

Dos and don'ts of reduced chi-squared

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Reduced chi-squared is a very popular method for model assessment, model comparison, convergence diagnostic, and error estimation in astronomy. In this manuscript, we discuss the pitfalls involved in using reduced chi-squared. There are two independent problems: (a) The number of degrees of freedom can only be estimated for linear models. Concerning nonlinear models, the number of degrees of freedom is unknown, i.e., it is not possible to compute the value of reduced chi-squared. (b) Due to random noise in the data, also the value of reduced chi-squared itself is subject to noise, i.e., the value is uncertain. This uncertainty impairs the usefulness of reduced chi-squared for differentiating between models or assessing convergence of a minimisation procedure. The impact of noise on the value of reduced chi-squared is surprisingly large, in particular for small data sets, which are very common in astrophysical problems. We conclude that reduced chi-squared can only be used with due caution for linear models, whereas it must not be used for nonlinear models at all. Finally, we recommend more sophisticated and reliable methods, which are also applicable to nonlinear models.

1 Introduction

When fitting a model f with parameters $\vec{\theta}$ to N data values y_n , measured with (uncorrelated) Gaussian errors σ_n at positions \vec{x}_n , one needs to minimise

$$\chi^2 = \sum_{n=1}^N \left(\frac{y_n - f(\vec{x}_n; \vec{\theta})}{\sigma_n} \right)^2. \quad (1)$$

This is equivalent to maximising the so-called “likelihood function”. If the data’s measurement errors are not Gaussian, χ^2 should not be used because it is not the maximum-likelihood estimator. For the rest of this manuscript, we shall therefore assume that the data’s errors are Gaussian. If K denotes the number of degrees of freedom, reduced χ^2 is then defined by

$$\chi_{\text{red}}^2 = \frac{\chi^2}{K}. \quad (2)$$

χ_{red}^2 is a quantity widely used in astronomy. It is essentially used for the following purposes:

1. Single-model assessment: If a model is fitted to data and the resulting χ_{red}^2 is larger than one, it is considered a “bad” fit, whereas if $\chi_{\text{red}}^2 < 1$, it is considered an overfit.
2. Model comparison: Given data and a set of different models, we ask the question which model fits the data best. Typically, each model is fit to the data and their values of χ_{red}^2 are compared. The winning model is that one whose value of χ_{red}^2 is closest to one.

3. Convergence diagnostic: A fit is typically an iterative process which has to be stopped when converged. Convergence is sometimes diagnosed by monitoring how the value of χ_{red}^2 evolves during the iteration and the fit is stopped as soon as χ_{red}^2 reaches a value sufficiently close to one. Sometimes it is claimed then, that “the fit has reached noise level”.
4. Error estimation: One fits a certain model to given data by minimising χ^2 and then rescales the data's errors such that the value of χ_{red}^2 is exactly equal to one. From this one then computes the errors of the model parameters. (It has already been discussed by Andrae (2010) that this method is incorrect, so we will not consider it any further here.)

In all these cases, χ_{red}^2 excels in simplicity, since all one needs to do is divide the value of χ^2 by the number of degrees of freedom and compare the resulting value of χ_{red}^2 to one.

In this manuscript, we want to investigate the conditions under which the aforementioned applications are meaningful – at least the first three. In particular, we discuss the pitfalls that may severely limit the credibility of these applications. We explain the two major problems that typically arise in using χ_{red}^2 in practice: First, we discuss the issue of estimating the number of degrees of freedom in Sect. 2. Second, we explain how the uncertainty in the value of χ^2 may affect the above applications in Sect. 3. Section 4 is then dedicated to explain more reliable methods rather than χ_{red}^2 . We conclude in Sect. 5.

2 Degrees of freedom

Given the definition of χ_{red}^2 , it is evidently necessary to know the number of degrees of freedom of the model. For N data points and P fit parameters, a naïve guess is that the number of degrees of freedom is $N - P$. However, in this section, we explain why this is *not* true in general. We begin with a definition of “degrees of freedom” and then split this discussion into three parts: First, we discuss only linear models. Second, we discuss linear models with priors. Third, we discuss nonlinear models. Finally, we discuss whether linearisation may help in the case of nonlinear models.

2.1 Definition

For a given parameter estimate, e.g., a model fitted to data, the degrees of freedom are the number of independent pieces of information that were used. The concept of “degrees of freedom” can be defined in different ways. Here, we give a general and simple definition. In the next section, we give a more technical definition that only applies to linear models.

Let us suppose that we are given N measurements y_n and a model with P free parameters $\theta_1, \theta_2, \dots, \theta_P$. The best-fitting parameter values are found by minimising χ^2 . This means we impose P constraints of the type

$$\frac{\partial \chi^2}{\partial \theta_p} = 0 \quad \forall p = 1, 2, \dots, P \quad (3)$$

onto our N -dimensional system. Hence, the number of degrees of freedom is $K = N - P$. At first glance, this appears to be a concise and infallible definition. However, we shall see that this is not the case.

2.2 Linear models without priors

A linear model is a model, where *all* fit parameters are linear. This means it is a linear superposition of a set of basis functions,

$$f(\vec{x}, \vec{\theta}) = \theta_1 B_1(\vec{x}) + \theta_2 B_2(\vec{x}) + \dots + \theta_P B_P(\vec{x}) = \sum_{p=1}^P \theta_p B_p(\vec{x}) , \quad (4)$$

where the coefficients θ_p are the fit parameters and the $B_p(\vec{x})$ are some (potentially nonlinear) functions of the position \vec{x} . A typical example is a polynomial fit, where $B_p(x) = x^p$. Inserting such a linear model into χ^2 causes χ^2 to be a quadratic function of the fit parameters, i.e., the first derivatives – our constraints from Eq. (3) – form a set of linear equations that can be solved analytically under certain assumptions.

A natural approach to solve such sets of linear equations is to employ linear algebra. This will lead us to a quantitative definition of the number of degrees of freedom for linear models. Let us introduce the following quantities:

- $\vec{y} = (y_1, y_2, \dots, y_N)^T$ is the N -dimensional vector of measurements y_n .
- $\vec{\theta} = (\theta_1, \theta_2, \dots, \theta_P)^T$ is the P -dimensional vector of linear model parameters θ_p .
- Σ is the $N \times N$ covariance matrix of the measurements, which is diagonal in the case of Eq. (1), i.e., $\Sigma = \text{diag}(\sigma_1^2, \sigma_2^2, \dots, \sigma_N^2)$.
- \mathbf{X} is the so-called design matrix which has format $N \times P$. Its elements are given by $X_{np} = B_p(\vec{x}_n)$, i.e., the p -th basis function evaluated at the n -th measurement point.

Given these definitions, we can now rewrite Eq. (1) in matrix notation,

$$\chi^2 = (\vec{y} - \mathbf{X} \cdot \vec{\theta})^T \cdot \Sigma^{-1} \cdot (\vec{y} - \mathbf{X} \cdot \vec{\theta}) . \quad (5)$$

Minimising χ^2 by solving the constraints of Eq. (3) then yields the analytic solution

$$\hat{\vec{\theta}} = (\mathbf{X}^T \cdot \Sigma^{-1} \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \Sigma^{-1} \cdot \vec{y} , \quad (6)$$

where the hat in $\hat{\vec{\theta}}$ accounts for the fact that this is only an *estimator* for $\vec{\theta}$, but not the true $\vec{\theta}$ itself. We then obtain the prediction $\hat{\vec{y}}$ of the measurements \vec{y} by,

$$\hat{\vec{y}} = \mathbf{X} \cdot \hat{\vec{\theta}} = \mathbf{X} \cdot (\mathbf{X}^T \cdot \Sigma^{-1} \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \Sigma^{-1} \cdot \vec{y} = \mathbf{H} \cdot \vec{y} , \quad (7)$$

where we have introduced the $N \times N$ matrix \mathbf{H} , which is sometimes called “hat matrix”, because it translates the data \vec{y} into a model prediction $\hat{\vec{y}}$. The number of *effective* model parameters is then given by the trace of \mathbf{H} (e.g. Ye 1998; Hastie et al. 2009),

$$P_{\text{eff}} = \text{tr}(\mathbf{H}) = \sum_{n=1}^N H_{nn} = \text{rank}(\mathbf{X}) , \quad (8)$$

which also equals the rank of the design matrix \mathbf{X} .¹ Obviously, $P_{\text{eff}} \leq P$, where the equality holds if and only if the design matrix \mathbf{X} has full rank. Consequently, for linear models the number of degrees of freedom is

$$K = N - P_{\text{eff}} \geq N - P . \quad (9)$$

¹The rank of \mathbf{X} equals the number of linearly independent column vectors of \mathbf{X} .

The standard claim is that a linear model with P parameters removes P degrees of freedom when fitted to N data points, such that the remaining number of degrees of freedom is $K = N - P$. Is this correct? No, not necessarily so. The problem is in the required linear independence of the P basis functions. We can also say that the P constraints given by Eq. (3) are not automatically independent of each other. Let us consider a trivial example, where the basis functions are clearly not linearly independent:

Example 1 *The linear model $f(\vec{x}, \vec{\theta}) = \theta_1 + \theta_2$ is composed of two constants, θ_1 and θ_2 , i.e., $B_1(\vec{x}) = B_2(\vec{x}) = 1$. Obviously, this two-parameter linear model cannot fit two arbitrary data points and its number of degrees of freedom is not given by $N - 2$ but $N - 1$, because the design matrix \mathbf{X} only has rank 1, not rank 2. In simple words, the two constraints $\frac{\partial \chi^2}{\partial \theta_1} = 0$ and $\frac{\partial \chi^2}{\partial \theta_2} = 0$ are not independent of each other.*

From this discussion we have to draw the conclusion that for a linear model the number of degrees of freedom is given by $N - P$ if and only if the basis functions are linearly independent for the given data positions \vec{x}_n , which means that the design matrix \mathbf{X} has full rank. In practice, this condition is *usually* satisfied, but not always. In the more general case, the true number of degrees of freedom for a linear model may be anywhere between $N - P$ and $N - 1$.

2.3 Linear models with priors

Priors are commonly used to restrict the possible values of fit parameters. In practice, priors are usually motivated by physical arguments, e.g., a fit parameter corresponding to the mass of an object must not be negative. Let us consider a very simple example of a prior:

Example 2 *A linear model $f(x, a_0, a_1) = a_0 + a_1x$ is given. The value of parameter a_0 is not restricted, but a_1 must not be negative. Figure 1 demonstrates that this two-parameter model is incapable of sensibly fitting two arbitrary data points because of this prior.*

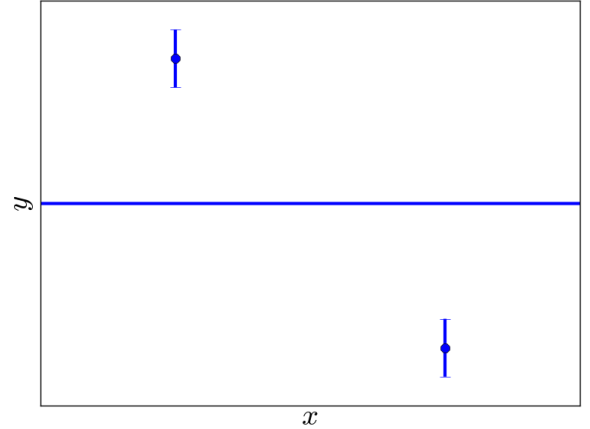


Figure 1: Example of a two-parameter model, $f(x) = a_0 + a_1x$, that is incapable of fitting two data points perfectly because it involves a prior $a_1 \geq 0$. We show the optimal fit for the given data. The model is discussed in Example 2.

Obviously, priors reduce the flexibility of a model, which is actually what they are designed to do. Consequently, they also affect the number of degrees of freedom. In this case, the prior was a step function (zero for $a_1 < 0$ and one otherwise), i.e., it was highly nonlinear. Consequently, although $f(x, a_0, a_1) = a_0 + a_1x$ is itself a linear function of all fit parameters, the overall model including the prior is not linear anymore. This leads us directly to the issue of nonlinear models.

2.4 Nonlinear models

We have seen that estimating the number of degrees of freedom is possible in the case of linear models with the help of Eq. (8). However, for a nonlinear model, we cannot rewrite χ^2 like in Eq. (5), because a nonlinear model cannot be written as $\mathbf{X} \cdot \vec{\theta}$. Therefore, \mathbf{H} does not exist and we cannot use Eq. (8) for estimating the number of degrees of freedom. Ye (1998) introduces

the concept of “generalised degrees of freedom”, but concludes that it is infeasible in practice. We now consider two examples in order to get an impression why the concept of degrees of freedom is difficult to grasp for nonlinear models:

Example 3 *Let us consider the following model $f(x)$, having three free parameters A , B , C ,*

$$f(x) = A \cos(Bx + C) . \quad (10)$$

If we are given a set of N measurement (x_n, y_n, σ_n) such that no two data points have identical x_n , then the model $f(x)$ is capable of fitting any such data set perfectly. The way this works is by increasing the “frequency” B such that $f(x)$ can change on arbitrarily short scales.² As $f(x)$ provides a perfect fit in this case, χ^2 is equal to zero for all possible noise realisations of the data. Evidently, this three-parameter model has infinite flexibility (if there are no priors) and $K = N - P$ is a poor estimate of the number of degrees of freedom, which actually is $K = 0$.

Example 4 *Let us modify the model of Example 3 slightly by adding another component with additional free parameters D , E , and F ,*

$$f(x) = A \cos(Bx + C) + D \cos(Ex + F) . \quad (11)$$

If the fit parameter D becomes small such that $|D| \ll |A|$, the second component cannot influence the fit anymore and the two model parameters E and F are “lost”. In simple words: This model may change its flexibility during the fitting procedure.

Hence, for nonlinear models, K may not even be constant.³ Of course, these two examples do *not* verify the claim that always $K \neq N - P$ for nonlinear models. However, acting as counter-examples, they clearly falsify the claim that $K = N - P$ is always true for nonlinear models.

2.5 Local linearisation

As we have seen above, there is no well-defined method for estimating the number of degrees of freedom for a truly nonlinear model. We may now object that any well-behaved nonlinear model⁴ can be *linearised* around the parameter values which minimise χ^2 . Let us denote the parameter values that minimise χ^2 by $\vec{\Theta}$. We can then Taylor-expand χ^2 at $\vec{\Theta}$ to second order,

$$\chi^2(\vec{\theta}) \approx \chi^2_{\min} + \sum_{p,q=1}^P \left. \frac{\partial^2 \chi^2}{\partial \theta_p \partial \theta_q} \right|_{\vec{\theta}=\vec{\Theta}} (\theta_p - \Theta_p)(\theta_q - \Theta_q) , \quad (12)$$

where the first derivative is zero at the minimum. Apparently, χ^2 is now a quadratic function of the model parameters, i.e., the model is linearised. Does this mean that we can simply linearise the model in order to get rid of the problems with defining the number of degrees of freedom for a nonlinear model?

The answer is definitely no. The crucial problem is that linearisation is just an *approximation*. The Taylor expansion of Eq. (12) has been truncated after the second-order term. There

²In practice, there is of course a prior forbidding unphysically large frequencies. But there is no such restriction in this thought experiment.

³For linear models this cannot happen, since products (or more complicated functions) of model parameters are nonlinear.

⁴With “well-behaved” we mean a model that can be differentiated twice with respect to all fit parameters, including mixed derivatives.

are two issues here: First, in general, we do not know how good this approximation really is for a given data sample. Second, we have no way of knowing how good the approximation *needs* to be in order to sufficiently linearise the model from the number-of-degrees-of-freedom point of view.

Even if these issues did not concern us, would linearising the model really help? Again, the answer is no. As we have seen in Sect. 2.2, the number of degrees of freedom is also not necessarily given by $N - P$ for a linear model. Moreover, the truly worrisome result of Sect. 2.4 – that the number of degrees of freedom is not constant – is *not* overcome by the linearisation. The reason is that the expansion of Eq. (12), and thereby the linearisation, depends nonlinearly upon *where* the maximum is.⁵ Consequently, the uncertainties in the maximum position inherited from the data's noise propagate nonlinearly through the expansion of Eq. (12). Therefore, we have to draw the conclusion that there is no way of reliably estimating the number of degrees of freedom for a nonlinear model.

2.6 Summary

Summarising the arguments brought up so far, we have seen that estimating the number of degrees of freedom is absolutely nontrivial. In the case of linear models, the number of degrees of freedom is given by $N - P$ if and only if the basis functions are indeed linearly independent in the regime sampled by the given data. Usually, this is true in practice. Otherwise, the number of degrees of freedom is somewhere between $N - P$ and $N - 1$. However, in the case of nonlinear models, the number of degrees of freedom can be anywhere between 0 and $N - 1$ and it is even not necessarily constant during the fit. Linearising the model at the optimum does not really help to infer the number of degrees of freedom, because the linearised model still depends on the optimum parameters in a nonlinear way. Hence, it is questionable whether it is actually *possible* to compute χ_{red}^2 for nonlinear models in practice.

3 Uncertainty in χ^2

We now discuss another problem, which is completely independent of our previous considerations. Even if we were able to estimate the number of degrees of freedom reliably, this problem would still interfere with any inference based on χ_{red}^2 . This problem stems from the fact that the value of χ^2 is subject to noise, which is inherited from the random noise of the data.⁶ Consequently, there is an “uncertainty” on the value of χ^2 and hence on χ_{red}^2 , which is typically ignored in practice. However, we show that this uncertainty is usually large and must not be neglected, because it may have a severe impact on the intended application.

Given some data with Gaussian noise, the true model having the true parameter values will generate a $\chi^2 = N$ and has N degrees of freedom because there is no fit involved. Hence, it results in a χ_{red}^2 of 1. We therefore compare the χ_{red}^2 of our trial model to 1 in order to assess convergence or to compare different models. Is this correct?

In theory, yes. In practice, no. Even in the case of the true model having the true parameter values, where there is no fit at all, the value of χ^2 is subject to noise. In this case, we are fortunate enough to be able to quantify this uncertainty. For the true model having the true

⁵For a linear model the second derivatives of χ^2 do not depend on any model parameters, i.e., they are constant.

⁶For a given set of data, χ^2 can of course be computed. However, consider a second set of data, which was drawn from the same physical process such that only the noise realisation is different. For this second set of data, the value of χ^2 will differ from that of the first set.

parameter values and *a-priori* known measurement errors σ_n , the normalised residuals,

$$R_n = \frac{y_n - f(\vec{x}_n, \vec{\theta})}{\sigma_n} \quad (13)$$

are distributed according to a Gaussian with mean $\mu = 0$ and variance $\sigma^2 = 1$.⁷ In this case only, χ^2 is the sum of $K = N$ Gaussian variates and its probability distribution is given by the so-called χ^2 -distribution,

$$\text{prob}(\chi^2; K) = \frac{1}{2^{K/2}\Gamma(K/2)} (\chi^2)^{K/2-1} e^{-\chi^2/2}. \quad (14)$$

Figure 2 shows some χ^2 -distributions with different values of K . The expectation value of the χ^2 -distribution is,

$$\langle \chi^2 \rangle = \int_0^\infty \chi^2 \text{prob}(\chi^2; K) d\chi^2 = K. \quad (15)$$

In fact, this expectation value is sometimes used as an alternative definition of “degrees of freedom”. As the χ^2 -distribution is of non-zero width, there is however an uncertainty on this expectation value. More precisely, the variance of the χ^2 -distribution is given by $2K$. This means the expectation value of χ_{red}^2 for the true model having the true parameter values is indeed one, but it has a variance of $2/K = 2/N$. If N is large, the χ^2 -distribution becomes approximately Gaussian and we can take the root of the variance, $\sigma = \sqrt{2/N}$, as an estimate of the width of the (approximately Gaussian) peak. Let us consider a simple example in order to get a feeling how severe this problem actually is:

Example 5 *We are given a data set comprised of $N = 1,000$ samples. Let the task be to use χ_{red}^2 in order to compare different models to select that one which fits the data best, or to fit a single model to this data and assess convergence. The true model having the true parameter values – whether it is given or not – will have a value of χ_{red}^2 with an (approximated) Gaussian standard deviation of $\sigma = \sqrt{2/1000} \approx 0.045$. Consequently, within the 3σ interval $0.865 \leq \chi_{\text{red}}^2 \leq 1.135$ we can neither reliably differentiate between different models nor assess convergence.*

This simple example clearly shows that this problem is very drastic in practice. Moreover, astronomical data sets are often much smaller than $N = 1,000$, which increases the uncertainty of χ_{red}^2 .

Of course, there is not only an uncertainty on the comparison value of χ_{red}^2 for the true model having the true parameter values. There is also an uncertainty on the value of χ_{red}^2 for any other model. Unfortunately, we *cannot* quantify this uncertainty via $\sigma \approx \sqrt{2/K}$ in

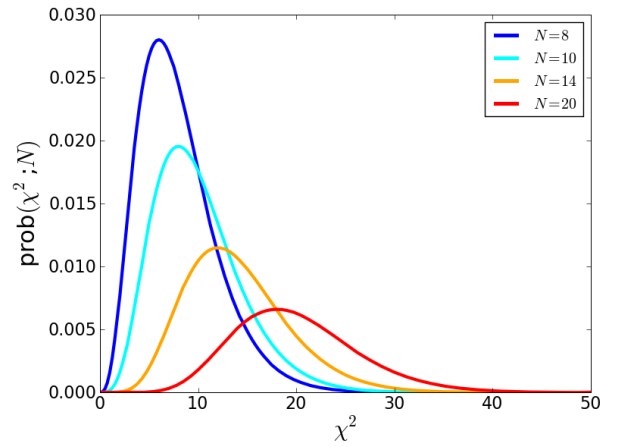


Figure 2: χ^2 -distributions for different values of $K = N$ degrees of freedom. The distributions are asymmetric, i.e., mean and maximum (mode) do not coincide. For increasing $K = N$, the distributions become approximately Gaussian.

⁷Again, we implicitly assume that the Gaussian errors are uncorrelated, as in Eq. (1). If the measurement errors σ_n are not known a priori but have been estimated from the data, the normalised residuals R_n are drawn from Student's *t*-distribution (e.g. Barlow 1993). With increasing number of data points Student's *t*-distribution approaches a Gaussian distribution.

practice anymore, because the χ^2 -distribution applies only to the true model having the true parameter values. For any other model the normalised residuals (cf. Eq. (13)) are not Gaussian with mean $\mu = 0$ and variance $\sigma^2 = 1$. Hence, χ^2 is *not* the sum of K Gaussian variates and the derivation of the χ^2 -distribution is invalid.

4 Alternative methods

If χ_{red}^2 does not provide a reliable method for assessing and comparing model fits, convergence tests or error estimation, what other methods can then be used with more confidence? An in-depth survey of alternative methods would be beyond the scope of this manuscript. Therefore, we restrict our discussion on some outstanding methods. Concerning methods for error estimation, we refer the interested reader to Andrae (2010).

4.1 Residuals

The first and foremost thing to do in order to assess the goodness of fit of some model to some data is to inspect the residuals. This is indeed trivial, because the residuals have already been computed in order to evaluate χ^2 (cf. Eq. (1)). For the true model having the true parameter values and *a-priori* known measurement errors, the distribution of normalised residuals (cf. Eq. (13)) is by definition Gaussian with mean $\mu = 0$ and variance $\sigma^2 = 1$. For any other model, this is not true. Consequently, all one needs to do is to plot the distribution of normalised residuals in a histogram and compare it to a Gaussian of $\mu = 0$ and $\sigma^2 = 1$. If the histogram exhibits a statistically *significant* deviation from the Gaussian, we can rule out that the model is the truth. If there is no significant difference between histogram and Gaussian, this can mean (a) we found the truth, or (b) we do not have enough data points to discover the deviation. The comparison of the residuals to this Gaussian should be objectively quantified, e.g., by using a Kolmogorov-Smirnov test⁸ (Kolmogorov 1933; Smirnov 1948).

In theory, this method may be used as a convergence diagnostic. In an iterative fit procedure, compare the distribution of normalised residuals to the Gaussian with $\mu = 0$ and $\sigma^2 = 1$ in each iteration step, e.g., via a Kolmogorov-Smirnov test. At first, the likelihood of the residuals to be Gaussian will increase as the model fit becomes better. *If* the fit finds a suitable local minimum, the model may eventually start to *overfit* the data and the likelihood of the residuals to be Gaussian will decrease again, as the residuals will peak too sharply at zero. When this happens, the fitting procedure should be stopped. In practice, there is no guarantee that this works, as the fit may end up in a local minimum with residuals too widely spread to resemble the Gaussian with $\mu = 0$ and $\sigma^2 = 1$.

Similarly, this method may also be used for model comparison. Given some data and a set of models, the model favoured by the data is that whose normalised residuals match the Gaussian with $\mu = 0$ and $\sigma^2 = 1$ best. The winning model does not need to be the truth. Let us consider the following example:

Example 6 *Vogt et al. (2010) analysed radial-velocity data of the nearby star GJ 581 and came to the conclusion that the data suggests the presence of six exoplanets instead of four as claimed by other authors using different data (e.g. Mayor et al. 2009). Vogt et al. (2010) assumed circular orbits, which result in nonlinear models of the form of Eq. (10) in Example 3. Their claim that two additional planets are required is primarily justified from the associated χ_{red}^2 (cf.*

⁸The Kolmogorov-Smirnov (KS) test compares the empirical cumulative distribution function (CDF) of a sample to a theoretical CDF by quantifying the distance between the distributions. Under the (null) hypothesis that the sample *is* from the given distribution, this distance (called the KS-statistic) has a known probability distribution. Now, the test calculates the KS-statistic and compares it to its known probability distribution.

Planets	1	2	3	4	5	6
p -value	$8.71 \cdot 10^{-11}$	$2.97 \cdot 10^{-9}$	$2.51 \cdot 10^{-7}$	$1.28 \cdot 10^{-4}$	$1.47 \cdot 10^{-5}$	$6.97 \cdot 10^{-8}$
χ^2_{red}	8.426	4.931	4.207	3.463	2.991	2.506

Table 1: p -values from KS-test and χ^2_{red} for 1–6 planets for the data of Vogt et al. (2010) discussed in Example 6.

Table 1). We take the identical data as Vogt et al. (2010) and their asserted orbital parameters of the six planets (their Table 2). For every number of planets, we apply the KS-test to the normalised residuals. Table 1 gives the resulting p -values⁹ for the six models. In terms of the KS-test, the data used by Vogt et al. (2010) strongly favour the model using four planets over the model using six planets. Furthermore, Fig. 3 displays the distributions of normalised residuals for the models using four and six planets. Evidently, both distributions deviate significantly from the Gaussian with $\mu = 0$ and $\sigma^2 = 1$, which implies that neither model is compatible with the truth. The most likely explanation for this discrepancy is that planetary orbits may be elliptical, whereas Vogt et al. (2010) assumed circular orbits.

There is a pitfall here, as well. The likelihood of the normalised residuals to come from a Gaussian with $\mu = 0$ and $\sigma^2 = 1$ is also subject to noise, as in the case of the value of χ^2 . However, these uncertainties surely cannot explain the large differences in Table 1.

4.2 Cross-validation

Cross-validation is one of the most powerful and most reliable methods for model comparison. Unfortunately, it is usually also computationally expensive. However, if χ^2_{red} is not applicable, e.g., because the model is nonlinear, computational cost cannot be used as an argument in disfavour of cross-validation.

The most straightforward (and also most expensive) flavour of cross-validation is “leave-one-out cross-validation”. We are given N data points and a set of models, and we want to know which model fits the data best. For each model, the goodness of fit is estimated in the following way:

1. Remove the n -th data point from the data sample.
2. Fit the model to the remaining $N - 1$ data points.
3. Take the model fitted to the $N - 1$ data points and compute its likelihood for the n -th data point that has been left out.

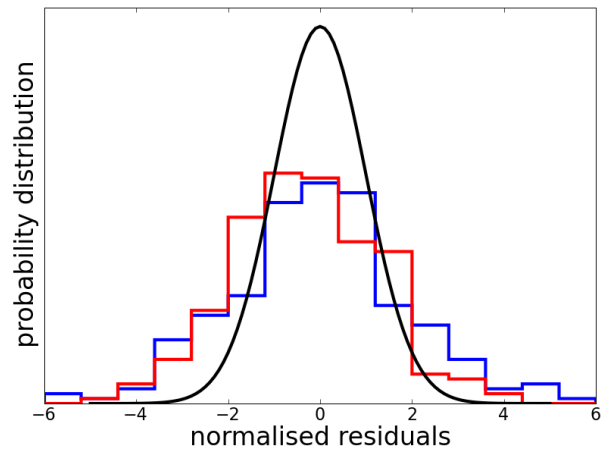


Figure 3: Distributions of normalised residuals for the data and models of Vogt et al. (2010) using four planets (blue histogram) and six planets (red histogram). For comparison we also show the Gaussian with $\mu = 0$ and $\sigma^2 = 1$. As the number of data points is large ($N = 241$), there is no difference between this Gaussian and Student’s t -distribution.

⁹Loosely speaking, in this case, the p -value is the probability that the true model can generate residuals that agree with the standard Gaussian as badly as or worse than the actually observed ones.

4. Repeat steps 1 to 3 from $n = 1$ to $n = N$ and compute the goodness of the prediction of the whole data set by multiplying the likelihoods obtained in step 3.

Steps 3 and 4 require the data's error distribution to be known in order to evaluate the goodness of the prediction for the left-out data point through its likelihood. For instance, if the data's errors are Gaussian, the goodness of the prediction is simply given by Eq. (13) as usual. Evidently, repeating steps 1 to 3 N times is what makes leave-one-out cross-validation computationally expensive. It is also possible to leave out more than one data point in each step.¹⁰ However, if the given data set is very small, cross-validation becomes unstable. A nice application of cross-validation can be found, e.g., in Hogg (2008).

4.3 Bootstrapping

Bootstrapping is somewhat more general than cross-validation, meaning it requires less knowledge about the origin of the data. Cross-validation requires the data's error distribution to be known in order to evaluate the likelihoods, whereas bootstrapping does not. Of course, this is an advantage if we do *not* have this knowledge. However, if we do know the data's errors, we should definitely exploit this knowledge by using cross-validation. Bootstrapping is discussed in Andrae (2010) in the context of error estimation. Therefore, we restrict its discussion here on the context of model comparison.

Let us suppose we are given 4 measurements y_1, y_2, y_3, y_4 . We then draw subsamples of size 4 from this data set with replacement. These subsamples are called bootstrap samples. Examples are:

- y_1, y_2, y_3, y_4 itself,
- y_1, y_2, y_2, y_4 ,
- y_2, y_4, y_4, y_4 ,
- y_1, y_1, y_1, y_1 ,
- etc.

We draw a certain number of such bootstrap samples, and to every such sample we then fit all the models that are to be compared.

In the context of model comparison, bootstrapping is typically used as “leave-one-out bootstrap” (e.g. Hastie et al. 2009). The algorithm is given by:

1. Draw a certain number of bootstrap samples from a given data set.
2. Fit all the models to every bootstrap sample.
3. For the n -th data point y_n in the given data set, consider only those bootstrap samples that do *not* contain y_n . Predict y_n from the models fitted to these bootstrap samples.
4. Repeat step 3 from $n = 1$ to $n = N$ and monitor the goodness of the predictions, e.g., by least squares.

Like cross-validation, bootstrapping aims at the prediction error of the model. Therefore, it is sensitive to over- and underfittings.

¹⁰The reason why cross-validation is so reliable is that it draws on the predictive error of the model, rather than the fitting error. Therefore, cross-validation can detect underfitting (the model is not flexible enough to describe the data) and also overfitting (the model is too flexible compared to the data). The fitting error is only sensitive to underfitting, but not to overfitting (χ^2 always decreases if the model becomes more complex).

5 Conclusions

We have argued that there are two fundamental problems in using χ_{red}^2 , which are completely independent of each other:

1. In Sect. 2, we have seen that estimating the number of degrees of freedom, which is necessary for evaluating χ_{red}^2 , is absolutely nontrivial in practice:
 - Concerning *linear* models, for N given data points and P fit parameters the number of degrees of freedom is *somewhere* between $N - P$ and $N - 1$, where it is $N - P$ if and only if the basis functions of the linear model are linearly independent for the given data. Equation (8) provides a quantification for the effective number of fit parameters of a linear model. Priors can cause a linear model to become nonlinear.
 - Concerning *nonlinear* models, the number of degrees of freedom is *somewhere* between zero and $N - 1$ and it may not even be constant during a fit, i.e., $N - P$ is a completely unjustified guess. The authors are not aware of any method that reliably estimates the number of degrees of freedom for nonlinear models. Consequently, it appears to be impossible to compute χ_{red}^2 in this case.
2. In Sect. 3, we have seen that the actual value of χ_{red}^2 is *uncertain*. If the number N of given data points is large, the uncertainty of χ_{red}^2 is approximately given by the Gaussian error $\sigma = \sqrt{2/N}$. For $N = 1,000$ data points, this means that within the 3σ -interval $0.865 \leq \chi_{\text{red}}^2 \leq 1.135$ we cannot compare models or assess convergence.

Given these considerations, it appears highly questionable whether the popularity of χ_{red}^2 – which is certainly due to its apparent simplicity – is indeed justified. As a matter of fact, χ_{red}^2 cannot be evaluated for a nonlinear model, because the number of degrees of freedom is *unknown* in this case. This is a severe restriction, because many relevant models are nonlinear. Moreover, even for linear models, χ_{red}^2 has to be used with due caution, considering the uncertainty in its value.

Concerning alternative methods for model comparison, we have explained cross-validation and bootstrapping in Sect. 4. We also explained how the normalised residuals of a model can be used to infer how close this model is to the true model underlying the given data. Concerning alternative methods for error estimation, we refer the interested reader to Andrae (2010).

Finally, we want to emphasise that the above considerations concerning χ_{red}^2 have *no* impact on the correctness of minimising a χ^2 in order to fit a model to data. Fitting models to data is a completely different task that should not be confused with model comparison or convergence testing. Minimising χ^2 is the correct thing to do whenever the data's measurement errors are Gaussian and a maximum-likelihood estimate is desired.

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References

- Andrae, R. 2010, ArXiv e-prints 1009.2755
- Barlow, R. 1993, Statistics: A Guide to the Use of Statistical Methods in the Physical Sciences (Wiley VCH)

- Hastie, T., Tibshirani, R., & Friedman, J. 2009, The Elements of Statistical Learning: Data Mining, Inference, and Prediction. (Springer-Verlag)
- Hogg, D. W. 2008, ArXiv e-prints 0807.4820
- Kolmogorov, A. 1933, Giornale dell' Istituto Italiano degli Attuari, 4, 83
- Mayor, M., Bonfils, X., Forveille, T., et al. 2009, A&A, 507, 487
- Smirnov, N. 1948, Annals of Mathematical Statistic, 19, 279
- Vogt, S. S., Butler, R. P., Rivera, E. J., et al. 2010, ApJ, 723, 954
- Ye, J. 1998, Journal of the American Statistical Association, 93, 120