## 3.2 Error propagation

There are two approaches to propagating the age uncertainties in 40Ar/39Ar geochronology. The first is to explicitly calculate the errors for each analysis separately. The second is to process multiple analyses together by matrix algebra. Although the first approach is the most common one, the second one is actually more practical and offers significant advantages for higher order data processing steps (Section 3.3).

**Separate error propagation**

Let be one of (i.e. ) 40Ar/39Ar age estimates:

where is the irradiation constant, is the 40Ar/39Ar-ratio and is the 40K decay constant. Then the uncertainty (standard error) of can be estimated as (McDougall and Harrison 1999):

Equation [2](#eq:sti) assumes that the uncertainties of and (i.e., and ) are *independent* of each other, and that the decay constant is known with zero uncertainty. In reality, neither of these assumptions is correct (Vermeesch 2015). But for the purpose of this paper, we will assume that this makes little difference.

**Joint error propagation**

In an alternative approach, we can also propagate the uncertainties of all the s together, forming a *covariance matrix* :

where is the covariance matrix of the 40Ar/39Ar-ratios and the irradiation constant:

where the zero values mean that the uncertainties of and are uncorrelated. This assumption is, of course, not correct in the general case. But we are making it here for the sake of consistency with the previous paragraph. is the Jacobian matrix (and its transpose) of partial derivatives of Equation [1](#eq:ti) w.r.t. and :

Even though the off-diagonal terms of are zero, those of generally are not. In other words, the uncertainties of the different age estimates are correlated with each other. This is important if we want to further process those estimates to calculate a weighted average, say.

## 3.3 Random vs. systematic uncertainties

Equation [2](#eq:sti) contains two sources of analytical uncertainty:

* is a *random* error, which differs for each .
* is a *systematic* error, which is the same for all .

The random (or ‘internal’) uncertainties can be reduced to arbitrarily low levels by simply increasing the number of aliquots (). Their effect on the standard error of the mean scales with . In contrast, the systematic (or ‘external’) uncertainties cannot be reduced. They impose a hard lower limit on the precision of the weighted mean.  
There are two different but equivalent ways to address the difference between these two types of analytical uncertainty. Hierarchical error propagation (Renne et al. 1998; Min et al. 2000) processes the random uncertainties first, and only then adds the systematic uncertainties. In an alternative approach, the random and systematic sources of uncertainty can also be processed jointly, using matrix algebra. Let us illustrate these two approaches by calculating the weighted mean of single grain age estimates.

**Hierarchical error propagation**  
We first calculate the variance-weighted mean 40Ar/39Ar-ratio :

and its standard error:

Then, we use Equations [1](#eq:ti) and [2](#eq:sti) to calculate the weighted mean age and its uncertainty:

and

**Joint error propagation**  
Instead of the two-step procedure of the previous paragraph, the weighted mean age and its uncertainty can also be obtained in one step.

where is a row vector with the individual age estimates , is a column vector of ones, is the inverse of the covariance matrix (calculated using Equation [3](#eq:Sigmat)), and is given by

## 3.4 Dispersion

The degree to which the analytical uncertainties account for the observed scatter between multiple measurements from the same sample may be assessed by means of the Mean Square of the Weighted Deviates (, McIntyre et al. 1966), which is also known as the ‘reduced Chi-square statistic’ outside of geochronology.

**Hierarchical error propagation**

In the context of the weighted mean age, the of age estimates is given by:

If the analytical uncertainties are the only source of scatter between the aliquots, then .

-values that are considerably greater than one indicate that there is some excess scatter in the data, which cannot be explained by the analytical uncertainties alone. This usually reflects the presence of some geological *dispersion*. Possible causes of such dispersion may be the protracted crystallisation history of a sample, variable degrees of inheritance, or partial loss of radiogenic 40Ar by thermally activated volume diffusion.

-values that are close to zero indicate that the analytical uncertainties have not been propagated correctly. In practice, this often reflects the presence of undetected error correlations. For example, if we were to apply Equation [11](#eq:MSWD) to the actual ages estimates () instead of the 40Ar/39Ar-ratios, then that would lower the -value. This is because the uncertainty of the irradiation constant is shared by all the age estimates, and this is not accounted for by Equation [11](#eq:MSWD).

**Joint error propagation**

In contrast with Equation [11](#eq:MSWD), the matrix definition of the can use either the 40Ar/39Ar or the actual age estimates:

So the same -value is obtained if is replaced with , with , and with , where the latter matrix groups the first rows and columns of Equation [4](#eq:SigmaRJ).

## 3.5 A synthetic example

Consider the dataset of ten 40Ar/39Ar-ratio measurements shown on the first row of Table 1. Assume that these measurements are associated with a 2% analytical uncertainty (i.e. for ).

**Hierarchical error propagation**

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | 0.9847 | 1.0033 | 0.9996 | 1.0335 | 0.9953 | 1.0072 | 0.9625 | 1.0046 | 1.0006 | 1.0314 |
|  | 1239.4 | 1256.3 | 1253.0 | 1283.4 | 1249.1 | 1259.8 | 1219.1 | 1257.5 | 1253.9 | 1281.5 |
|  | 25.4 | 25.6 | 25.6 | 26.0 | 25.5 | 25.7 | 25.1 | 25.6 | 25.6 | 26.0 |

Table 1: Example of 10 synthetic 40Ar/39Ar measurements drawn from a population with true 40Ar/39Ar=1, an irradiation parameter and a 2% analytical uncertainty for both and .

The 40Ar/39Ar-ages and uncertainties, given by Equations [1](#eq:ti) and [2](#eq:sti), are shown on the second and third row of Table 1. The weighted mean 40Ar/39Ar-ratio is (from Equation [5](#eq:Rbar)) with a standard error of (from Equation [6](#eq:sRbar)). Plugging these values into Equations [7](#eq:bart) and [8](#eq:sbart) yields a weighted mean age and error of and , respectively.  
Plugging and into Equation [11](#eq:MSWD) yields a value of . This is close to unity and consistent with the fact that the 2% analytical uncertainty fully accounts for the scatter in the synthetic dataset. However, if we were to substitute and for and in Equation [11](#eq:MSWD), then we would obtain . In other words, the age estimates are *underdispersed* with respect to the analytical uncertainties if the random and systematic sources of uncertainty are lumped together. As explained in the previous sections, these problems can be avoided by jointly propagating all the measurements together.

**Joint error propagation**

Using Equation [3](#eq:Sigmat) to obtain the covariance matrix of the age estimates:

Taking the square root of the diagonal terms of gives exactly the same values for as shown in Table 1. Similarly, we can calculate the weighted mean age and its uncertainty using Equations [9](#eq:bart2) and [10](#eq:sbart2) instead of Equations [7](#eq:bart) and [8](#eq:sbart). Doing so yields in values of and . This only differs slightly from the value obtained by hierarchical error propagation because of numerical rounding errors. Similarly, the MSWD-value obtained from Equation [12](#eq:MSWD2) is (virtually) identical to that obtained from Equation [11](#eq:MSWD) at .

## 3.6 Uncertainty budget of the 40Ar/39Ar method

Sections 3.2-3.5 have shown that identical results can be obtained by hierarchical error propagation of the random and systematic uncertainties, or by jointly propagating them using matrix algebra. This is true for simple data processing steps such as age calculation and averaging. But things are not so simple for more complex operations such as radioactive decay, atmospheric argon, and Ca-, Cl- or K-interference corrections. In those cases, the matrix approach is the only practical way to keep track of all the error correlations (Vermeesch 2015).

Figure 1 shows the results of a sensitivity analysis performed at the WiscAr lab using a Nu Instruments Noblesse multicollector mass spectrometer. The data processing chain for this dataset involves (1) blank correction; (2) regression to the time of gas inlet; (3) detector calibration and mass bias correction by comparison with a synthetic gas mixture of known composition (Jicha, Singer, and Sobol 2016); (4) correction of the sample and the calibration gas for the radioactive decay of 39Ar and 37Ar; (5) correction for interfering neutron reactions on K (on 40Ar), Ca (on 36Ar and 39Ar), and Cl (on 36Ar); (6) calculation and interpolation of the irradiation constant () using a reference material of independently known age; and (7) age calculation using the 40K decay constant and its uncertainty.

All these steps involve both random and systematic errors, which are impossible to separate from each other. Thus, the hierarchical error propagation approach is not possible in this case. Joint error propagation by matrix algebra is the only option to keep track of the complex interactions between the different sources of uncertainty. By eliminating individual steps of this processing chain, Figure 1 reveals the relative effect of the different corrections. These will differ for samples of different age and composition.



Figure 1: Sensitivity analysis for a single total fusion analysis of a sanidine crystal, showing the effect of omitting specific steps in the data processing chain on the accuracy (horizontal axis) and precision (vertical axis) of the results. The white square in the right panel shows the best age estimate using all corrections.

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