Error analysis for stellar population synthesis as an inverse problem

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Abstract
Stellar population synthesis can be approached as an inverse problem. The physical information is extracted from the observations through an inverse model. The process requires the transformation of the observational errors into model errors. A description is given for the error analysis to obtain objectively the errors in the model.

Finding a solution for overdetermined and underdetermined cases was the purpose of two preceding papers. This new one completes the problem of stellar population synthesis by means of a data base, by providing practical formulae defining the set of acceptable solutions. All solutions within this set are compatible, at a given confidence level, with the observations.

Key words: methods: data analysis – methods: numerical – galaxies: stellar content.

1 Introduction
Important astrophysical issues could be solved if we were able to deduce the stellar population from the integrated light received from a far-away galaxy (or a region of a galaxy). Two methods try to solve this problem: the stellar data base synthesis and the evolutionary population synthesis. The first method is a more empirical approach, which relies strictly on the spectral data base of stars or stellar aggregates; while the second one is a more theoretical approach, which relies on our best knowledge on the formation and evolution of stars and stellar aggregates. Stellar data base synthesis is used in both inverse and forward modelling, while evolutionary population synthesis is mostly applied as a forward model. In our opinion the two methods are complementary and should be used jointly in an effort to solve this difficult problem. Both methods are subject to errors and ideally their results should always be presented with a set of acceptable solutions rather than just a solution. The purpose of this paper is to establish this set of acceptable solutions for the stellar data base synthesis.

Pelat (1997, 1998, hereafter Papers I and II) reinvestigated the stellar data base synthesis method and proposed new and fast algorithms to search for physical solutions. The sensitivity of this solution to the observational errors was discussed in general terms: Monte Carlo simulations were performed but no real error analysis had been done. This paper provides the user with practical formulae which give an estimate of the domain of acceptable solutions around the solution.

In Section 2, we recall briefly the solution we have proposed and then we focus in great detail on the question of error analysis.

2 Population synthesis as an inverse problem
First we specify what is meant by observables and parameters in the description of the physical model.

Observables. It is usually agreed to adopt equivalent widths as spectral observables, in order to avoid data reduction errors and to minimize extinction problems. These observables are noted here as the vector \( W_{\text{obs}} \). The aim of the stellar population synthesis is to find the combinations of stars which best reproduce the equivalent widths \( W_{\text{obs}} \) of the observed object (say, a galaxy).

Model parameters. The galaxy is described by the unknowns \( k_i \). They give the proportional contribution to the luminosity due to stars of type \( i \) at a reference wavelength \( \lambda_0 \). The assembly of \( k_i \) is described by the vector \( k \).

The equation governing the stellar population synthesis problem is a non-linear one, where a set of synthetic equivalent widths is a function of a set of stellar luminosity contributions \( k_i \). We have

\[
W_{\text{syn}} = \frac{\sum_{i=1}^{n_{\lambda}} W_i I_{ji} k_i}{\sum_{i=1}^{n_{\lambda}} I_{ji} k_i}, \quad j = 1, \ldots, n_{k},
\]

where \( n_{\lambda} \) is the number of observed equivalent widths; \( n_k \) is the number of stars used for the synthesis; and \( W_i \) and \( I_{ji} \) are respectively the equivalent width and continuum flux at wavelength \( \lambda_i \) of stars of kind \( i \). The continuum fluxes are normalized to unity at the reference wavelength \( \lambda_0 \). For short we write equation (1): \( W_{\text{syn}} = \varphi(k) \).

In addition we have the condition that the contribution of a star to the luminosity cannot be negative and that the normalized proportions \( k_i \) add up to unity. A physical solution of equation (1)
therefore lies in the vector set
\[ S = \left\{ (k_1, \ldots, k_n) | k_i \geq 0, \sum_{i=1}^{n} k_i = 1 \right\}. \]  
(2)

This set \( S \) is a simplex (e.g. an equilateral triangle for a data base of three stars, a tetrahedron for a data base of four and so on). The set of all equivalent widths which are able to be exactly synthesized by the data base is the image of \( S \) by \( \varphi \). This is the synthetic domain \( \mathcal{W} \) introduced in Paper I:
\[ \mathcal{W} = \{ W | W = \varphi(k), \forall k \in S \}. \]  
(3)

If \( W_{\text{obs}} \in \mathcal{W} \) there is at least one exact solution \( k \) such that \( \varphi(k) = W_{\text{obs}} \).

The set \( \mathcal{K} \) of all exact solutions is given formally by \( \mathcal{K} = \varphi^{-1}(W_{\text{obs}}) \). This set may be empty. The solution set \( \mathcal{K} \) is non-empty if there exists at least one vector \( k \) solution of the following system:
\[ \begin{align*}
  k & \geq 0, \\
  A k & = 0, \\
  b^T k & = 1.
\end{align*} \]  
(4)

The matrix elements of \( A \) are \( [A]_{ji} = (W_{\text{obs}} - W_j)I_{ji} \) and \( b^T \) is a line of ‘ones’. This system may or may not possess a solution.

### 2.1 Test for the existence of an exact solution

It is very easy to check if the above system (4) possesses at least one solution. If we add to it a linear equation to be maximized (e.g. \( c^T k = \max \)), this system turns into a linear program. In fact, it is not necessary to make explicit that supplementary linear system:
\[ \begin{align*}
  k & \geq 0, \\
  A k & = 0, \\
  b^T k & = 1.
\end{align*} \]  
(5)

The matrix elements of \( A \) are \( [A]_{ji} = (W_{\text{obs}} - W_j)I_{ji} \) and \( b^T \) is a line of ‘ones’. This system may or may not possess a solution.

### 2.2 Underdetermined case: \( n_\lambda \leq n_s - 1 \)

If the set \( \mathcal{K} \) is non-empty, it has been demonstrated in Paper II that \( \mathcal{K} \) is a polytope, i.e. it is the convex hull of some finite extreme solutions. A solution \( k \) is extreme if it possesses at least \( n_0 = 1 \) components (stellar contributions) equal to zero. The key parameter \( n_0 \) is the dimension of the null space associated with matrix \( A \). The data base is non-degenerate for the observation if we have \( n_0 = n_s - n_\lambda \).

If the galaxy cannot be synthesized, an approximate solution is found with a data base reduced to at most \( n_\lambda \) stars. The procedure is described in the next section.

### 2.3 Overdetermined case: \( n_\lambda \geq n_s \)

In the overdetermined case, there is most probably no exact solution of (4), the observation is not on the synthetic surface and one must content oneself with an approximate solution. This approximate solution \( k \) is usually accepted in the least-square meaning, that is \( k \) must minimize a quadratic form:
\[ D^2 = [W_{\text{obs}} - \varphi(k)]^T \Sigma^{-1} [W_{\text{obs}} - \varphi(k)]. \]  
(6)

where \( \Sigma^{-1} \) is a positive definite ‘weight’ matrix. It has been shown in Paper I that a very successful estimate of \( k \) is found near the ‘first-guess’ \( k_0 \):
\[ k_0 = (B^T B)^{-1} b^T b (B^T B)^{-1} b]^T \]

where \( B \) is equal to the matrix \( A \) augmented with the line \( b^T \). It is shown in Appendix A how one can get rid of the positivity constraint \( k \geq 0 \) when searching for a minimum in the neighbourhood of \( k_0 \). The estimate \( k_0 \) is the unique solution of the problem if the matrix \( \Sigma^{-1} \) is diagonal with diagonal elements equal to \( \sum_{i=1}^{n_s} I_{ji} k_j \). It was argued in Paper I that a reasonable weight matrix should not be very different from this particular diagonal matrix.

### 3 PURPOSES OF THE ERROR ANALYSIS

An observation of a galaxy is not just the point \( W_{\text{obs}} \) in \( W \)-space, it includes all points interior to an error zone around the observation. If we assume the observational errors to be Gaussian, this error zone is a hyper-ellipsoid around \( W_{\text{obs}} \). We have observed \( W_{\text{obs}} \) but we consider that we could have observed, with probability \( \gamma \), any other point in the interior of this hyper-ellipsoid. This set of ‘probable’ points, \( \mathcal{E}_\gamma \), is formally defined as
\[ \mathcal{E}_\gamma = \{ W | (W - W_{\text{obs}})^T V^{-1} (W - W_{\text{obs}}) \leq F_{\gamma}^{-1}(\gamma) \}, \]  
(7)

where \( V \) is the variance–covariance matrix of the observation and \( F_{\gamma} \) is the distribution function of a \( \chi^2 \) variate with \( n_\lambda \) degrees of freedom. For short, we call \( \mathcal{E}_\gamma \), the ‘error ellipsoid’. We recall that \( \mathcal{E}_\gamma \) is the ‘error ellipsoid’. We recall that \( \mathcal{E}_\gamma \) is the ‘error ellipsoid’. We recall that \( \mathcal{E}_\gamma \) is the ‘error ellipsoid’. We recall that \( \mathcal{E}_\gamma \) is the ‘error ellipsoid’. We recall that \( \mathcal{E}_\gamma \) is the ‘error ellipsoid’. We recall that \( \mathcal{E}_\gamma \) is the ‘error ellipsoid’. We recall that \( \mathcal{E}_\gamma \) is the ‘error ellipsoid’. We recall that \( \mathcal{E}_\gamma \) is the ‘error ellipsoid’. We recall that \( \mathcal{E}_\gamma \) is the ‘error ellipsoid’. We recall that \( \mathcal{E}_\gamma \) is the ‘error ellipsoid’. We recall that \( \mathcal{E}_\gamma \) is the ‘error ellipsoid'. We have
\[ \mathcal{K}_\gamma \approx \{ k | (k - k_0)^T P (k - k_0) \leq F_{\gamma}^{-1}(\gamma) \}. \]  
(8)

The matrix \( P \) would be equal to \( V^{-1} \) if \( V \) were invertible, but this is not the case here: the matrix \( V \) is singular because of the normalization constraint on \( k \). Using the definition of \( \mathcal{K}_\gamma \) (7), one is able to test if an alternative solution \( k' \) is acceptable at the confidence level \( \gamma \).

The results of the error analysis are given in Section 5. Before that, we give in Section 3.1 an overview of the main processes at the origin of the observational errors, and in Section 4 we introduce information content held by an observation with regard to the synthesis problem we want to solve.

### 3.1 Origin of the errors

Errors on equivalent widths from spectra of galaxies have several origins. The most important one is induced by the empirical process of continuum intensity plotting. This leads to a wide uncertainty on equivalent width estimates, caused by the fact that the continuum intensity lies in the denominator of the expression for the equivalent width. Contributing to the uncertainties in this empirical approach are the blending of the absorption lines plus the possible presence of emission lines as in active galactic nuclei.
spectra. The limited wavelength range of the study also plays a crucial role in this domain.

Another phenomenon in active galactic nuclei spectra is the presence of an additional non-stellar continuum which leads to the dilution of lines, i.e. the reduction of equivalent widths in comparison with those of normal galaxies. The effect of this non-stellar continuum can be estimated and equivalent widths can be corrected; but obviously, this estimation is also subject to errors. Finally, velocity dispersion in the galaxies broadens lines and is also a source of errors. Considering these facts, typical errors of 10 per cent are present in the equivalent widths of strong lines.

We did not take into account the errors in the equivalent width of the lines in the data base itself because they are supposed to be negligible compared with errors in the equivalent width of the lines from the galaxy. However, in Section B1.3 we provide the user with a test able to validate this hypothesis. If these errors were not negligible, one should not perform the synthesis.

4 INFORMATION CONTENT OF AN OBSERVATION

It is clear that if the synthetic domain $\mathcal{W}$ is entirely contained within the observational error $\mathcal{E}_\gamma$, the observation cannot discriminate, at the level $\gamma$, between the different stellar populations. All possible models that fall within $\mathcal{E}_\gamma$ must be considered as indistinguishable. In other words, the observation does not bear enough information to differentiate between various possible stellar populations of the galaxy. The size of the error ellipsoid $\mathcal{E}_\gamma$ is in some way the resolution at which we try to sort between the different models.

On the contrary, if the observation is so good that one can consider the ‘error bars’ to be null, the observation indeed conveys maximum information: $\mathcal{W}_{\text{obs}}$ must be synthesized by the data base. Under this extreme hypothesis, $\mathcal{E}_\gamma$ is reduced to the single point $\{\mathcal{W}_{\text{obs}}\}$ which has a zero measure in $\mathcal{W}$.

Following a suggestion of R. Barrett we define the information $I_\gamma$ brought by the observation as being a function of the measure of $\mathcal{E}_\gamma$ within $\mathcal{W}$. More precisely $I_\gamma$ will be a function of the probability $p_\gamma$ that the image by $\varphi$ of a point drawn at random from the a priori distribution of the stellar populations falls within the error ellipsoid. That is,

$$p_\gamma = \int_{\mathcal{E}_\gamma \cap \mathcal{W}} \pi(w) \, dw, \quad w = \varphi(k),$$

where $\pi$ is the a priori probability density function of the equivalent widths. We shall evaluate this $n_s$-dimensional integral by a Monte Carlo method (see Appendix A).

The probability $p_\gamma$ may be zero under two circumstances: (i) $\mathcal{W}_{\text{obs}}$ is within the synthetic domain and $\mathcal{E}_\gamma$ is reduced to $\{\mathcal{W}_{\text{obs}}\}$ only; (ii) the observation and its associated error domain are outside the synthetic domain: $\mathcal{E}_\gamma \cap \mathcal{W} = \emptyset$. In each case we have maximum information of different nature conveyed by the observation: (i) we know that the true stellar population lies in the solution set (provided that all stars present in the galaxy are also present in the data base); (ii) we know that the data base is incomplete, more stars must be added.

In a first approach, it seems reasonable to define the information brought by an observation by $I = 1 - p_\gamma$, i.e. it is the probability that a stellar population drawn at random from the simplex $S$ induces equivalent widths that do not fall within the error domain. By ‘at random’ we mean according to $\pi$, the a priori distribution of the equivalent widths. In practice we use the

Figure 1. Illustration of the error analysis for the extreme solution $k$. Around the observation $\mathcal{W}_{\text{obs}} = (4, 6)$ there is an error ellipsoid defined by a variance–covariance matrix $V$. Here this matrix is diagonal – the square roots of its diagonal elements (the standard deviations of the observations) are set to 10 per cent of $W_{\text{obs}}$. The synthetic domain is defined by a data base of five stars identical to those given in table 1 of Paper II. This observation and its error ellipsoid contain the information $I_\gamma = 0.92$ at the 1σ confidence level: $\gamma = 0.683$. 

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5 ERROR ANALYSIS IN PRACTICE

In this section, we limit ourselves to the practical results of the error analysis. We refer to Appendix B for all the computations needed to derive the various matrices that appear below.

The key parameter here is the number of stars necessary to define the solution (or the extreme solutions). In the overdetermined case \( n_s = n_k \), while in the underdetermined case \( n_s = n_k + 1 \) if the galaxy can be synthesized and \( n_s = n_k \) if it cannot. In both under- and overdetermined cases, it is less than or equal to \( n_k + 1 \). We have a regular case if \( n_s = n_k + 1 \) and a singular case if \( n_s < n_k + 1 \). We consider these two cases separately. In both cases, \( V \) stands for the variance–covariance matrix of the observations and \( s \) for the list of the indices of the stars retained in the solution.

5.1 Regular case \( n_s = n_k + 1 \)

Note that in this case the galaxy belongs to the synthetic domain. A solution \( k \) is any barycentric combination of \( n_k \) extreme solutions denoted by \( k_i \) (\( n_k \) may be equal to unity). At least \( n_s - (n_k + 1) \) components of \( k_i \) are equal to zero. The components of \( k_i \) are in addition subject to errors, as a result of the presence of errors in the data. In the tangent approximation (small errors), the variance–covariance matrix of the extreme solutions is a singular matrix given by

\[
V_k = K \begin{pmatrix} V & 0 \\ 0 & 0 \end{pmatrix} K^T, \quad K = W^{-1}.
\]

The elements of the matrix \( W \) are

\[
[W]_{ij} = (W_{obs} - W_{syn}) \frac{I_{j(i)}}{I_{syn}}, \quad j = 1, \ldots, n_s - 1,
\]

\[
= 1, \quad j = n_s,
\]

where \( s(i), i = 1, \ldots, n_s \), runs over the stars retained in the solution. The set of acceptable extreme solutions is an ellipsoid centred around the extreme solution \( k_i \). Its characteristic matrix \( P_s \) is given by

\[
P_s = W^T \begin{pmatrix} V^{-1} & 0 \\ 0 & 0 \end{pmatrix} W = J^T B.
\]

where \( J \) is an \((n_k + 1) \times (n_s + 1) \) diagonal matrix:

\[
[J]_{jj} = I_{syn}, \quad j = 1, \ldots, n_k,
\]

\[
[J]_{jj} = 1, \quad j = n_s + 1.
\]

Table 1. The extreme solutions and errors associated with the observation and data base illustrated in Fig. 1. Solution \( s \) is \( k_s \); \( \sigma k_s \) is the standard deviation vector associated with this solution. For the extreme solution \( 1 \), we also give \( \Delta = \sigma k_s \) in order to allow a direct comparison with Fig. 1. The parameter \( c_y \) determines the size of the error ellipsoids. We have \( c_y = \frac{[F_x^2 \gamma ]^{1/2}}{\gamma} \), e.g. with \( \gamma = 0.683 \) and \( n_k = 2 \) degrees of freedom one gets \( c_y = 1.515 \). The quantity \( \Delta \) is the difference between the maximum and the minimum attained by the stellar contributions of an observation that is constrained to move on the error ellipsoid. In spite of the non-linear nature of the problem illustrated here, it is clear from Fig. 1 that the error analysis under the tangent approximation is excellent.

| \( k_s \) | \( k_1 \) | \( k_2 \) | \( k_3 \) | \( k_4 \) | \( k_5 \) |
|---|---|---|---|---|---|
| \( k_i \) | 0.306 | 0.245 | 0.000 | 0.449 | 0.000 |
| \( \sigma k_1 \) | ±0.115 | ±0.094 | ±0.119 | ±0.119 |
| \( \Delta \) | 0.347 | 0.286 | 0.361 |
| \( k_2 \) | 0.491 | 0.000 | 0.218 | 0.291 | 0.000 |
| \( \sigma k_2 \) | ±0.094 | ±0.111 | ±0.124 |
| \( k_3 \) | 0.231 | 0.000 | 0.000 | 0.308 | 0.462 |
| \( \sigma k_3 \) | ±0.111 | ±0.115 | ±0.150 |

The set of acceptable solutions may be considered as the convex hull of all these acceptable extreme solutions.

We have illustrated in Fig. 1 the error analysis performed on an observation subject to errors of 10 per cent. The population synthesis was done with the same data base as used in Paper II. The results are given in Table 1. The \( k_s, s = 1, 2, 3 \), are the three extreme solutions; \( \sigma k_s \) is the standard deviation vector associated with the solution (it is the square root of the diagonal of \( V_k \)); and \( \Delta \) is the extreme range attained by the \( k_s \) by a point, which is constrained to move on the error ellipsoid. The analysis was done at the confidence level of 1σ, that is \( \gamma = 0.683 \).

5.1.1 Merit order among extreme solutions

The product of the non-zero eigenvalues of \( V_k \) is proportional to the surface of the ellipsoid \( K_{1\gamma} \). This quantity allows the extreme solutions to be sorted in order of merit, from the smallest surface (highest merit) to the greatest surface (smallest merit). In a synthesis with many extreme solutions it is advisable to retain only the solutions that possess the highest merit.

5.2 Singular case \( n_s < n_k + 1 \)

In the singular case, an approximate solution is sought by minimizing a distance from the observation to the synthetic domain. This distance is usually the elliptical distance \( D \), defined by equation (5), and it requires a positive definite matrix \( D \). However, we suppose below that \( D \) is the Euclidean distance through the variable transformation described in Appendix B2.5. The ellipse has been transformed into the unit circle and \( \Sigma = I \).

The error analysis is complicated by the fact that one must perform a projection on a plane that is tangent to the synthetic domain around the approximate solution. We describe step by step the operations that lead to the result.

Step A: First, construct the \( n_s \times n_k \) matrix \( \hat{A} \) of elements:

\[
[A]_{j(i)} = (W_{syn} - W_{j(i)}) I_{j(i)}.
\]

The index \( s(i) \) runs over the \( n_s \) stars defining the solution. We also need the diagonal matrix \( J_k = \text{diag}(I_{syn1}, \ldots, I_{synn_k}) \).

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The matrix $Q$ in the singular case we have $K$ blocks:

$$Q = \begin{pmatrix} \text{supplementary line of 'ones'} & \text{matrix } K \end{pmatrix},$$

and we can write $Q = (p^T q)$. The first block is formed by the $n_s - 1$ first columns of $Q$. An orthogonal projector $H = pp^T$ is constructed.

Step V: We define the matrix $B$ equal to $A$ with a supplementary line of 'ones' and the matrix $K = (B^T B)^{-1} B^T J$ where $J$ has already been defined [$J = \text{diag}(I_{\text{syn} 1}, \ldots, I_{\text{syn} n_s}, 1)$].

The variance–covariance matrix of the solution is $V_s = K \begin{pmatrix} HVH^T & 0 \\ 0 & 0 \end{pmatrix} K^T$.

Step P: We define the oblique projector $M$:

$$M = pp^T + qq^T V_p p^T p^T,$$

and compute $W = J^{-1} \hat{B}$. The matrix $P$ entering the definition of the acceptance zone in equation (7) is given by

$$P = W^T \begin{pmatrix} M^T V^T M & 0 \\ 0 & 0 \end{pmatrix} W, \quad W = J^{-1} \hat{B}.$$

Note that in the regular case we have $K = B^{-1} J$, and in the singular case we have $K = (B^T B)^{-1} B^T J$. Therefore $K$ is always the least-square solution of the linear system $BK = J$. (In both cases $B$ is constructed with $W_{\text{syn}}$ and the stars contributing to the synthesis.)

6 THE EXAMPLE OF NGC 3521

To illustrate our study we take, as an example, the clusters of Bica’s data base (see Bica 1988) and its galaxy S3 (NGC 3521). As our aim is to visualize the error zone, we shall use only two lines (i.e. $n_s = 2$) – this means two degrees of freedom for the error analysis. (Indeed our analysis is valid for any number of lines.) From the 35 clusters constituting the data base, we select according to Bica’s results the eight clusters (i.e. $n_s = 8$) contributing to the synthesis. We have chosen the two largest equivalent widths of the galaxy which correspond to the CaII K line ($\lambda_K = 3933$ Å) and the CH G band ($\lambda_H = 4301$ Å); the reason for this choice is that the relative errors on the strongest lines are generally the smallest. Typical errors on such equivalent widths are in the order of 10 per cent, but for the sake of argument, we take an error of only 3 per cent. We also assume that there is no correlation between equivalent width errors ($\rho = 0$) even if this is probably not the case in reality.

Fig. 2 shows that the galaxy can be synthesized exactly. Our method gives 16 different extreme solutions. Table B1 shows these several extreme solutions $k_s$ where $s = 1, \ldots, 16$; also shown are the standard deviation vectors $\sigma k_s$ corresponding to $1\sigma$ confidence level, and the standard deviation $\sigma k_s$ taking into account a 1 per cent error in the data base. The solutions are sorted by increasing order of merit (i.e. surface$^{-1}$).

Fig. 2 demonstrates clearly the impact of the synthetic domain structure $D$ on the solution errors. Indeed, the clusters constituting the data base are nearly aligned in $W$-space and their continuum intensities are such that the synthetic domain is compressed (i.e. the lines joining the clusters are very close and nearly parallel to...
each other). As a consequence, large errors are present in the extreme solutions (see also Fig. 3). It is important to bear this situation in mind when a data base of clusters (or stars) is chosen. Ideally the resolution at which the equivalent width space is sampled should be adapted to the quality of the observations. Better observations allow a finer coverage of the $W$-space, i.e. more clusters (or stars) may be added. We see in Table B1 that the contribution of data base errors to the solution errors is negligible. Finally, the best solution (as defined in Section 5.1.1) is solution 1; solutions 1, 4 and 11 are the three solutions among the 16 extreme solutions that agree well with Bica’s solution (see $k_{Bica}$ in Table B1). This result is very satisfying, because we used minimal information by considering only two equivalent widths.

7 CONCLUSION

We provide explicit formulae to perform a complete error analysis on stellar population synthesis by means of a data base. The hypothesis underlying the results is that errors on the data base itself are negligible compared with errors on the observed galaxy. The method also supposes that the errors are reasonably Gaussian and further demands knowledge of the error matrix (the variance–covariance matrix) of the observed equivalent widths. The results provided are: (i) the variance–covariance matrix of the extreme solutions (regular case) or of the approximate solution (singular case); (ii) the matrix defining a zone in the solution space where the stellar populations are indistinguishable at a confidence level $\gamma$.

We also introduced information contained in an observation with respect to the problem to be solved. This information is evaluated by a Monte Carlo method using as input the a priori knowledge about the type 0 and further demands knowledge of the error matrix (the variance–covariance matrix) of the observed equivalent widths. The transformation

\[ f_{n*}(k_1, \ldots, k_{n*}) = \prod_{i=1}^{n*} f(k_i) = \exp\left(-\sum_{i=1}^{n*} k_i\right) \]

and is constant on \(\sum_{i=1}^{n*} k_i = a\). The conditional density on \(\sum_{i=1}^{n*} k_i = a\) is therefore uniform for any $a > 0$, in particular for $a = 1$.

Now the random variable

\[ U_i = \int_0^{k_i} f(k) \, dk = 1 - \exp(-K_i) \]

is uniformly distributed on $0 \leq u_i < 1$ so, $K_i = -\ln(1 - U_i)$ or equivalently $K_i = -\ln(U_i)$ is exponentially distributed. In conclusion, the mapping $\psi$ defined by

\[ k_i = -\ln(u_i), \quad i = 1, \ldots, n*, \quad 0 < u_i \leq 1, \]

(A1)

ensures (i) $k_i \geq 0$; (ii) a uniform coverage of the $k_i$ domain; and (iii) that $u_i$ is only subject to simple bounds constraints $0 \leq u_i \leq 1$, $i = 1, \ldots, n*$.

The only problem with this method is that we use $n*$ parameters while only $n* - 1$ are necessary. The search algorithm may lose time exploring those lines in $u$ space where $W_{syn}$ does not change because the $k_i$ differ only by a scaling factor. We thus designed ‘method 2’ in order to solve this problem.

A2 Method 2

Here we want to map the $k_i$ using only $n* - 1$ parameters of type $u_i$. Again the $K_i$ are exponentially distributed as in ‘method 1’; this ensures, as shown above, that the density is uniform on \(\sum_{i=1}^{n*} k_i = 1\).

We now introduce the new variables $Q_i$. For the sake of argument we limit ourselves to an $n* = 4$ example, but it should

\[ Q_i = \frac{k_i}{\sum_{i=1}^{n*} k_i}, \quad i = 1, \ldots, n* \]

\[ Q_n = 1 - \sum_{i=1}^{n-1} Q_i \]

The transformation $\psi$ allows a simplification of the constraints $k_i \geq 0$ subject to $\sum_{i=1}^{n*} k_i = 1$ (or $k_i \leq 1$) through the mapping $k = \phi(u)$ of the variables $u_i$ subject to simple bounds constraints of the type $0 \leq u_i \leq 1$. At the same time the uniform coverage of the hyper-tetrahedron $S$ permits evaluation of the information integral (8).

We also want the change of variables $\psi$ to be continuous and twice derivable, so that $\psi$ can be used in an optimization program where the variables are subject to the constraints $k_i \in S$ as needed in Section 2.3.

One can think of several ways to map $k = \phi(u)$, but if the transformation is not chosen carefully there is a risk that $\psi$ preferentially selects certain zones of the $k$ parameter space. In order to avoid this possible bias, we would like to find a change of variable ensuring that a uniform coverage of the $u$ space (the cube) transforms to a uniform coverage of the $k$ space (the tetrahedron). We found two methods satisfying these requirements.

A1 Method 1

Let us consider the $n*$ independent random variables $K_i$, all following the same exponential distribution. This distribution is, for $k \geq 0$, a probability density function: $f(k) = \exp(-k)$. The joint distribution of the multiplet $(K_1, \ldots, K_{n*})$ has the density

\[ f_{n*}(k_1, \ldots, k_{n*}) = \prod_{i=1}^{n*} f(k_i) = \exp\left(-\sum_{i=1}^{n*} k_i\right) \]

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APPENDIX A: UNIFORM MAPPING OF A SIMPLEX

In this appendix we show how to transform a hyper-cube into a hyper-tetrahedron. This operation is continuous and transforms a uniform density on the hyper-cube into a density equally uniform on the hyper-tetrahedron.

Let us consider the $k_1, \ldots, k_{n*}$ subject to $\sum_{i=1}^{n*} k_i = 1$ (or $k_i \leq 1$) through the mapping $k = \phi(u)$ of the variables $u_i$ subject to simple bounds constraints of the type $0 \leq u_i \leq 1$. At the same time the uniform coverage of the hyper-tetrahedron $S$ permits evaluation of the information integral (8).

We also want the change of variables $\psi$ to be continuous and twice derivable, so that $\psi$ can be used in an optimization program where the variables are subject to the constraints $k_i \in S$ as needed in Section 2.3.

One can think of several ways to map $k = \phi(u)$, but if the transformation is not chosen carefully there is a risk that $\psi$ prefersentially selects certain zones of the $k$ parameter space. In order to avoid this possible bias, we would like to find a change of variable ensuring that a uniform coverage of the $u$ space (the cube) transforms to a uniform coverage of the $k$ space (the tetrahedron). We found two methods satisfying these requirements.

A1 Method 1

Let us consider the $n*$ independent random variables $K_i$, all following the same exponential distribution. This distribution is, for $k \geq 0$, a probability density function: $f(k) = \exp(-k)$. The joint distribution of the multiplet $(K_1, \ldots, K_{n*})$ has the density

\[ f_{n*}(k_1, \ldots, k_{n*}) = \prod_{i=1}^{n*} f(k_i) = \exp\left(-\sum_{i=1}^{n*} k_i\right) \]

and is constant on $\sum_{i=1}^{n*} k_i = a$. The conditional density on $\sum_{i=1}^{n*} k_i = a$ is therefore uniform for any $a > 0$, in particular for $a = 1$.

Now the random variable

\[ U_i = \int_0^{k_i} f(k) \, dk = 1 - \exp(-K_i) \]

is uniformly distributed on $0 \leq u_i < 1$ so, $K_i = -\ln(1 - U_i)$ or equivalently $K_i = -\ln(U_i)$ is exponentially distributed. In conclusion, the mapping $\psi$ defined by

\[ k_i = -\ln(u_i), \quad i = 1, \ldots, n*, \quad 0 < u_i \leq 1, \]

(A1)

ensures (i) $k_i \geq 0$; (ii) a uniform coverage of the $k_i$ domain; and (iii) that $u_i$ is only subject to simple bounds constraints $0 \leq u_i \leq 1$, $i = 1, \ldots, n*$.

The only problem with this method is that we use $n*$ parameters while only $n* - 1$ are necessary. The search algorithm may lose time exploring those lines in $u$ space where $W_{syn}$ does not change because the $k_i$ differ only by a scaling factor. We thus designed ‘method 2’ in order to solve this problem.

A2 Method 2

Here we want to map the $k_i$ using only $n* - 1$ parameters of type $u_i$. Again the $K_i$ are exponentially distributed as in ‘method 1’; this ensures, as shown above, that the density is uniform on \(\sum_{i=1}^{n*} k_i = 1\).

We now introduce the new variables $Q_i$. For the sake of argument we limit ourselves to an $n* = 4$ example, but it should
be clear that the method works for any $n_+ > 0$. We define
\[ Q_1 = K_4 + K_3 + K_2 + K_1, \quad 0 \leq Q_1 < \infty; \]
\[ Q_2, Q_3 = K_4 + K_3 + K_2, \quad 0 \leq Q_2, Q_3 \leq 1; \]
\[ Q_4 = K_4 + K_3, \quad 0 \leq Q_4 \leq 1. \]

The Jacobian of this change of variables,
\[ J_4 = \frac{\partial(k_1, \ldots, k_4)}{\partial(q_1, \ldots, q_4)}, \]
is given by $J_4 = q_1^3 q_2^2 q_3$. The four values ($Q_1, Q_2, Q_3, Q_4$) have the density
\[ f(q_1, q_2, q_3, q_4) = \exp(-q_1) q_1^3 q_2^2 q_3. \quad (A2) \]

This demonstrates that the $Q_i$ are independent and have densities
\[ f_1(q_1) = \frac{1}{3!} q_1^3 e^{-q_1}, \quad 0 \leq q_1 < \infty; \]
\[ f_2(q_2) = 2q_2^2, \quad 0 \leq q_2 < 1; \]
\[ f_3(q_3) = 2q_3, \quad 0 \leq q_3 < 1; \]
\[ f_4(q_4) = 1, \quad 0 \leq q_4 < 1. \quad (A3) \]

The variable $Q_1$ follows a gamma distribution (as required for a sum of independent exponential random variables) and the other variables follow a power distribution of decreasing index, the last one being uniform.

Now if $Q_1$ is given, say $Q_1 = \sum_{i=1}^{n_+} K_i = 1$, the remaining $Q_2, Q_3$ and $Q_4$ cover uniformly (because the $K_i$ are exponential) the hyper-tetrahedron defined by equation (2). We have
\[ K_4 = Q_2 Q_3 Q_4, \]
\[ K_3 = (1 - Q_3) Q_4, \]
\[ K_2 = (1 - Q_2) Q_4, \]
\[ K_1 = 1 - Q_2. \quad (A4) \]

Finally if we define
\[ U_n = \int_0^{Q_{n-1}} q^{n-1} dq = Q_n, \quad (A5) \]
for $n = 1, \ldots, n_+ - 1$, the variables $U_n$ are uniform and independent. We then have a power distribution of index $n$: $Q_{n-1} = U_n^{1/n}$ (for $n = 1, \ldots, n_+ - 1$) when $U_n$ is uniformly distributed in $[0,1]$. Therefore the change of variables $\psi$:
\[ k_4 = u_{1/2} u_2^{1/3}; \]
\[ k_3 = (1 - u_1) u_2^{1/3}; \]
\[ k_2 = (1 - u_2^{1/3}); \]
\[ k_1 = 1 - u_1^{1/3}, \quad (A6) \]
maps the $k$ space uniformly if $u_1, u_2, u_3$ are drawn from three independent random variables $U_1, U_2, U_3$ uniformly distributed in $[0,1]$. Now for any $n_+ > 1$, $\psi$ is defined by
\[ k_1 = 1 - u_{1/(n_+ - 1)}^{1/(n_+ - 1)}; \]
\[ k_{n_+} = \prod_{i=1}^{n_+ - 1} u_i^{1/i}, \quad (A7) \]
and for $n = 2, \ldots, n_+ - 1$:
\[ k_n = [1 - u_{n_+ - n}^{1/(n_+ - n)}] \prod_{i=n_+ - n+1}^{n_+ - 1} u_i^{1/i}, \quad (A8) \]
where all $u_i$ are subject to the constraint $0 \leq u_i < 1$. We present in Fig. A1 an example of such a mapping for $n_+ = 3$.

### APPENDIX B: COMPUTATIONS NEEDED FOR THE ERROR ANALYSIS

We would like to establish a relationship between a small variation $dW$ around $W_{\text{obs}}$ and the resulting variation $dk$ around the solution $k$. The variation $dk$ is constrained to $\sum_{i=1}^{n_+} dk_i = 0$ by $\sum_{i=1}^{n_+} k_i = 1$.

#### B1 The galaxy can be synthesized

$W_{\text{obs}}$ belongs to the synthetic domain ($W_{\text{obs}} \in W$) if the galaxy can be synthesized and the many solutions are contained within the convex hull of a set of extreme solutions (see Paper II). An extreme solution has by definition at least $n_+ - (n_+ + 1)$ components $k_i$ equal to zero; what remains is the evaluation of $n_+ + 1$ components of $k$.

#### B1.1 Error analysis of the extreme solutions

We discard the stars with zero contribution and set $n_+ = n_+$ (recall that $n_+ = n_+ + 1$). This allows us to keep the same notation. Note that the new matrix $A$ is formed of the $n_+ + 1$ columns of the original matrix in system (4) corresponding to the stars that have not been set to zero. In the same way $\varphi$ stands here for the original $\varphi$ restricted to these stars.

By adding the line $b^T$ to $A$ we form an $(n_+ + 1) \times (n_+ + 1)$ matrix $B$, and $B^{-1}$ exists, because the problem has an (extreme) solution. We have
\[ k = B^{-1} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad B = \begin{pmatrix} A \\ b^T \end{pmatrix}. \quad (B1) \]

From here we have $dBk + B\; dk = 0$, the matrix $dB$ is $dA$ supplemented with a line of zeros. We have $dA_{ji} = dw_j / \partial y_i$ and

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Table B1. The Bica solution and our 16 extreme solutions of galaxy NGC 3521 synthesis using as data base the eight clusters (2–7, 9, 15) retained by E. Bica in his synthesis. Under column $k_i$ is the contribution to the galactic luminosity of cluster number $i$; $\sigma k_i$ ($s = 1, 2, \ldots, 16$) is the standard deviation corresponding to the extreme solution $k_s$, assuming only errors on galactic data and $\sigma' k_s$ is the standard deviation corresponding to the same extreme solution taking into account errors in the data base. Finally, ‘Surface’ is the value of the ellipsoid’s surface for each extreme solution. The solutions are sorted according to a decreasing order of merit (increasing order of surface).

|     | $k_2$ | $k_3$ | $k_4$ | $k_5$ | $k_6$ | $k_7$ | $k_8$ | $k_9$ | $k_{10}$ | $k_{11}$ | $k_{12}$ | $k_{13}$ | $k_{14}$ | $k_{15}$ | Surface |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|----------|----------|----------|----------|----------|----------|---------|
| $k_{\text{Bica}}$ | 0.510 | 0.090 | 0.080 | 0.070 | 0.060 | 0.050 | 0.050 | 0.080 | 0.060 | 6.462 x 10^{-5} |
| $k_1$ | 0.561 | 0.000 | 0.000 | 0.000 | 0.000 | 0.091 | 0.000 | 0.348 | 0.407 | 7.779 x 10^{-5} |
| $\sigma k_1$ | ±0.334 | ±0.067 | ±0.069 | ±0.418 | |
| $\sigma' k_1$ | ±0.353 | ±0.474 | ±0.498 | ±0.520 | |
| $k_2$ | 0.000 | 0.875 | 0.000 | 0.000 | 0.000 | 0.075 | 0.000 | 0.050 | 8.759 x 10^{-5} |
| $\sigma k_2$ | ±0.454 | ±0.048 | ±0.050 | ±0.520 | |
| $\sigma' k_2$ | ±0.474 | ±0.520 | ±0.520 | ±0.520 | |
| $k_3$ | 0.390 | 0.000 | 0.601 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 2.085 x 10^{-4} |
| $\sigma k_3$ | ±0.451 | ±0.581 | ±0.132 | ±0.136 | |
| $\sigma' k_3$ | ±0.463 | ±0.598 | ±0.136 | ±0.136 | |
| $k_4$ | 0.570 | 0.000 | 0.000 | 0.000 | 0.000 | 0.146 | 0.000 | 0.284 | 1.456 x 10^{-4} |
| $\sigma k_4$ | ±0.339 | ±0.104 | ±0.106 | ±0.438 | |
| $\sigma' k_4$ | ±0.347 | ±0.448 | ±0.448 | ±0.448 | |
| $k_5$ | 0.000 | 0.868 | 0.000 | 0.086 | 0.000 | 0.046 | 0.000 | 0.000 | 2.121 x 10^{-4} |
| $\sigma k_5$ | ±0.515 | ±0.842 | ±0.328 | ±0.343 | |
| $\sigma' k_5$ | ±0.538 | ±0.880 | ±0.343 | ±0.343 | |
| $k_6$ | 0.267 | 0.000 | 0.000 | 0.000 | 0.000 | 0.165 | 0.568 | 0.000 | 2.121 x 10^{-4} |
| $\sigma k_6$ | ±0.724 | ±0.032 | ±0.700 | ±0.723 | |
| $\sigma' k_6$ | ±0.748 | ±0.723 | ±0.723 | ±0.723 | |
| $k_7$ | 0.000 | 0.885 | 0.000 | 0.000 | 0.105 | 0.010 | 0.000 | 0.000 | 3.098 x 10^{-4} |
| $\sigma k_7$ | ±0.345 | ±1.029 | ±0.684 | ±0.717 | |
| $\sigma' k_7$ | ±0.361 | ±1.077 | ±0.717 | ±0.717 | |
| $k_8$ | 0.366 | 0.000 | 0.000 | 0.000 | 0.231 | 0.000 | 0.403 | 0.000 | 3.162 x 10^{-4} |
| $\sigma k_8$ | ±0.664 | ±0.042 | ±0.633 | ±0.648 | |
| $\sigma' k_8$ | ±0.680 | ±0.043 | ±0.648 | ±0.648 | |
| $k_9$ | 0.395 | 0.000 | 0.589 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 3.261 x 10^{-4} |
| $\sigma k_9$ | ±0.520 | ±0.773 | ±0.255 | ±0.262 | |
| $\sigma' k_9$ | ±0.535 | ±0.795 | ±0.262 | ±0.262 | |
| $k_{10}$ | 0.000 | 0.824 | 0.116 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 3.769 x 10^{-4} |
| $\sigma k_{10}$ | ±0.944 | ±1.133 | ±0.190 | ±0.198 | |
| $\sigma' k_{10}$ | ±0.983 | ±1.179 | ±0.198 | ±0.198 | |
| $k_{11}$ | 0.546 | 0.000 | 0.000 | 0.268 | 0.000 | 0.000 | 0.000 | 0.186 | 3.986 x 10^{-4} |
| $\sigma k_{11}$ | ±0.308 | ±0.180 | ±0.480 | ±0.490 | |
| $\sigma' k_{11}$ | ±0.315 | ±0.183 | ±0.490 | ±0.490 | |
| $k_{12}$ | 0.428 | 0.000 | 0.000 | 0.352 | 0.000 | 0.000 | 0.000 | 0.220 | 5.458 x 10^{-4} |
| $\sigma k_{12}$ | ±0.609 | ±0.060 | ±0.564 | ±0.576 | |
| $\sigma' k_{12}$ | ±0.621 | ±0.061 | ±0.576 | ±0.576 | |
| $k_{13}$ | 0.014 | 0.864 | 0.000 | 0.000 | 0.122 | 0.000 | 0.000 | 0.000 | 6.746 x 10^{-4} |
| $\sigma k_{13}$ | ±1.010 | ±1.124 | ±0.117 | ±0.122 | |
| $\sigma' k_{13}$ | ±1.055 | ±1.174 | ±0.122 | ±0.122 | |
| $k_{14}$ | 0.000 | 0.756 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 8.087 x 10^{-4} |
| $\sigma k_{14}$ | ±1.174 | ±0.178 | ±1.538 | ±1.589 | |
| $\sigma' k_{14}$ | ±1.771 | ±1.83 | ±1.589 | ±1.589 | |
| $k_{15}$ | 0.401 | 0.000 | 0.556 | 0.044 | 0.000 | 0.000 | 0.000 | 0.000 | 2.269 x 10^{-3} |
| $\sigma k_{15}$ | ±0.611 | ±1.281 | ±0.671 | ±0.689 | |
| $\sigma' k_{15}$ | ±0.627 | ±1.315 | ±0.689 | ±0.689 | |
| $k_{16}$ | 0.162 | 0.601 | 0.000 | 0.236 | 0.000 | 0.000 | 0.000 | 0.000 | 2.604 x 10^{-3} |
| $\sigma k_{16}$ | ±1.154 | ±1.379 | ±0.228 | ±0.234 | |
| $\sigma' k_{16}$ | ±1.184 | ±1.414 | ±0.234 | ±0.234 | |
Error analysis for stellar population synthesis

At the level $B_1$, the acceptance region of the extreme solutions 

\[ B_{1, \text{syn}} \] 

can be expressed by

\[ \mathcal{K}_{\gamma} = \{ k' \mid \mathbf{W}^{-1} \mathbf{V}^{-1} (\mathbf{V} - k) \leq F^{-1}_{\chi^2}(\gamma) \}, \]

where we have set $\mathbf{W} = \mathbf{V} - k$. The above expression is equivalent to

\[ \mathcal{K}_{\gamma} = \{ k' \mid (\mathbf{dW})^T \mathbf{V}^{-1} \mathbf{dW} \leq F^{-1}_{\chi^2}(\gamma) \}. \]

The choice of the extra elements in the central matrix is arbitrary. We chose zero for simplicity. We can now use equation (B3) and write

\[ \mathcal{K}_{\gamma} = \{ k' \mid (\mathbf{dW})^T \mathbf{V}^{-1} \mathbf{dW} \leq F^{-1}_{\chi^2}(\gamma) \}. \]

Therefore,

\[ \mathbf{P} = \mathbf{W}^T \left( \begin{array}{cc} \mathbf{V}^{-1} & 0 \\ 0 & 0^T \end{array} \right) \mathbf{W}. \]

B1.3 Contributions to errors coming from stellar library

Let us call $\mathbf{J}_W$ and $\mathbf{J}_B$ the diagonal matrices such that for $j = 1, \ldots, n_s$ we have $[\mathbf{J}_W]_{jj} = I_{j, k_i}$ and $[\mathbf{J}_B]_{jj} = (\mathbf{W}_{\text{syn}} - \mathbf{W}_j)k_i$. In addition we have for $j = n_s + 1$ that $[\mathbf{J}_W]_{jj} = [\mathbf{J}_B]_{jj} = 1$. Define further $\mathbf{K}_W = \mathbf{B}^{-1} \mathbf{J}_W$ and $\mathbf{K}_B = \mathbf{B}^{-1} \mathbf{J}_B$. Following the same reasoning as in Section B1.1 we find that the contribution of the stellar library to the total variance–covariance matrix of a solution is

\[ \mathbf{V}_{k(i)} = \sum_{j=1}^{n_s+1} \left( \mathbf{K}_W \left( \begin{array}{c} \mathbf{V}_W \\ 0^T \end{array} \right) \mathbf{K}_W^T + \mathbf{K}_B \left( \begin{array}{c} \mathbf{V}_B \\ 0^T \end{array} \right) \mathbf{K}_B^T \right), \]

where $\mathbf{V}_W$ and $\mathbf{V}_B$ are the variance–covariance matrices of the $W_j$ and $B_j$ of star $i$. A comparison of $\mathbf{V}_{k(i)}$ and $\mathbf{V}_k$ is able to tell if the errors introduced by the stellar library are negligible relative to the errors on the observed galaxy.

B2 The galaxy cannot be synthesized

An approximate solution $\mathbf{W}_{\text{syn}}$ is found if the galaxy cannot be synthesized. A manifold of solutions is defined by a number of stars $n_s$ less than or equal to the number of equivalent widths. Here we distinguish $n_s$ from the $n_s$ number of stars in the data base. This manifold is called the synthetic ‘surface’ in Paper I.

B2.1 Projector on the tangent plane

If the observational errors $\mathbf{dW}_{\text{obs}}$ are small around $\mathbf{W}_{\text{obs}}$, we can expect small deviations $\mathbf{dW}_{\text{syn}}$ around $\mathbf{W}_{\text{syn}}$. In this context, we can approximate the synthetic surface by a plane tangent to this surface at $\mathbf{W}_{\text{syn}}$. The results obtained in equation (B1) can be applied to $\mathbf{W}_{\text{syn}}$ since, by definition, $\mathbf{W}_{\text{syn}}$ belongs to the synthetic domain. In this context let $\mathbf{A}$ and $\mathbf{B}$ stand for the matrices $\mathbf{A}$ and $\mathbf{B}$, where $\mathbf{W}_{\text{obs}}$ have been replaced by $\mathbf{W}_{\text{syn}}$. By equation (B2) $\mathbf{W}_{\text{syn}} + \mathbf{dW}_{\text{syn}}$ belongs to the tangent plane if the $\mathbf{dW}$ are such that

\[ \begin{bmatrix} \mathbf{dW}_{\text{syn}} \\ 0 \end{bmatrix} = -\mathbf{J}^{-1} \mathbf{B} \mathbf{dW} \quad \text{or} \quad \mathbf{dW}_{\text{syn}} = -\mathbf{J}^{-1} \mathbf{A} \mathbf{dW}. \]

\[ \begin{bmatrix} \mathbf{dW}_{\text{syn}} \\ 0 \end{bmatrix} = -\mathbf{J}^{-1} \mathbf{B} \mathbf{dW} \quad \text{or} \quad \mathbf{dW}_{\text{syn}} = -\mathbf{J}^{-1} \mathbf{A} \mathbf{dW}. \]
with $J_\kappa = \text{diag}(I_{n_1}, \ldots, I_{n_n})$. This means that $dW_{\text{syn}}$ belongs to the linear hull of the columns of $J_\kappa^T A$ provided that $\sum d_k = 0$. We maintain that $dW_{\text{syn}}$ belongs to this linear hull even if $\sum d_k \neq 0$.

In fact $\sum d_k = 0$ is the equation of a hyperplane $\Sigma_0$ orthogonal to the subspace of dimension 1 generated by e.g. the vector $(1, \ldots, 1)$. The hyperplane $\Sigma_0$ is itself a subspace since it includes the origin; therefore any vector $d_k$ is the sum of a vector $d_k \in \Sigma_0$ plus a vector $v \notin \Sigma_0$. By construction the solution $k \notin \Sigma_0$ since $\sum d_k = 1$, then $d_k$ can be written $d_k = d_k + \alpha \kappa$, where $\alpha \kappa$ is a scalar. Now we have

$$J^{-1} \hat{B} d_k = J^{-1} B (d_k + \alpha \kappa),$$

$$= J^{-1} B d_k + \alpha \kappa J^{-1} B \kappa,$$

$$= \left( \begin{array}{c} dW_{\text{syn}} \\ \alpha \kappa \end{array} \right).$$

Therefore $dW_{\text{syn}}$ belongs to the linear hull of the columns of $G = J_\kappa^{-1} A$, i.e. it belongs to the range of $G$.

The range of $G$ is obtained by the rank deficiency QR algorithm (see Golub & Van Loan 1996, chapter 5, section 5.4.1). According to this algorithm it is possible to write, after a permutation $\Pi$, $G_\Pi = QR$. The array $Q$ is an $n_3 \times n_\lambda$ matrix. The first $n_3 - 1$ columns of $Q$ span the range of $G$ (i.e. they are an orthonormal basis of the tangent plane) and the remaining columns span the subspace orthonormal to it. If, following this partition, we write $Q = (p|q)$, one can construct the orthogonal projector $H$ on the tangent plane; we have

$$H = pp^T.$$

The projector $H$ is an $n_3 \times n_\lambda$ matrix of rank $n_3 - 1$.

### B2.2 Least-squares solution of the linearized problem

One obtains $W_{\text{syn}}' = W_{\text{syn}} + dW_{\text{syn}}$ from $W_{\text{obs}}' = W_{\text{obs}} + dW_{\text{obs}}$ by minimizing a ‘distance’ between these $W_{\text{syn}}'$ and $W_{\text{obs}}'$. This distance is usually defined as a positive definite quadratic form; therefore the correction $dW_{\text{syn}}$ is implicitly defined by

$$(W_{\text{obs}}' - W_{\text{syn}}') \Sigma^{-1} (W_{\text{obs}}' - W_{\text{syn}}') = \min_{W}(W_{\text{obs}}' - W_{\text{obs}}') \Sigma^{-1} (W_{\text{obs}}' - W_{\text{obs}}').$$

Via a change of variables, one can describe the ‘weight’ matrix $\Sigma^{-1}$ by the identity matrix (see Section B2.5). We hereafter consider that $\Sigma^{-1} = I$, then the synthesis is obtained by the orthogonal projection of $W_{\text{obs}}$ on the synthetic surface, i.e. using $H$. Consequently one obtains $W_{\text{syn}}'$ by adding $dW_{\text{syn}} = H (W_{\text{obs}}' - W_{\text{syn}})$ to $W_{\text{syn}}$. Taking into account that $H (W_{\text{obs}}' - W_{\text{syn}}) = 0$ we obtain

$$dW_{\text{syn}} = H dW_{\text{obs}}.$$

### B2.3 Variance–covariance matrix of $k$

The second step is to find a relation between $dW_{\text{syn}}$ and $d\kappa$, where $d\kappa$ is restricted to the $n_3$ stars that contribute to the synthesis. Since, by definition $W_{\text{syn}} \in W'$, the overdetermined system $B \kappa = (0 \ 1)^T$ possesses an exact solution in the least-squares sense. Therefore $k$ is also the solution of the invertible square system $B^T B \kappa = B^T (0 \ 1)^T$. In this linear analysis, the perturbed $W_{\text{syn}}$ is close to the synthetic surface and the normalization constraint $b^T k = 1$ is approximately satisfied. It follows that $\hat{B}^T dB k + B^T B \kappa = 0$. Again $dB \kappa$ is given by equation (B2), where $J$ is the diagonal matrix of the synthetic continua $J = \text{diag} (I_{n_1}, \ldots, I_{n_n}, 1)$. This leads to

$$d\kappa = -(\hat{B}^T \hat{B})^{-1} \hat{B}^T dW_{\text{syn}}.$$  (B8)

Note that $\hat{B}$ being of full column rank, the expression $(\hat{B}^T \hat{B})^{-1} \hat{B}^T$ is equal to $\hat{B}^T (\hat{B}^T \hat{B})^{-1}$, the Moore–Penrose pseudo-inverse of $\hat{B}$ (for a definition see e.g. Harville 1997, chapter 20.1). Let us define here $K = (\hat{B}^T \hat{B})^{-1} \hat{B}^T J$, and recalling that $dW_{\text{syn}} = H dW_{\text{obs}}$ we obtain the variance–covariance matrix of the synthesis:

$$V \hat{\kappa} = K \left( \begin{array}{cc} HH^T & 0 \\ 0 & 0 \end{array} \right) K^T,$$  (B9)

where $V = (dW_{\text{obs}} dW_{\text{obs}}^T)$ is the variance–covariance matrix of the observations.

### B2.4 Acceptance region of the least-squares solutions

An alternative solution $k'$ is considered acceptable, at the level $\gamma$, if there exists a $W_{\text{obs}}'$ within the ‘error’ region $\gamma$ around $W_{\text{obs}}$ such that $H (W_{\text{obs}}' - W_{\text{syn}}') = \varphi (k')$. According to this definition, $k'$ is acceptable if it belongs to the following set:

$$\gamma = \{ k' | dW_{\text{obs}} V^{-1} dW_{\text{obs}} < F_{\chi^2}(\gamma) \},$$

$$H dW_{\text{obs}} = dW_{\text{syn}} = \varphi (k') - \varphi (k),$$  (B10)

where $V$ is the variance–covariance matrix of the observational errors.

Among all the solutions of $H dW_{\text{obs}} = dW_{\text{syn}}$ we choose the one which is ‘closest’ to $W_{\text{obs}}$ in the $V^{-1}$ norm. This ensures that the solution is within $\gamma$. The minimum of $dW_{\text{obs}} V^{-1} dW_{\text{obs}}$, which satisfies the constraint $H dW_{\text{obs}} = dW_{\text{syn}}$ is given by

$$dW_{\text{obs}} = M dW_{\text{syn}},$$

where

$$M = pp^T + q(p^T V p)^{-1} p^T.$$

The matrix $M$ is an oblique projector on the regression plane defined by the constraint. We indeed have

$$\left( \begin{array}{c} dW_{\text{obs}} \\ 0 \end{array} \right) = \left( \begin{array}{c} M dW_{\text{syn}} \\ 0 \end{array} \right).$$  (B11)

One cannot invert equation (B8) in order to introduce $d\kappa$, but we can use equation (B5) since $K_{\gamma}$ is in the set where $\sum d_k = 0$:

$$dW_{\text{syn}} = -J^{-1} B d\kappa.$$  (B12)

Combining equations (B12) and (B11) and proceeding like in Section B1.2, we find

$$K_{\gamma} = [k' (k' - k)^T P(k' - k)] \leq F_{\chi^2}(\gamma),$$  (B13)

where

$$P = W^T \left( \begin{array}{cc} M & 0 \\ 0 & 0 \end{array} \right) W,$$  (B14)

We consider now the case where the distance between two points...
of the W-space is not the Euclidean distance but an elliptical distance. This elliptical distance is subordinated to a symmetric definite positive matrix $\Sigma$. We have $d_2(W_1, W_2) = (W_1 - W_2)^T \Sigma^{-1} (W_1 - W_2)$. Usually one chooses $\Sigma$ equal to $V$, the variance–covariance matrix of the data, but it may not be always the case.

A substitution of variables transforms the elliptical distance into a spherical (i.e. Euclidean) one. We want in other words that $d(W_1, W_2) = \hat{d}(W_1, W_2)$, where $d$ is the Euclidean distance. If $W_0$ stands for the original variables and $W$ for the new variables, we define the matrix $N$ by $W_0 = NW$. It now follows that

$$d(W_1, W_2) = (W_1 - W_2)^T N \Sigma^{-1} N (W_1 - W_2).$$

This imposes the condition $N^T \Sigma^{-1} N = I$, which is satisfied if we choose $N$ as the matrix appearing in the Choleski factorization of $\Sigma$ (see Golub & Van Loan 1996, section 4.2.1). We have $\Sigma = NN^T$, where $N$ is lower triangular. It is straightforward to verify that $N$ satisfies the condition.

Finally we need to compute the variance–covariance matrix $V$ appearing in equations (B9) and (B14) from the variance–covariance matrix $V_0$ of the original variables. We have $V = (dW dW^T) = N^{-1} (dW_0 dW_0^T) N^{-1 T}$, and therefore

$$V = N^{-1} V_0 N^{-1 T}. \quad (B15)$$

This paper has been typeset from a \TeX/LaTeX file prepared by the author.