositions also bring up (without justification) the incomplete gamma function at this point. It is easy to see why such an approach is so popular: For a given dataset and a given theory/model, Eq. (9) allows one (even one who is unfamiliar with modern statistics) to produce a single number and thereby draw the conclusion whether or not the fit is good. As the authors of Ref. [43] put it: “The most pernicious idea in statistics is the idea that we can produce a single-number summary of any dataset and this will be enough to make a decision.”

Before we turn to a general discussion of what’s wrong with this specific single-number summary, let us look at a couple of examples. For the dataset from the left panel of Fig. 1, the maximum-likelihood estimate leads to a (minimum) $\chi^2 / \nu$ of 1.28, whereas the dataset from the right panel corresponds to an MLE parameter set with a $\gamma^2$ course, in practical applications the dataset (and the MLE prediction and corresponding $\gamma^2$ large (especially if an amazing thing happened to me tonight. I was coming here, on the way to the lecture, and I came in through the parking lot. And you
won't believe what happened. I saw a car with the license plate ARW 357. Can you imagine? Of all the millions of license plates in
the state, what was the chance that I would see that particular one tonight? Amazing!

Things are even worse when it comes to model selection [46]: Our argument in Eq. (10) relied on our having access to the
true theory with the true parameter values, so we could employ the noise term Eq. (1). When you do not know those (i.e.,
nearly always) the numerator in the exponent in Eq. (3) is not the error term $E_j$, so you cannot follow the derivation from standard
normal random variables to the Chi-squared distribution of Eq. (11). (Incidentally, if you truly did know the true theory and the
true parameter values, you would not be interested in model selection in the first place.) This means that you cannot quantify the
spread in $\chi^2$ values by using the variance of $2\nu$ corresponding to Eq. (11). Without going into more detail, we note in passing that
in frequentist inference (where, e.g., employing a Bayes factor [47] is not an option) there are alternative techniques available that
can help with model selection, e.g., cross-validation or bootstrapping. Putting it all together:

Correction #2 You should avoid over-relying on single-number summaries of complex datasets; the $\chi^2$ statistic is no exception
to this general point. Blindly aiming for a $\chi^2/\nu$ of 1 (e.g., over-worrying about underestimated input data uncertainties) might
lead you to ignore rare (but possible) statistical fluctuations. Similarly, $\chi^2$-based model selection is problematic, as the statistical
foundation of thinking in terms of the Chi-squared distribution is invalid. Statisticians have developed several alternative tools that
help one to assess the goodness of fit or to do model selection.

3.3 Confidence intervals for model parameters

Sections 3.1 and 3.2 focus on different aspects of essentially the same task: parameter estimation given a dataset and a model form.
Of course, just as important (if not more important) is the question of the uncertainty associated with the point estimates provided by
likelihood maximization/$\chi^2$ minimization. The $\hat{c}$ of Eq. (4) is a statistic (i.e., a function of the data $Y$) so it inherits the randomness of
the data: This is why Eq. (4) also includes an expression for the variance in each parameter estimate, $\Sigma_{kk}$. Qualitatively, if you have
a huge dataset whose data points have tiny uncertainties, and your theory captures the overall trend very well, then you would expect
that your parameter estimates have small associated uncertainties. The meaning and relevance of these parameter uncertainties are
very often mishandled in the literature, bringing us to:

Mistake #3 “Confidence intervals—probabilistic bounds on the errors in the parameters. Confidence intervals are determined
from the standard errors in the parameters together with a desired probability that the bounds are correct. Under the assumptions
that the model errors are independent and normally distributed, the true value of the parameter will lie within the interval with,
say, 90% or 95% probability.”

Let us immediately get something out of the way: the modifier confidence interval is clearly a misnomer: One’s confidence is
typically low when the interval is big. Other terms have been proposed in the literature (e.g., uncertainty interval or compatibility
interval) but have not been widely adopted. Turning now to the interpretation of a confidence interval: In one dimension, the idea is
motivated by what is known as the empirical rule for the normal distribution (which will re-appear below). As you can see in the
left panel of Fig. 4, for the density function $N(\mu, \sigma)$ of Eq. (2) the fractional area in the interval ($\mu - \sigma, \mu + \sigma$) is approximately
$0.683$, i.e., 68.3%. Similarly, the fractional area in ($\mu - 2\sigma, \mu + 2\sigma$) is 95.4% and that in ($\mu - 3\sigma, \mu + 3\sigma$) is 99.7%. This is why
the term “empirical rule” is sometimes used interchangeably with the term “$68.3 - 95.4 - 99.7$ rule” (see, however, Sect. 3.4). As the right panel of Fig. 4 shows, you do not have to limit yourself to integer multiples of the standard deviation: For example, the
fractional area in ($\mu - 1.645\sigma, \mu + 1.645\sigma$) is roughly 90% and the fractional area in ($\mu - 1.96\sigma, \mu + 1.96\sigma$) is roughly 95%.

The previous paragraph, and Fig. 4, corresponded to a simple Gaussian probability density $N(\mu, \sigma)$, i.e., had nothing to do with
parameter estimation. The intricacy arises (as in the quote above) when one tries to use the language of confidence intervals. To see
what is wrong with the (quite popular) Mistake #3, let us (once again) turn to the two datasets in Fig. 1 for which, as you may recall, the true parameter value for the first parameter was $c_{true} = 2$. Applying the spirit of our quote would imply that there is a 68.3% probability that the interval $(c_0 - \sqrt{\Sigma_{00}}, c_0 + \sqrt{\Sigma_{00}})$ contains the true parameter value $c_{true} = 2$. (To streamline the presentation, we are here ignoring the fact that we are faced with an ellipse (not a simple interval), given that $\Sigma$ is in general not diagonal—see Sect. 3.4.) But what exactly does that mean? Applying this prescription to the dataset (and MLE evaluation) of the left panel, we find the interval $(1.807, 2.117)$, whereas for the right panel we find the interval $(1.681, 1.966)$. What does it mean to say that there is a 68.3% probability that the interval $(1.807, 2.117)$ contains the number 2? This is nonsensical: The interval $(1.807, 2.117)$ clearly contains the number 2 (and if you choose to employ the language of probability, then the corresponding probability is obviously 100%). Similarly, the interval $(1.681, 1.966)$ clearly does not contain the number 2, with a probability of 100% (i.e., contains the number 2 with a probability of 0%). In both cases, the relative fraction 68.3% seems to be totally irrelevant.

At its core, Mistake #3 arises from a fundamental misunderstanding of the meaning of probability: In frequentist statistics, probability refers to the long-run relative frequency of occurrences. Symbolically, our confidence interval gives rise to the equation:

$$P\left(\hat{c}_0 - \sqrt{\Sigma_{00}} \leq c_{true} \leq \hat{c}_0 + \sqrt{\Sigma_{00}}\right) \approx 0.683$$

(12)

For a single interval, e.g., $(1.681, 1.966)$ there is no “long” run involved. Instead, Eq. (12) should be interpreted as follows: Since what is random is the interval (not the true parameter), to compute the probability of Eq. (12) you need many different confidence interval evaluations, each corresponding to a different dataset. We have done this in Fig. 5, for which we generated 100 datasets (from the same underlying function, adding noise terms of the same form but different value each time) and the corresponding 100 confidence intervals for the parameter $c_0$. For this specific case, 67 out of 100 confidence intervals contain the true parameter value; we are dealing with a $1\sigma$ random interval, for which we expect a coverage of 68.3%. (Reader, these are “typical” results.) Similarly, for $2\sigma$ confidence intervals we find the proportion of those that contain the true parameter value to be 98 out of 100 (and for $3\sigma$ confidence intervals it is 99 out of 100). Simply put, it is wrong to take a single one of these confidence intervals and try to interpret it as “mostly” containing the true parameter value: for a frequentist interpretation of probability, you need a long run.

A fine-grained analysis of this misconception is carried out in Ref. [48], which is characteristically titled “The fallacy of placing confidence in confidence intervals.” The authors of that reference distinguish between three interrelated issues: (a) the fundamental confidence fallacy (i.e., making the leap from a 68.3% probability that a random interval contains the true value to a 68.3% probability that a given observed interval contains the true value), (b) the precision fallacy (i.e., that a confidence interval’s width tells us how precisely we know the parameter) and (c) the likelihood fallacy (i.e., that a confidence interval indicates the likely values of the parameter). All three of these very widespread misunderstandings follow from a folk understanding of confidence intervals.

Before concluding this subsection, we note that one can arrive at an interval that is interpreted as per the “folk expectation”: In a Bayesian framework, where the likelihood is folded together with the prior to produce the posterior distribution, one may generate a credible interval with the desired interpretation (i.e., a 68.3% rational degree of belief given the single dataset at our disposal). Of course, as with everything in life, this is a mixed blessing: the credible interval that is intuitively easy/natural to interpret, will not in general have the same frequency coverage properties, i.e., after generating many datasets and the corresponding credible intervals, it will not be true that 68.3% of the credible intervals will contain the true parameter.

**Correction #3** A single confidence interval should never be interpreted in terms of the probability that it contains the true parameter value. Since the true parameter value is fixed (though unknown), a given confidence interval either contains the true parameter or it does not. The (frequentist) concept of a confidence interval coverage takes on a probabilistic interpretation when you consider many experiments, i.e., distinct datasets giving rise to distinct confidence intervals ($Q\%$ of which will contain the true parameter).
parameter value). If you really want to interpret a given interval in terms of the probability that it contains the true parameter, you should be using a (Bayesian) credible interval.

3.4 Empirical rule in the multivariate case

The previous subsection addressed the problem of constructing a confidence interval for a single model parameter. Of course, in practical applications we are typically faced with multivariate problems, in which case we have to construct confidence regions (sometimes known as confidence sets). Human intuition does not work very well in many dimensions, but we are fortunate that our running example from Fig. 1 involves only two parameters, in which case visualizing things is still a possibility. The next mistake in our list relates to the aforementioned empirical rule, namely the rule that tells us what the probability enclosed in a given number of standard deviations is. Even if you have mastered Correction #3, namely the meaning of the term probability in this context, perusing our list relates to the aforementioned empirical rule, namely the rule that tells us what the probability enclosed in a given number of standard deviations is. Even if you have mastered Correction #3, namely the meaning of the term probability in this context, perusing the introductory literature (or even research works) will convince you that there is still room for a further misunderstanding:

Mistake #4 "The result of the measurement can be visualized as iso-density contours in the parameter space. These contours are elliptical in the case of Gaussian likelihood functions and are therefore called 'error ellipses.' Typically one is interested in the contour that encloses 68.3% of the likelihood, corresponding to one Gaussian deviation or 'one sigma,' or 95.4% corresponding to two Gaussian standard deviations or 'two sigma'."

Basically, the claim here is that the empirical rule is equivalent to the 68.3 — 95.4 — 99.7 rule, even in more than one dimensions. To understand why this is wrong, let us turn to our expression in Eq. (12): it is hard to see how to generalize that to more dimensions, so let us first recast it into the form:

$$P\left( \left| \frac{\hat{c}_0 - c_0}{\sqrt{\Sigma_{00}}} \right| \leq 1 \right) \approx 0.683$$

(13)

where we would have $$|\hat{c}_0 - c_0|/\sqrt{\Sigma_{00}} \leq 2$$ for the 2σ interval and so on. The fraction inside the absolute value here takes the form $$|(X - \mu)/\sigma|$$, where X is a random variable. (This is a rescaling operation that is very common when dealing with Gaussian distributions.) You may recall that in Sect. 3.3 we, somewhat cryptically, referred to the fact that $$\Sigma$$ is in general not diagonal, implying that Eq. (12), and therefore also Eq. (13), does not tell us the full story; it is now time to see what this means. First, we recall from Eq. (4) that $$\hat{c}$$ is a linear transformation of Y; since we know from Eq. (3) that Y obeys a Gaussian distribution, then so will $$\hat{c}$$ (N- and n-dimensional, respectively). As mentioned in Sect. 3.1, the MLE estimator is unbiased, i.e., $$\hat{\mathbb{E}}(\hat{c}) = c_0$$. Combined with the covariance matrix for our parameter estimates, again from Eq. (4), we have thereby seen that $$\hat{c}$$ obeys the distribution:

$$P(\hat{c}; c_0, \Sigma) = N(c_0, \Sigma)$$

$$= \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left[ -\frac{1}{2}(\hat{c} - c_0)^T \Sigma^{-1}(\hat{c} - c_0) \right]$$

(14)

Observe that this is our first multivariate Gaussian: Eqs. (3) and (8) were written as products of univariate Gaussians. The form of Eq. (14) is more general, i.e., the prefactor involving the determinant also works when $$\Sigma$$ is not diagonal. Our result in Eq. (13) was implicitly assuming a univariate Gaussian; since we know that $$\hat{c}_0$$ is not an independent parameter, i.e., it is part of the random vector $$\hat{c}$$, let us now see how to generalize our statements on probability. The natural generalization of $$|\hat{c}_0 - c_0|/\sqrt{\Sigma_{00}}$$ to many dimensions is via the Mahalanobis distance, namely: $$\sqrt{(\hat{c} - c_0)^T \Sigma^{-1}(\hat{c} - c_0)}$$. The analogue of Eq. (13) would now be to check if the Mahalanobis distance is less than, say, 1 and thereby produce a 1σ interval. For example, a simple test with the 100 synthetic datasets used in Fig. 5 leads to 36, 88, 98 Mahalanobis distances enclosed within 1, 2, 3 σ, respectively. Of course, these are not asymptotic results (since they correspond to only 100 different instances of $$\hat{e}$$) but, still, you can already see that, for this two-dimensional problem, 1σ corresponds to roughly 40% contra what the quote in Mistake #4 claimed.

Let us try to be a bit more systematic: [49] we already know from Eq. (14) that $$\hat{c}$$ obeys a normal distribution; this means that $$\Sigma^{-1/2}(\hat{c} - c_0)$$ obeys a standard normal distribution. But then we see that the argument of the square root in the Mahalanobis distance definition, $$(\hat{c} - c_0)^T \Sigma^{-1}(\hat{c} - c_0)$$, is simply the square of a (multivariate) standard normal distribution so, as per the same lemma we employed in Sect. 3.2, it will obey an n-dimensional—not ν-dimensional as in Eq. (11)—Chi-squared distribution. We have thereby shown that:

$$P\left( \sqrt{(\hat{c} - c_0)^T \Sigma^{-1}(\hat{c} - c_0)} \leq p \right)$$

$$= P\left( (\hat{c} - c_0)^T \Sigma^{-1}(\hat{c} - c_0) \leq p^2 \right) = F_n(p^2)$$

(15)

In the first equality, we simply eliminated the square root. In the second equality, we made use of $$F_n$$, the cumulative distribution function corresponding to the Chi-squared distribution.
3.5 What is random in frequentist versus Bayesian regression

As noted above, most of our discussion up to this point has been (sometimes implicitly) focused on frequentist approaches to linear regression; this is merely a consequence of the fact that the relevant textbooks with a scientific or engineering readership are still largely unBayesian in their outlook; despite the well-known inertia exhibited by physical scientists, this is, thankfully, now beginning to change. On the other hand, machine learning textbooks are overwhelmingly Bayesian in their viewpoint; more often than not, these works remind one of so many histories of philosophy, hurriedly dispatching alternative viewpoints, in the process throwing the methodological principle of charity out the window.

Obviously, we cannot discuss philosophical/conceptual issues in depth in the present article, so let us, instead, briefly outline the different approaches to probability; on this topic, the reader may appreciate Ref. [50]. In the frequentist viewpoint, as we’ve already seen, probability represents the long-run relative frequency of occurrences; for example, after a large number of coin flips, a table shows us that roughly half were heads and half tails. In the Bayesian viewpoint, probability represents a rational degree of belief about something given current knowledge; for example, we expect that for a fair coin the next flip is just as likely to give heads as tails. Almost everyone is in agreement on such summaries; things get a bit unsettled when we turn to the interpretation of regression:

**Mistake #5** “In the frequentist approach, c is treated as an unknown fixed constant, and the data is treated as random. In the Bayesian approach, we treat the data as fixed (since it is known) and the parameter as random (since it is unknown).”
There is quite a bit to unpack here. Let us start from what we touched upon more often above, namely the frequentist approach: it is true that a frequentist would take the data-generating parameters $c_*$ appearing in Eq. (1) to be constant. (Of course, it is not clear what the quote above meant by emphasizing that the parameter is unknown in the Bayesian approach, since $c_*$ is unknown in the frequentist approach, as well.) That being said, the main set of parameters appearing in a frequentist approach is not $c_*$ but the $c$ of Eq. (4), namely the result of thinking in terms of a general likelihood $L(c) = P(y; c, \Phi, \Sigma_d)$ and then finding the argument which maximizes that. But, as Eq. (4) clearly shows, $c$ is a function of the data and is therefore a random vector. That being said, even in a frequentist approach you are typically faced with only a single dataset $y$ (so you produce a single $c$ point estimate). The dataset $y$ is, indeed, treated as random in the sense of being a realization of the random vector $Y$ (but that is relevant only when one considers, e.g., the interpretation of the covariance matrix for our parameter estimates, $\Sigma$). In short, insofar as the frequentist approach is concerned, you could interpret the above quote to be correct, but you could also read it as being completely wrong.

Turning now to the Bayesian viewpoint, let us start from the (easier) point regarding the data: While it is true that we wrote down Bayes’ rule in Eq. (5) for a single dataset $y$, that same equation contains the likelihood $P(y|c; \Phi, \Sigma_d)$ in the numerator, an entity which most clearly shows that the dataset $y$ is a realization of a general distribution for $Y$. In other words, while you focus on a single dataset (as aforementioned, just as you did in the frequentist approach to get the point estimate $c$), you are also dealing with a statistical model reflecting what you know about how a given $c$ gives rise to $y$’s. Finally, while we noted in Sect. 3.3 that (frequentist) confidence intervals will have the expected coverage (across alternative datasets in the absence of systematic errors), [51] and (Bayesian) credible intervals will in general not exhibit that coverage, there is nothing keeping you from examining the frequentist coverage (across alternative datasets) of your Bayesian theory; as a matter of fact, this is something that is routinely done in Bayesian approaches, as reflected already in chapter 1 of Ref. [52].

Still on the subject of the Bayesian approach to regression, we now turn to the (thornier) question of the status of the parameters. Somewhat frustratingly, many Bayesian expert treatments are tight-lipped on the matter of the underlying function/the true parameters $c_*/the$ data-generating distribution. We believe there are two reasons for this: first, when studying other fields it is often awkward to be thinking in terms of “true fixed parameters” (consider, e.g., the study of economic growth). Things are considerably different in physical science, where nearly all physicists would agree that, e.g., the mass of the electron is a constant that we should ideally be able to compute from first principles—and, absent that, try to extract from experimental measurements (of course, even in physics, advocates of Quantum Bayesianism would advocate against thinking in terms of “elements of physical reality”) [53]. Second, a careful study of the foundations of the subject will expose you to an (orthodox) viewpoint [54, 55] which is subjectivist and operational, namely one in which the focus is on individual beliefs about how to make decisions (i.e., not on the true parameters). In lieu of entering that discussion ourselves, we simply reach for an argumentum ab auctoritate, quoting two prominent Bayesians on the subject: “Notice that (in sharp contrast to conventional statistics) parameters are treated as random variables within the Bayesian paradigm. This is not a description of their variability (parameters are typically fixed unknown quantities) but a description of the uncertainty about their true values.” (Bernardo) [56] and “This would be another form of the mind projection fallacy, confusing reality with a state of knowledge about reality. In the problem we are discussing, $c_*$ is simply an unknown constant parameter; what is distributed is not the parameter, but the probability.” (Jaynes). [57]

Obviously, quoting from the works of acknowledged experts does not rise to the level of a sustained argument, but this should suffice to show that the (extremely widespread) summarization in Mistake #5 is certainly oversimplified and arguably flat-out incorrect. There are several corollaries to this haphazard treatment of the conceptual underpinnings of frequentist vs Bayesian approaches to regression; for example, one often hears mention of the “dataset likelihood,” though the term “likelihood” should be more properly reserved for the parameters. Similarly, we broke with the overwhelming majority of the literature by not using in the $P(y|c, \Phi, \Sigma_d)$ of Eq. (3), since $c$ is not (the realization of) a random vector there. (Compare with the Bayesian setting of Eq. (5), which does employ $\\cdot$). Even so, these questions are not as important as the central issue discussed above, namely what is random (and what is not) in frequentist vs Bayesian approaches to regression. It is fair to say that this is considerably more involved than introductory treatments let on. (Again, this is perhaps understandable, though not excusable.)

**Correction #5** It should come as no surprise that hypercondensed formulations can lead one astray: there is no substitute for careful thinking and clear exposition. It is certainly defensible (both from frequentist and from Bayesian viewpoints) to take the data-generating parameters $c_*$ to be unknown constants. Similarly, both frequentist and Bayesian approaches can view the data as being a single realization $y$ of the random vector $Y$. The real difference between the two approaches (except for the inclusion or not of prior information) is on whether the parameters are taken to be a random vector or not. Of course, even in a frequentist setting the MLE estimator $\hat{c}$ is a random vector; the crucial difference is that expectations there are taken across datasets (i.e., in $N$ dimensions) whereas in a Bayesian approach they are across parameter values (i.e., in $n$ dimensions).

### 3.6 Posterior predictive distribution, noise and samples

While Sect. 3.5 changed gears (transitioning from a frequentist to a Bayesian viewpoint), it was quite abstract, involving no equations or figures. With the conceptual background now in place, we turn to more practical aspects of what is entailed by a Bayesian approach to regression. As it so happens, our next general theme (predictive distributions) is actually of relevance even in a frequentist/MLE setting. Simply put, the idea is as follows: After one has somehow determined the parameter values (either as a point estimate or
For the dataset from the left panel of Fig. 1, we show predictions corresponding to samples drawn from the posterior distribution (left) and from the posterior predictive distribution (right).

in the form of the posterior distribution), one would typically like to find which predictions correspond to that set of parameters; in the language of Eq. (7), this means introducing a new random variable \( \tilde{Y} \) starting from the (random) parameters \( C \):

\[
\tilde{Y} = \sum_{k=0}^{n-1} C_k \phi_k(\tilde{x}) = \tilde{\Phi} C
\]

To ensure this point does not get muddled in a sea of formalism, we immediately note that this equation (modulo a change or two in the notation) is precisely of the same form as what is given in countless discussions of least-squares fitting in numerical methods textbooks. In an MLE setting, the \( C \) in Eq. (16) would be \( \hat{c} \) (this is precisely how the MLE predictions in Fig. 1 were produced); in a Bayesian setting, it could correspond to the maximum of the posterior distribution, but it would be best to somehow fold in the entirety of the posterior (i.e., not just a point estimate). Eventually, one would like to go beyond Eq. (16) by producing, e.g., a 3σ uncertainty band in predicted values. Before we go too far, let us examine our sixth (and final) quote:

**Mistake #6** “[W]e can show that the posterior predictive distribution at a test point \( \tilde{x} \) is also Gaussian:

\[
P(\tilde{y}|c; \tilde{\Phi}) = \int d^n c \mathcal{N}(\tilde{\Phi} c, \sigma) \mathcal{N}(\mu_c, \Sigma_c) = \mathcal{N}(\tilde{\phi} \mu_c, \tilde{\sigma})
\]

where \( \tilde{\sigma}^2 = \sigma^2 + \tilde{\phi} \Sigma_c \tilde{\phi}^T \) is the variance of the posterior predictive distribution at point \( \tilde{x} \) after seeing the \( N \) training examples. The predicted variance depends on two terms: the variance of the observation noise, \( \sigma^2 \), and the variance in the parameters, \( \Sigma_c \).

[...The left panel of Fig. 7 shows 10 samples from the true posterior predictive distribution."

This mistake is made up of two sub-fallacies, one relating to noise and the other relating to samples; let us examine them in turn. First, we discuss the meaning of noise; as you may recall, this is the term we used to describe the continuous random variable \( E_j \) in Eq. (1). In the present context, “noise” plays an additional role: in Eq. (17) we are faced with an integral over a product of two terms, both Gaussian density functions; this is a specific version of the product that we wrote down as \( P(\tilde{y}|c; \tilde{\phi})P(c; \Phi, \Sigma_c) \) in Eq. (7). The second term in \( \mathcal{N}(\tilde{\phi} c, \sigma) \mathcal{N}(\mu_c, \Sigma_c) \) is easy enough to interpret: If you take Bayes’ rule of Eq. (5) and apply it for the case of a Gaussian likelihood and a Gaussian prior distribution, the result is a Gaussian posterior distribution, with mean vector \( \mu_c \) and covariance matrix \( \Sigma_c \) as per Eq. (6). The first term is a bit more involved: Many sources in the literature employ it without comment, calling it a “prediction” or (as in the quote above) an “observation.” To assume that our model for producing an \( \tilde{y} \) given the values of \( c \) and \( \tilde{\phi} \), namely \( P(\tilde{y}|c; \tilde{\phi}) \), is Gaussian is to have “one thought too many” (to borrow Bernard Williams’ inimitable phrase). [58] While such an assumption allows one to use a standard property of multivariate Gaussians—thereby reaching the second line in Eq. (17)—it has to be juxtaposed with the inconvenient fact that we (together with the entire numerical methods community) already assumed a perfectly natural (yet non-Gaussian) model in Eq. (16), namely:

\[
P(\tilde{y}|c; \tilde{\phi}) = \delta(\tilde{y} - \tilde{\phi} c)
\]

To be fair, some authors make the distinction between noisy observations and noise-free function values; sometimes, there is even an attempt to use prediction for a noisy quantity and regression for a noise-free quantity, but other authors employ the exact opposite
nomenclature; quite confusingly, a given author often employs both (‘). Here, prediction will always be noise-free, i.e., will take the logically true form of Eq. (18). Let us now see what this implies regarding the posterior predictive distribution:

\[
P(\tilde{y}|y; \phi, \Phi, \Sigma_d, \mu_0, \Sigma_0) = \int d^n c\, \delta(\tilde{y} - \tilde{\phi}c) \exp\left[-\frac{1}{2}(c - \mu_c)^T \Sigma_c^{-1} (c - \mu_c)\right]
\]

(19)

In the first step, we plugged in the (one-dimensional) Dirac delta function from Eq. (18) and the Gaussian corresponding to Eq. (6) into Eq. (7). We do not explicitly derive the second step, pointing instead to Ref. [2], pp. 405–407; we merely note that we used a straightforward argument involving, among other things, rotation matrices as well as the fact that Gaussians are closed under marginalization. Note that our final result is identical to that in Eq. (17) if one simply sets \( \sigma^2 = 0 \) for the \textit{ad hoc} observation noise employed there (as it should, given that a zero-width Gaussian is one definition of a Dirac delta function).

Next, we turn to the second sub-fallacy, this one relating to samples. We first observe that the posterior predictive distribution of Eq. (19) takes in a dataset (i.e., many \( x_j \)'s, \( y_j \)'s and \( \sigma_j \)'s), a set of basis functions (i.e., many \( \phi_k \)'s), as well as a prior distribution and a given \( \tilde{x} \); it folds in the posterior distribution’s mean \( \mu_c \) and covariance matrix \( \Sigma_c \) from Eq. (6) to tell us which \( \tilde{y} \) values we should expect. Crucially, Eq. (19) shows a univariate Gaussian in \( \tilde{y} \); observe that the mean \( \tilde{\phi}\mu_c \) and the variance \( \tilde{\phi} \Sigma_c \tilde{\phi}^T \) are numbers (i.e., not vectors/matrices). It is therefore very strange to read in Mistake #6 that samples drawn from the posterior predictive distribution look like the left panel of Fig. 7: Should not samples from a univariate Gaussian have a “jittery” look? As it so happens, if you do produce 100 samples from the posterior predictive distribution of Eq. (19) you will find the, decidedly non-smooth, results shown in the right panel of Fig. 7. Note that this is not a simple typo (e.g., a confusion of left vs right panel): We have not actually encountered (nary a reference to) a plot like that in the right panel of Fig. 7 in the literature (outside Ref. [2]). As it so happens, the smooth results shown in the left panel of Fig. 7 (which frequently appear in textbooks) were produced in a totally different way: They result from taking samples of the \( n \)-dimensional Gaussian posterior distribution with mean vector \( \mu_c \) and covariance matrix \( \Sigma_c \) from Eq. (6), each sample giving rise to a single set of parameters \( c \) and then plotting \( \tilde{y} \) (a given realization of Eq. (16)); in other words, the results shown in the left panel have nothing to do with the posterior predictive distribution of Eq. (19).

Finally, note that some references (somewhat more carefully than the quote given above) claim that the left panel shows “samples from the posterior predictive distribution induced by the parameter posterior”: This is obscure at best and misleading at worst. The posterior predictive distribution integrates out the parameters \( c \), as you can see in Eq. (19) or Eq. (7); it is therefore hard to see how 10 samples from the posterior distribution can play the same role as a full integral over the entire posterior distribution.

\textbf{Correction #6} \textit{The natural definition of a predictive distribution, in keeping with what is done in least-squares fitting, is to include no \textit{ad hoc} noise term. For the case of a Gaussian posterior distribution, this implies that the posterior predictive distribution is given by an expression that you are not likely to encounter in a textbook (an integral over all parameter values of the product of a one-dimensional Dirac delta function and a multivariate Gaussian). On a different note, if you wish to draw samples from the posterior predictive distribution then you have to acknowledge that you are dealing with a univariate Gaussian and the results will therefore look jagged.}

\section{4 Summary and conclusion}

In this article, we encountered a sampling of mistaken claims in the introductory literature on data analysis, machine learning or computational science and engineering, all having to do with frequentist and Bayesian inference. The themes touched upon ranged from maximum-likelihood estimation to the meaning of the \( \chi^2 \) statistic, Gaussian distributions (and the corresponding confidence regions) in one or many dimensions, the question of random vs non-random in frequentist versus Bayesian regression, as well as the derivation of (and samples from) the posterior predictive distribution. With the exception of Mistake #5, all of these were very practical; some were computational questions (e.g., is \( \tilde{c} \) equal to \( c \), or what does 1\( \sigma \) mean in many dimensions), but nearly all of them involved a fair bit of interpretation (e.g., of the magnitude of \( \chi^2 \), of the meaning of a confidence interval, of what is random or of what constitutes a prediction). While we tried above, where possible, to explain why a given misconception arose in the first place, we consciously stay away from the question of why these issues have been propagating through the introductory (or sometimes not-so-introductory) literature.

Before closing, we note that we are well aware that debunking itself has its pitfalls: There is certainly the danger that a careless reader may replace one set of claims that drops from the sky with another one of the same provenance. Put another way, while it is reasonable to begin a myth-busting process having Alexander Pope’s “a little learning is a dangerous thing” in mind, this has to be balanced against Heraclitus’ “the learning of many things does not teach understanding.” Our motivation in collecting these misconceptions and discussing them in some detail is broader than the specific mistakes encountered above; we wish to promote understanding from first principles and this is something that one has to arrive at for oneself. Even so, we hope that our article is read and appreciated by data analysis instructors and may therefore contribute toward improved teaching and learning; similarly,
we hope that our pointing out of previously unperceived subtleties may help elevate the level of the discussion in related research works.

Acknowledgements A.G. would like to thank Andrew Gelman for help navigating the relevant literature. This work was supported in part by the Natural Sciences and Engineering Research Council (NSERC) of Canada and the Canada Foundation for Innovation (CFI). Computational resources were provided by SHARCNET and NERSC.

Data availability statement Not applicable.

References

1. A. Gezerlis, M. Williams, Six textbook mistakes in computational physics. Am. J. Phys. 89, 51–60 (2021)
2. A. Gezerlis, Numerical Methods in Physics with Python, 2nd edn. (Cambridge University Press, Cambridge, 2023)
3. A. Gelman, J. Hill, A. Vehtari, Regression and Other Stories (Cambridge University Press, Cambridge, 2020), p.154
4. A. Gelman, Going beyond the book: tomorrow’s readings in statistics teaching. Teach. Stat. 34(3), 82–86 (2011)
5. R.J. Barlow, Statistics: A Guide to the Use of Statistical Methods in the Physical Sciences (Wiley, New Jersey, 1989)
6. K.J. Beers, Numerical Methods for Chemical Engineering (Cambridge University Press, Cambridge, 2007)
7. D.P. Bertsekas, J.N. Tsitsiklis, Introduction to Probability, 2nd edn. (Athena Scientific, Massachusetts, 2008)
8. P.R. Bevington, D.K. Robinson, Data Reduction and Error Analysis in the Physical Sciences, 3rd edn. (McGraw-Hill, New York, 2003)
9. C.M. Bishop, Pattern Recognition and Machine Learning (Springer, Berlin, 2006)
10. G. Bohn, G. Zech, Introduction to Statistics and Data Analysis for Physicists, 3rd edn. (Verlag Deutsches Elektronen-Synchrotron, Hamburg, 2017)
11. J. Boudreau, T. Giroldi, A First Course in Computational Physics (Oxford University Press, Oxford, 2018)
12. R.L. Burden, D.J. Faires, A.M. Burden, Numerical Analysis, 10th edn. (Cengage Learning, Massachusetts, 2015)
13. S.C. Chapra, R.P. Canale, Numerical Methods for Engineers, 7th edn. (McGraw-Hill, New York, 2014)
14. M.H. DeGroot, M.J. Schervish, Probability and Statistics, 4th edn. (Addison-Wesley, Massachusetts, 2012)
15. M.P. Deisenroth, A.A. Faisal, C.S. Ong, Mathematics for Machine Learning (Cambridge University Press, Cambridge, 2020)
16. P.L. DeVries, A First Course in Computational Physics (Wiley, New Jersey, 1994)
17. A. Gilat, V. Subramanian, Numerical Methods for Engineers and Scientists, 3rd edn. (Wiley, New Jersey, 2013)
18. H. Gould, J. Tobochnik, W. Christian, An Introduction to Computer Simulation Methods, Rev., 3rd edn. (CreateSpace, California, 2017)
19. R.W. Hamming, Numerical Methods for Scientists and Engineers, 2nd edn. (McGraw-Hill, New York, 1973)
20. H. Jiang, Machine Learning Fundamentals (Cambridge University Press, Cambridge, 2021)
21. D. Kahaner, C. Moler, S. Nash, Numerical Methods and Software (Prentice Hall, New Jersey, 1989)
22. J. Kiussalaas, Numerical Methods for Engineers with Python 3 (Cambridge University Press, Cambridge, 2013)
23. S. Koonin, D.C. Meredith, Computational Physics (Addison-Wesley, Massachusetts, 1990)
24. R.H. Landau, M.J. Páez, C.C. Bordeianu, Computational Physics, 3rd edn. (Wiley-VCH, New Jersey, 2015)
25. L. Lyons, Statistics for Nuclear and Particle Physicists (Cambridge University Press, Cambridge, 1986)
26. J. Mandel, The Analysis of Experimental Data (Wiley, New Jersey, 1964)
27. J. Mathews, R.L. Walker, Mathematical Methods of Physics, 2nd edn. (Pearson, London, 1971)
28. K.P. Murphy, Probabilistic Machine Learning (The MIT Press, Massachusetts, 2022)
29. W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes in Fortran, 2nd edn. (Cambridge University Press, Cambridge, 1992)
30. C.A. Prumeau, Data Analysis Techniques for Physical Scientists (Cambridge University Press, Cambridge, 2017)
31. J.A. Rice, Mathematical Statistics and Data Analysis (Duxbury, California, 2007)
32. B.P. Roe, Probability and Statistics in the Physical Sciences (Wiley, New Jersey, 2000), p.236
33. D.P. Roe, Numerical Methods in Physics with Python, 2nd edn. (Cambridge University Press, Cambridge, 2020)
34. S. Širca, M. Horvat, Computational Methods in Physics, 34. S. Širca, M. Horvat, Bayesian Philosophy of Science (Oxford University Press, Oxford, 2019), p.28
35. M.H. DeGroot, M.J. Schervish, Mathematical Statistics: A Concise Course in Statistical Inference, 2nd edn. (Springer, Berlin, 2004)
36. M.P. Deisenroth, A.A. Faisal, C.S. Ong, Mathematics for Machine Learning (Cambridge University Press, Cambridge, 2020)
37. M.P. Deisenroth, A.A. Faisal, C.S. Ong, Mathematics for Machine Learning (Cambridge University Press, Cambridge, 2020)
38. K.P. Murphy, Probabilistic Machine Learning (The MIT Press, Massachusetts, 2022)
39. W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes in Fortran, 2nd edn. (Cambridge University Press, Cambridge, 1992)
40. C.A. Prumeau, Data Analysis Techniques for Physical Scientists (Cambridge University Press, Cambridge, 2017)
41. J.A. Rice, Mathematical Statistics and Data Analysis (Duxbury, California, 2007)
42. B.P. Roe, Probability and Statistics in the Physical Sciences, 3rd edn. (Springer, Berlin, 2020)
43. S. Širca, M. Horvat, Numerical Methods in Physics with Python, 2nd edn. (CRC Press, Florida, 2017)
44. S. Širca, M. Horvat, Numerical Methods in Physics with Python, 2nd edn. (CRC Press, Florida, 2017)
45. D.S. Sivia, J. Skilling, Data Analysis: A Bayesian Tutorial, 2nd edn. (Oxford University Press, Oxford, 2006)
46. S. Theodoridis, Machine Learning: A Bayesian and Optimization Perspective, 2nd edn. (Academic Press, London, 2020)
47. W.J. Thompson, Computing for Scientists and Engineers (Wiley, New Jersey, 1992)
48. S.S.M. Wong, Computational Methods in Physics and Engineering, 2nd edn. (World Scientific, Singapore, 1997)
49. A. Zielesny, From Curve Fitting to Machine Learning, 2nd edn. (Springer, Berlin, 2016)
50. A. Vehtari, A. Gelman, A. Simpson, E. Gabry, P. Vehtari, `Interpreting draws from the posterior distribution', Ann. Rev. Nucl. Part. Sci. 70, 22–27 (2019)
51. C.P. Robert, The Bayesian Choice, 2nd edn. (Springer, Berlin, 2007), p.350
52. R.D. Morey, R. Hoekstra, J.N. Rouder, M.D. Lee, E.-J. Wagenmakers, The fallacy of placing confidence in confidence intervals. Psychon. Bull. Rev. 23, 103–123 (2016)
53. C.A. Fuchs, R. Schack, QBism and the Greeks: Why a quantum state does not represent an element of physical reality. Phys. Scr. 90, 015104 (2015)
54. J.M. Bernardo, A.F.M. Smith, Bayesian Theory (Wiley, New Jersey, 2000), p.236
55. J. Sprenger, S. Hartmann, Bayesian Philosophy of Science (Oxford University Press, Oxford, 2019), p.28
56. J. M. Bernardo, Interpretation of Electoral Results: A Bayesian Analysis, in Proceedings of Teias Matemáticas, pp. 63–75 (2004)
57. E.T. Jaynes, *Probability Theory: The Logic of Science* (Cambridge University Press, Cambridge, 2003), p.108  
58. B. Williams, *Moral Luck: Philosophical Papers 1973–1980* (Cambridge University Press, Cambridge, 1982), p.18

Springer Nature or its licensor (e.g. a society or other partner) holds exclusive rights to this article under a publishing agreement with the author(s) or other rightsholder(s); author self-archiving of the accepted manuscript version of this article is solely governed by the terms of such publishing agreement and applicable law.