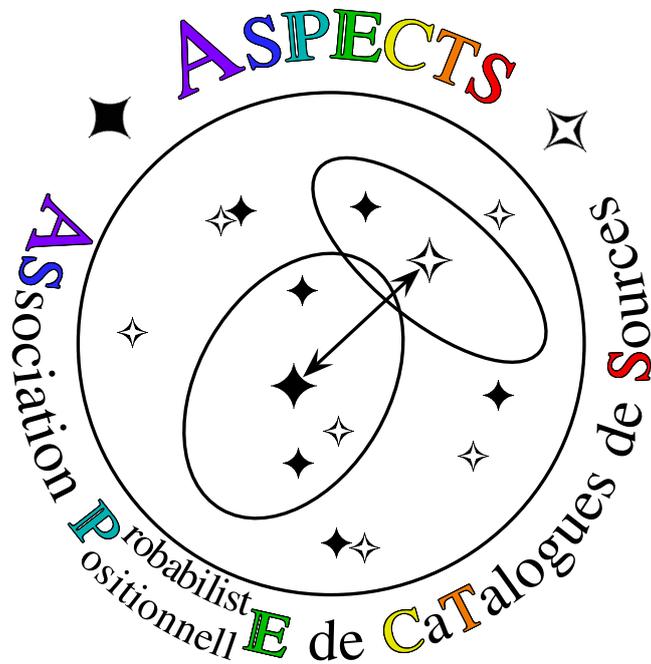


# The ASPECTS code for probabilistic cross-identification of astrophysical sources

Version 2.0.1, 2014-4-29

[«www2.iap.fr/users/fioc/Aspects/v2.0/»](http://www2.iap.fr/users/fioc/Aspects/v2.0/)



## Documentation and complements

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# Documentation

## I. Introduction

ASPECTS<sup>\*1</sup> is a code for the probabilistic cross-identification of astrophysical sources. Version 2.0 of the code fully supersedes the version 1.0 described in Fioc (2012)<sup>\*2</sup> and is an implementation in Fortran 95 of the relations established in Fioc (2014)<sup>\*3</sup>. Its source files are freely<sup>\*4</sup> available at

«<http://www2.iap.fr/users/fioc/Aspects/v2.0/>»

in tar file «Aspects\_v2.0.tar». Type `<tar xvf Aspects_v2.0.tar>` to extract them in «Aspects\_v2.0/».

## II. Overview

Given two catalogs  $K$  and  $K'$  of  $n$  and  $n'$  astrophysical sources, respectively, ASPECTS computes, for any objects  $M_i \in K$  and  $M'_j \in K'$ , the probability that  $M'_j$  is a *counterpart* of  $M_i$ , i.e. that they are the same source. To determine this *probability of association*, denoted by  $P(A_{i,j} | C \cap C')$  in Fioc (2014), the code takes into account the coordinates and positional uncertainties of all the  $K$ -sources ( $C$ ) and of all the  $K'$ -sources ( $C'$ ). ASPECTS also computes the probabilities  $P(A_{i,0} | C \cap C')$  and  $P(A_{0,j} | C \cap C')$  that  $M_i$  or  $M'_j$  has no counterpart.

Three exclusive hypotheses are considered for these calculations:

- $H_{s:o}$ : a  $K$ -source has at most one counterpart in  $K'$ , but a  $K'$ -source may have several counterparts in  $K$  (**several-to-one K-K' associations**).
- $H_{o:s}$ : a  $K'$ -source has at most one counterpart in  $K$ , but a  $K$ -source may have several counterparts in  $K'$  (**one-to-several K-K' associations**).
- $H_{o:o}$ : a  $K$ -source has at most one counterpart in  $K'$  and vice versa (**one-to-one associations**).

All quantities derived under either  $H_{s:o}$ ,  $H_{o:s}$  or  $H_{o:o}$  have a subscript “s:o”, “o:s” or “o:o”, respectively.

Although  $H_{o:o}$  is the most natural assumption because of its symmetry, the other two deserve some consideration too. For instance, if the spatial resolution is much lower in  $K'$  than in  $K$ , several distinct  $K$ -sources may be merged in  $K'$ ;  $H_{s:o}$  might then be preferred. On the opposite, if objects are more patchy at the wavelength of  $K'$  than at that of  $K$ , single extended  $K$ -sources may look as several objects in  $K'$ ;  $H_{o:s}$  should be more appropriate in this case. Additional reasons for making computations under  $H_{s:o}$  and  $H_{o:s}$  is that they are much simpler and faster than under  $H_{o:o}$ , and that they are used in the first step of the iterative procedure leading to the probabilities  $P_{o:o}(A_{i,j} | C \cap C')$ ...

To compute the probabilities of association, ASPECTS needs the a priori (i.e., ignoring  $C$  and  $C'$ ) probability  $f$  (or  $f'$ ) that any object in  $K$  (or  $K'$ ) has a counterpart in the other catalog. The code obtains estimates  $\hat{f}_{s:o}$ ,  $\hat{f}_{o:s}$  and  $\hat{f}_{o:o}$  (or  $\hat{f}_{o:o} = n \hat{f}_{o:o}/n'$ ) of  $f$  or  $f'$  by maximizing the *likelihood*  $L$  to observe all the sources at their effective positions under assumptions  $H_{s:o}$ ,  $H_{o:s}$  and  $H_{o:o}$ , respectively.

ASPECTS computes these likelihoods, and in particular their maxima  $\hat{L}_{s:o} := L_{s:o}(\hat{f}_{s:o})$ ,  $\hat{L}_{o:s} := L_{o:s}(\hat{f}_{o:s})$  and  $\hat{L}_{o:o} := L_{o:o}(\hat{f}_{o:o})$ <sup>\*5</sup>. The assumption for which the maximum likelihood is the largest should be the most appropriate to compute the probabilities of association.

## III. Contents of the «Aspects\_v2.0/» directory

A large variety of cases may be considered, depending on whether the positional uncertainties are known in both catalogs, only one or none. If not fully known, they may be modelled with some additional parameters

1. Pronounced [aspɛ] in International Phonetic Alphabet transcription, not [æspekts], and preferentially written “Aspects” if small capitals are not available.  
“ASPECTS” is a French acronym for “*Association positionnelle/probabiliste de catalogues de sources*” (“Positional/probabilistic association of catalogs of sources” in English). The French word “*Aspect*” (pluralized in the acronym) has the same general meaning as the corresponding English word; interestingly, it signifies in particular the relative position of heavenly bodies...
2. The latter provided biased probabilities (and therefore also biased values of the likelihood and of estimators of unknown parameters) under assumption  $H_{o:o}$  (cf. § II).
3. Available as file «paper.pdf» in directory «v2.0/» (see below). References to sections or equations of this paper are preceded by “P-”. A basic presentation of ASPECTS is also given in Fioc (2013) (file «IAP\_seminar.pdf»).
4. The *Numerical Recipes* routines in Fortran 90 (Press *et al.*, 1992) mentioned in Fioc (2014) have been replaced by free equivalents.
5. All quantities computed at  $f = \hat{f}$  or  $f' = \hat{f}'$  under the corresponding assumption bear a circumflex accent hereafter. For instance,  $\hat{P}_{s:o}(A_{i,j} | C \cap C')$  is the value of  $P_{s:o}(A_{i,j} | C \cap C')$  for  $f = \hat{f}_{s:o}$ .

(e.g.  $\hat{\sigma}$  and  $\hat{\nu}$ ; cf. § P-A), to be determined by likelihood maximization; galaxy positional uncertainties, for instance, might be expressed as a function of the size of objects.

It would be impractical to cover all the cases in a single general-purpose main program. Therefore, besides the main module, `«mod_Aspects.f90»`, and a series of minor modules, we provide two main programs as examples: `«example_simul.f90»` and `«example_read.f90»` (cf. § V). These programs assume that positional uncertainties are known, but extensive comments should make them easy to adapt to other cases (cf. § VI).

The complete list of files in `«Aspects_v2.0/»` is the following:

<code>«Read_me.pdf»</code>	<code>«paper.pdf»</code>	<code>«Makefile»</code>
<code>«example_simul.f90»</code>	<code>«example_read.f90»</code>	<code>«mod_Aspects.f90»</code>
<code>«mod_simul_catalogs.f90»</code>	<code>«mod_output_prob.f90»</code>	<code>«mod_read_catalog.f90»</code>
<code>«mod_variables.f90»</code>	<code>«mod_constants.f90»</code>	<code>«mod_types.f90»</code>
<code>«mod_files.f90»</code>	<code>«mod_heap_index.f90»</code>	<code>«input_example_simul.dat»</code>
<code>«input_example_read.dat»</code>	<code>«K_p.dat»</code>	<code>«K_u.dat»</code>
<code>«IAP_seminar.pdf»</code>		

The current version, v2.0.1, only differs from v2.0[.0] by a few minor changes in the formatting of outputs produced by `«example_read.f90»` and by subroutine `«write_prob»` of `«mod_output_prob.f90»`.

## IV. Compilation

The default compiler is `<i>fort>`. To choose instead `<g>fortran>`, edit file `«Makefile»`: comment line 4 (insert a `<#>` before `<f95_compiler>`) and uncomment line 9. The code is written in standard Fortran 95, so other compilers should also work. Note that none of the options of compilation (set by variable `<f95_options>`) is mandatory: they provide various checks during the compilation and the execution, but might actually slow down the latter.

To compile the code, just type `<make>` on the keyboard. This will produce two executables: `«example_simul»` and `«example_read»`. To recompile from scratch, type first `<make clean_all>`: this will delete the executables and the objects (`«*.o»`) and `«*.mod»` files. To clean the directory while keeping the executables, type just `<make clean>`.

## V. Execution

### 1. Code `«example_simul»`

This executable simulates a sequence of twin mock catalogs and analyzes them.

#### a. Inputs

`«example_simul»` first asks for the following input parameters:

<code>&lt;n_simul&gt;</code>	integer	Number of simulations requested.
<code>&lt;n_u&gt;</code>	integer	Number $n$ of $K$ -sources.
<code>&lt;n_p&gt;</code>	integer	Number $n'$ of $K'$ -sources.
<code>&lt;input_f_u&gt;</code>	real	Requested fraction $f$ of $K$ -sources with a counterpart in $K'$ .
<code>&lt;semi_axis_a_u&gt;</code>	real	$1\text{-}\sigma$ positional uncertainty in radians along the major axis for $K$ -sources.
<code>&lt;semi_axis_b_u&gt;</code>	real	The same along the minor axis.
<code>&lt;semi_axis_a_p&gt;</code>	real	$1\text{-}\sigma$ positional uncertainty in radians along the major axis for $K'$ -sources.
<code>&lt;semi_axis_b_p&gt;</code>	real	The same along the minor axis.
<code>&lt;one_to_one&gt;</code>	boolean	<code>&lt;T&gt;</code> for simulations of one-to-one $K$ - $K'$ associations; <code>&lt;F&gt;</code> for simulations of several-to-one $K$ - $K'$ associations.
<code>&lt;area_S&gt;</code>	real	Area $S$ in steradians of the surface covered by $K$ and $K'$ ; set to $4\pi$ if the input value is not in $]0, 4\pi]$ .
<code>&lt;output_catalogs&gt;</code>	boolean	<code>&lt;T&gt;</code> to write the catalogs created by the <i>first</i> simulation; <code>&lt;F&gt;</code> otherwise.
<code>&lt;K_u_file&gt;</code>	string of characters	Name of the output file for catalog $K$ ; not required if <code>&lt;output_catalogs&gt;</code> is false.
<code>&lt;K_p_file&gt;</code>	string	The same for catalog $K'$ .

A set of input parameters is given as an example in `<input_example_simul.dat>`. Type

`<example_simul < input_example_simul.dat>`

to run the code with these values.

## b. Outputs

If requested, `<example_simul>` writes the catalogs created by the first simulation in the files designated by `<K_u_file>` and `<K_p_file>`. If any of these files already exists, new files with the same base names and a suffix derived from the current date and time are created.

For each simulation, `<example_simul>` returns the following quantities:

<b>Properties of the simulation</b>	
<code>&lt;seed&gt;</code>	Array of integers generating the sequence of random numbers used in the simulation.
<code>&lt;n_unavailable&gt;</code>	Number of $K$ -sources unassociated because no $K'$ -source was available ( $\neq 0$ only if <code>&lt;one_to_one&gt;</code> is true).
<code>&lt;n_side_effects&gt;</code>	Number of $K$ -sources unassociated because of side effects (only if <code>&lt;area_S&gt;</code> $< 4\pi$ ).
<code>&lt;eff_f_u&gt;</code>	Effective fraction of $K$ -sources with a counterpart in the other catalog.
<code>&lt;eff_f_p&gt;</code>	The same for $K'$ -sources.
<code>&lt;oto_deviation&gt;</code>	$= n \times \langle \text{eff\_f\_u} \rangle / (n' \times \langle \text{eff\_f\_p} \rangle)$ . Deviation with respect to one-to-one associations ( $= 1$ if <code>&lt;one_to_one&gt;</code> is true; $> 1$ otherwise, i.e. for several-to-one associations).
<b>Several-to-one computations</b>	
<code>&lt;sto_f_u&gt;</code>	$= \hat{f}_{s:o}$ : maximum likelihood estimator of $f$ under assumption $H_{s:o}$ .
<code>&lt;std_dev_sto_f_u&gt;</code>	Standard deviation of $\hat{f}_{s:o}$ .
<code>&lt;sto_f_p&gt;</code>	$= \hat{f}'_{s:o}$ : estimator of $f'$ under assumption $H_{s:o}$ .
<code>&lt;max_ln_sto_Lh&gt;</code>	$= \ln \hat{L}_{s:o}$ : maximum value of the log-likelihood under $H_{s:o}$ .
<b>One-to-several computations</b>	
<code>&lt;ots_f_p&gt;</code>	$= \hat{f}'_{o:s}$ : maximum likelihood estimator of $f'$ under assumption $H_{o:s}$ .
<code>&lt;std_dev_ots_f_p&gt;</code>	Standard deviation of $\hat{f}'_{o:s}$ .
<code>&lt;ots_f_u&gt;</code>	$= \hat{f}_{o:s}$ : estimator of $f$ under assumption $H_{o:s}$ .
<code>&lt;max_ln_ots_Lh&gt;</code>	$= \ln \hat{L}_{o:s}$ : maximum value of the log-likelihood under $H_{o:s}$ .
<b>One-to-one computations</b>	
<code>&lt;oto_f_u&gt;</code>	$= \hat{f}_{o:o}$ : maximum likelihood estimator of $f$ under assumption $H_{o:o}$ .
<code>&lt;std_dev_oto_f_u&gt;</code>	Standard deviation of $\hat{f}_{o:o}$ .
<code>&lt;oto_f_p&gt;</code>	$= \hat{f}'_{o:o} = n \hat{f}_{o:o} / n'$ .
<code>&lt;max_ln_oto_Lh&gt;</code>	$= \ln \hat{L}_{o:o}$ : maximum value of the log-likelihood under $H_{o:o}$ .

## 2. Code `<example_read>`

This executable reads two catalogs, analyzes them and computes the probabilities of association of the sources they contain. It also makes a few checks.

### a. Inputs

`<example_read>` asks for the following inputs:

<code>&lt;K_u_file&gt;</code>	Name of the input file containing the coordinates and positional uncertainties of $K$ -sources.
<code>&lt;K_p_file&gt;</code>	The same for $K'$ -sources.
<code>&lt;sto_prob_u_file&gt;</code>	Name of the output file containing the probabilities $\hat{P}_{s:o}(A_{i,j}   C \cap C')$ for all $M_i \in K$ .
<code>&lt;sto_prob_p_file&gt;</code>	The same for all $M'_j \in K'$ .
<code>&lt;ots_prob_u_file&gt;</code>	Name of the output file containing the probabilities $\hat{P}_{o:s}(A_{i,j}   C \cap C')$ for all $M_i \in K$ .
<code>&lt;ots_prob_p_file&gt;</code>	The same for all $M'_j \in K'$ .
<code>&lt;oto_prob_u_file&gt;</code>	Name of the output file containing the probabilities $\hat{P}_{o:o}(A_{i,j}   C \cap C')$ for all $M_i \in K$ .
<code>&lt;oto_prob_p_file&gt;</code>	The same for all $M'_j \in K'$ .
<code>&lt;skip_checks&gt;</code>	<code>&lt;T&gt;</code> to skip checks of one-to-one computations; <code>&lt;F&gt;</code> otherwise.

(All the `*_file` inputs are strings of characters.)

A set of input parameters is given as an example in `<input_example_read.dat>`. Type

```
<example_read < input_example_read.dat>
```

to run the code on the catalogs `<K_u.dat>` and `<K_p.dat>` (these have been created by `<example_simul>`).

### Warning

The subroutine `<read_catalog>` of `<mod_read_catalog.f90>` is called to read the files designated by `<K_u_file>` and `<K_p_file>` (the format of these files is described in the header of `<K_u.dat>` and `<K_p.dat>`). It reads in particular the surface area  $S$  covered by  $K$  and  $K'$ . This is used to set to  $1/S$  the quantities  $\xi_{i,0}$  (cf. § P-3.1.1) and  $\xi_{0,j}$  (cf. § P-3.2.1) for all  $M_i$  and  $M'_j$ , assuming that unrelated sources are uniformly and randomly distributed on the surface. The user must provide this quantity for real catalogs. If it is less than  $4\pi$  steradians, he also has to make sure that the catalogs cover the same surface: `<example_read>` checks only that the surface *areas* —not the *surfaces* themselves— are identical.

## b. Outputs

`<example_read>` provides the following outputs:

Fractions of sources with a counterpart		
<code>&lt;sto_f_u&gt;</code> , <code>&lt;std_dev_sto_f_u&gt;</code> , <code>&lt;sto_f_p&gt;</code>		Estimates under $H_{s:0}$ (cf. § V.1.b).
<code>&lt;ots_f_u&gt;</code> , <code>&lt;std_dev_ots_f_u&gt;</code> , <code>&lt;ots_f_p&gt;</code>		The same under $H_{0:s}$ .
<code>&lt;oto_f_u&gt;</code> , <code>&lt;std_dev_oto_f_u&gt;</code> , <code>&lt;oto_f_p&gt;</code>		The same under $H_{0:0}$ .
Choice of association model <sup>*6</sup>		
<code>&lt;max_ln_sto_Lh&gt;</code> , <code>&lt;max_ln_ots_Lh&gt;</code> , <code>&lt;max_ln_oto_Lh&gt;</code>		Maximum values of the log-likelihood under $H_{s:0}$ , $H_{0:s}$ and $H_{0:0}$ (cf. § V.1.b).
Probabilities of association		
<code>&lt;sto_prob_u(i)&gt;</code>	Written in <code>&lt;sto_prob_u_file&gt;</code> .	Probabilities $\hat{P}_{s:0}(A_{i,j}   C \cap C')$ for all $M_i \in K$ .
<code>&lt;sto_prob_p(j)&gt;</code>	Written in <code>&lt;sto_prob_p_file&gt;</code> .	The same for all $M'_j \in K'$ .
<code>&lt;ots_prob_u(i)&gt;</code>	Written in <code>&lt;ots_prob_u_file&gt;</code> .	Probabilities $\hat{P}_{0:s}(A_{i,j}   C \cap C')$ for all $M_i \in K$ .
<code>&lt;ots_prob_p(j)&gt;</code>	Written in <code>&lt;ots_prob_p_file&gt;</code> .	The same for all $M'_j \in K'$ .
<code>&lt;oto_prob_u(i)&gt;</code>	Written in <code>&lt;oto_prob_u_file&gt;</code> .	Probabilities $\hat{P}_{0:0}(A_{i,j}   C \cap C')$ for all $M_i \in K$ .
<code>&lt;oto_prob_p(j)&gt;</code>	Written in <code>&lt;oto_prob_p_file&gt;</code> .	The same for all $M'_j \in K'$ .

The quantities `<sto_prob_u(i)>`, etc., are records of type `<prob_struct>` (see `<mod_types.f90>`). Their fields are described in § VI.3. To read the list of possible counterparts and the corresponding probabilities of association from the output files designated by `<sto_prob_u_file>`, etc., see the header of these files.

As an illustration, `<example_read>` also computes  $\ln L_{0:0}(f)$  for a grid of equidistant values of  $f$  with the subroutine `<compute_ln_oto_Lh>` of `<mod_Aspects.f90>`<sup>\*7</sup>.

## c. Checks of results obtained under $H_{0:0}$

The code finally makes some checks if `<skip_checks>` is false. It first computes  $\ln \hat{L}_{0:0}$  (`<max_ln_oto_Lh_alt>`) again with the function `<func_ln_oto_Lh_alt>` of `<mod_Aspects.f90>`, which is based on the results of § C.2. As currently implemented, this procedure is however extremely slow and should generally be avoided.

`<example_read>` then swaps  $K$  and  $K'$ , and computes  $\hat{f}_{0:0}$ ,  $\hat{f}'_{0:0}$ ,  $\ln \hat{L}_{0:0}$  and the probabilities  $\hat{P}_{0:0}(A_{i,j} | C \cap C')$  again. The suffix `<_sw>` is appended to all these quantities, as well as to the files in which the probabilities are written.

## VI. Understanding and adapting the code

### 1. Terminological and typographical conventions

Here is a brief summary of the conventions used in the code and this file:

- In outputs to the terminal and comments, code fragments are written between `<`>` (grave accents), and filenames between `<">`. Non Fortran mathematical expressions, quantities and objects defined in the article are between dollars in pseudo-TeX.

6. `<example_read>` also recalls the recommendations given in the second paragraph of § P-6.4.

7. This subroutine has already been used to compute `<max_ln_oto_Lh>`. As calculations under  $H_{0:0}$  are lengthy, `<compute_ln_oto_Lh>` may be called to compute  $\ln L_{0:0}$  for a given  $f$  and for a grid of  $f$  at the same time.

In the documentation and the complements, code fragments are surrounded by “<” and “>”; file names, by “<<” and “>>”;

- Quantities chiefly or only related to catalog  $K$  are written with a suffix `<_u>` (for “unprimed”); those related to  $K'$ , with a suffix `<_p>` (for “prime”). In file `<mod_Aspects.f90>`, `<_1>` and `<_2>` are used instead because  $K$  and  $K'$  are sometimes swapped;
- The word “neighbor” (`<ngb>`) designates a nearby object in the same catalog; “counterpart” (`<ctp>`), a nearby object in the other catalog;
- The notations `<sto>`, `<ots>` and `<oto>` are used to distinguish the results obtained under the assumptions  $H_{s,o}$ ,  $H_{o,s}$  and  $H_{o,o}$ , respectively.

## 2. Coordinates and positional uncertainties

- The coordinates and positional uncertainties of  $K$ - and  $K'$ -sources are written in the records `<coord_u>` and `<coord_p>`. These records are of type `<coord_struct>` (see `<mod_types.f90>`) and contain the following fields:

<code>&lt;alpha&gt;</code>	Right ascension (or equivalent: Galactic longitude, etc.).
<code>&lt;delta&gt;</code>	Declination (or Galactic latitude, etc.).
<code>&lt;semi_axis_a&gt;</code>	Semi-major axis of the positional uncertainty ellipse.
<code>&lt;semi_axis_b&gt;</code>	Semi-minor axis.
<code>&lt;beta&gt;</code>	Positional angle of the ellipse.

For instance, the right ascension  $\alpha_i$  of the  $K$ -source  $M_i$  is `<coord_u(i)%alpha>`, and the semi-minor axis  $b'_j$  of the  $K'$ -source  $M'_j$  is `<coord_p(j)%semi_axis_b>`.

All these quantities are in radians.

- Right ascensions are in  $[0, 2\pi[$ . Sources must be ordered by increasing right ascension; this is done automatically when calling subroutine `<simul_catalogs>`, as in `<<example_simul>`, but you have to do it yourself if you read catalogs, as in `<<example_read>` (this is checked, however).
- The positional uncertainty angle  $\beta$  is counted eastward from the North to the semi-major axis and is in  $[0, \pi[$ .
- The distribution of the observed position of a source relative to its true position is described by a 2-dimensional normal (i.e. Gaussian) law<sup>\*\*8</sup>. The semi-major (resp. semi-minor) axis is the  $1\text{-}\sigma$  positional uncertainty along the major (resp. minor) axis, independently from the position along the minor (resp. major) axis. So, if  $a$ ,  $b$ ,  $X$  and  $Y$  are, respectively, the semi-major and semi-minor axes and the positional errors along each axis, then

$$P((X, Y) \in [x, x + dx[ \times [y, y + dy[) = \frac{1}{2\pi ab} \exp\left(-\frac{1}{2} \left[ \frac{x^2}{a^2} + \frac{y^2}{b^2} \right]\right) dx dy. \quad (1)$$

## 3. Probabilities of association

For any source, the probabilities of association are written in records of type `<prob_struct>` (see `<mod_types.f90>`) containing the following fields:

<code>&lt;n_ctp&gt;</code>	Number of possible real counterparts to the source.
<code>&lt;ctp&gt;</code>	For $k \in \llbracket 1, \langle n\_ctp \rangle \rrbracket$ , <code>&lt;ctp(k)&gt;</code> is the ordinal number of the $k$ -th counterpart; the fictitious counterpart <code>&lt;ctp(0)&gt;</code> (= 0) corresponds to no counterpart.
<code>&lt;prob&gt;</code>	For $k \in \llbracket 1, \langle n\_ctp \rangle \rrbracket$ , <code>&lt;prob(k)&gt;</code> is the probability that the source is associated with <code>&lt;ctp(k)&gt;</code> ; <code>&lt;prob(0)&gt;</code> is the probability that the source has no counterpart.

For instance, `<sto_prob_u(i)%n_ctp>` is the number of possible real counterparts of  $M_i$ , and `<sto_prob_u(i)%ctp(k)>` is the ordinal number  $j$  of the  $k$ -th counterpart  $M'_j$  of  $M_i$  under  $H_{s,o}$ . Similarly, if  $i = \langle oto\_prob\_p(j)\%ctp(k) \rangle$ , `<oto_prob_p(j)%prob(k)>` is the probability that  $M'_j$  is associated to  $M_i$  under  $H_{o,o}$ , and `<oto_prob_p(j)%prob(0)>` is the probability that  $M'_j$  has no counterpart.

## 4. Simulations

Mock catalogs are created with the subroutine `<simul_catalogs>` of `<mod_simul_catalogs.f90>`. Here are some details about it.

8. The sphere is locally assimilated to its tangent plane or to a tangent cylinder. Note that this would not be appropriate if the semi-major axis were not negligible with respect to  $\pi$  radians (!). A Kent distribution (Kent, 1982), for instance, would then seem a better choice, as it is one possible generalization of the normal law to the sphere, but, contrary to a Gaussian, it is not stable: the sum of independent Kent-distributed random variables does not follow a distribution of the same type.

## a. Generation of twin mock catalogs

### Shape of the surface

A spherical cap  $C$  covering a solid angle  $\langle \text{area}_S \rangle$ <sup>9</sup> and centered on the North pole is used in simulations. If  $\langle \text{area}_S \rangle \notin ]0, 4\pi]$  steradians, it is set to  $4\pi$  (with a warning), i.e.  $C$  is the whole sky.

### Associations, positions and positional uncertainty angles. Side effects

The procedure described in § P-6.1 has been slightly modified. The algorithm we now use is the following:

1. Draw the observed positions of all  $K'$ -sources on  $C$  randomly and uniformly;
2. Generate their true positions from their observed positions and from the  $\langle \text{semi\_axis\_*_p} \rangle$  parameters with the subroutine  $\langle \text{position} \rangle$  of  $\langle \text{mod\_simul\_catalogs.f90} \rangle$  (cf. § B). The observed positional uncertainty angles  $\beta'_i$  (i.e. with respect to the direction of the North at the observed position) are drawn randomly and uniformly in  $[0, \pi[$ ;
3. For each  $i$  from 1 to  $n$ ,
  - a. determine whether  $M_i$  is associated to some (yet unknown) counterpart in  $K'$ . Do this with probability  $\langle \text{input\_f\_u} \rangle$  if  $\langle \text{force\_ctp\_frac} \rangle$  (cf. § VI.5) is false, and for  $n \times \langle \text{input\_f\_u} \rangle$  of them otherwise.

If  $\langle \text{one\_to\_one} \rangle$  is true, consider  $M_i$  as unassociated if all the objects in  $K'$  are already associated. Jump then to point 4;
  - b. randomly select a counterpart  $M'_i$  to  $M_i$  among all the  $K'$ -sources if  $\langle \text{one\_to\_one} \rangle$  is false, and among all the  $K'$ -sources which are not associated yet if  $\langle \text{one\_to\_one} \rangle$  is true;
  - c. generate the observed position of  $M_i$  with subroutine  $\langle \text{position} \rangle$  from its true position (i.e. that of  $M'_i$ ) and from the  $\langle \text{semi\_axis\_*_u} \rangle$  parameters. The true positional uncertainty angle (i.e. with respect to the direction of the North at the true position) is drawn randomly and uniformly in  $[0, \pi[$ , and is converted to the observed angle<sup>10</sup> in this subroutine (cf. § B);
  - d. *side effects* may occur if  $C$  is a strict subset of the whole sky (i.e. if  $\langle \text{area}_S \rangle < 4\pi$ ): a  $K'$ -source observed within the spherical cap  $C$  but close to its boundary may indeed have a counterpart observed outside of  $C$ .

If the observed position of  $M_i$  falls outside of  $C$ , discard this position and consider  $M_i$  as unassociated. Jump then to point 4;
4. For each unassociated  $K$ -source, draw its observed position uniformly and randomly on  $C$ .

The positions of the sources are ordered by increasing right ascension only after this procedure.

## b. Effective fraction of $K$ -sources with a counterpart

The quantity  $\langle \text{eff\_f\_u} \rangle$  may be different from  $\langle \text{input\_f\_u} \rangle$  for several reasons:

- because the number of  $K$ -sources with a counterpart must be less than  $n'$  if  $\langle \text{one\_to\_one} \rangle$  is true;
- because the number of sources with a counterpart is an integer;
- if  $S < 4\pi$ , because of side effects (cf. point 3.d of § VI.4.a);
- if  $\langle \text{force\_ctp\_frac} \rangle$  is false, because (ignoring above constraints)  $\langle \text{input\_f\_u} \rangle$  is the probability that a  $K$ -source has a counterpart, so  $\langle \text{eff\_f\_u} \rangle$  is the same as  $\langle \text{input\_f\_u} \rangle$  only on average, i.e.

$$\langle n \times \langle \text{eff\_f\_u} \rangle + \langle \text{n\_unavailable} \rangle + \langle \text{n\_side\_effects} \rangle \rangle = n \times \langle \text{input\_f\_u} \rangle. \quad (2)$$

However, if  $\langle \text{force\_ctp\_frac} \rangle$  is true,

$$|n \times \langle \text{eff\_f\_u} \rangle + \langle \text{n\_unavailable} \rangle + \langle \text{n\_side\_effects} \rangle - n \times \langle \text{input\_f\_u} \rangle| < 1. \quad (3)$$

## c. Using $\langle \text{seed} \rangle$

The knowledge of  $\langle \text{seed} \rangle$  may be useful in case one of the simulations (let say the  $i$ -th) fails. To generate exactly the same random numbers as in the  $i$ -th simulation and to run the latter first, insert the line

```
 $\langle \text{call random\_seed}(\text{put} = (/s_1, \dots, s_q/)) \rangle$ 
```

in  $\langle \text{example\_simul.f90} \rangle$ , just before the call to  $\langle \text{simul\_catalog} \rangle$ . The integers  $s_1, \dots, s_q$  are the elements of the array  $\langle \text{seed} \rangle$  returned for the  $i$ -th simulation; do not forget the commas between them, nor the leading  $\langle (/ \rangle$  and the trailing  $\langle / \rangle$ . This procedure avoids to run all the simulations 1 to  $i - 1$  anew just to search where the problem comes from.

9. This parameter is actually optional in  $\langle \text{simul\_catalogs} \rangle$ . It is set to  $4\pi$  if absent.

10. Except near the poles, the difference between the true and observed angles is negligible.

## 5. Code constants

The default type used for reals is given by parameter `<real_type>`, which is defined in `<mod_types.f90>`.

All the following constants are defined and commented in `<mod_constants.f90>` (most of them control the accuracy of the results):

`<force_ctp_frac>`:

- `<.true.>` if the number  $n \times \langle \text{eff\_f\_u} \rangle$  of simulated  $K$ -sources associated to  $K'$ -ones is forced to be equal to  $n \times \langle \text{input\_f\_u} \rangle$ , up to one unit;
- `<.false.>` if the probability that any  $K$ -source is associated is drawn with probability `<input_f_u>`, independently from the association status of other  $K$ -sources.

(All this, ignoring side effects and, if `<one_to_one>` is true, the constraint  $n \times \langle \text{eff\_f\_u} \rangle \leq n'$ .)

Default value: `<.true.>`;

`<n_max_sigma>`: Value of

$$\frac{\langle R\_ctp \rangle}{\max_{M_i \in K, M'_j \in K'} \sqrt{a_i^2 + a'_j^2}},$$

where `<R_ctp>` is the radius within which counterparts are searched. Reasonable values of `<n_max_sigma>` should be in [5, 10].

Default value: 5;

`<min_xi_ratio>`: Minimum value of  $\xi_{i,j}/\xi_{i,0}$ , where  $\xi_{i,j}$  is the spatial probability density to observe the source  $M'_j$  at some position if it is a true counterpart of the object  $M_i$ , and  $\xi_{i,0}$  is the same quantity if they are unrelated. This ratio should be  $\ll 1$ : if  $\xi_{i,j}/\xi_{i,0} < \langle \text{min\_xi\_ratio} \rangle$ , then  $\xi_{i,j}$  is set to 0 and  $M'_j$  is not considered as a possible counterpart of  $M_i$ ; if `<min_xi_ratio>`  $\leq 0$ , this never happens.

Default value:  $10^{-10}$ ;

`<epsilon_f>`: Accuracy of maximum-likelihood estimates of  $f$  and  $f'$ : an estimate  $\hat{f}$  of  $f$  is the limit of a sequence  $f_{k+1} = g(f_k)$ , where  $g$  is the function defined in § P- 5.3; when  $|f_{k+1} - f_k| < \langle \text{epsilon\_f} \rangle$ , the iteration procedure stops and  $\hat{f}$  is set to  $f_{k+1}$ .

Default value:  $10^{-5}$ .

The constants below are used only in calculations under  $H_{0:0}$ :

`<R_ratio>`: Value of `<R_ngb>/<R_ctp>`, where `<R_ngb>` is the radius within which neighbors are searched in calculations under  $H_{0:0}$ . An `<R_ngb>` equal to a few times `<R_ctp>` seems reasonable.

Default value: 2;

`<n_max_ngb>`: Maximal number of neighbors (including the main source, so  $\geq 1$ ) considered for calculations under  $H_{0:0}$ .

Default value: 8;

`<epsilon_oto_prob>`: Parameter setting the accuracy of the iterative procedure computing the probabilities  $P_{0:0}(A_{i,j} | C \cap C')$ . See subroutine `<compute_oto_prob>` in `<mod_Aspects.f90>`.

Default value:  $10^{-5}$ ;

`<epsilon_ln_oto_Lh>`: Parameter setting the accuracy of  $\ln L_{0:0}$  when it is computed with `<compute_ln_oto_Lh>`. See subroutine `<refine_grid>` in `<mod_Aspects.f90>`.

Default value:  $10^{-5}$ ;

`<d_f>`: Shift of  $\hat{f}_{0:0}$  used in the subroutine `<oto_analysis>` of `<mod_Aspects.f90>` to compute the standard deviation of  $\hat{f}_{0:0}$  from a finite difference approximation to  $(\partial^2 \ln L_{0:0} / \partial f^2)_{f=\hat{f}_{0:0}}$ .

Default value:  $10^{-3}$ ;

`<f_max_shift>`: Under  $H_{0:0}$ , the theoretical maximal value of  $f$  is  $f_{\max} = \min\{1, n'/n\}$ . For numerical reasons, the maximal value of  $f$  effectively used in the subroutine `<compute_ln_oto_Lh>` of `<mod_Aspects.f90>` is  $f_{\max} - \langle \text{f\_max\_shift} \rangle$ .

Default value:  $10^{-3}$ .

## 6. Modules used in `<example_simul>` and `<example_read>`

A few modules are loaded by `<example_simul>` and `<example_read>` (see the `<use mod_*>` statements at the beginning of these programs<sup>\*11</sup>). All of them are in the corresponding `<mod_*.f90>` files.

The file `<mod_variables.f90>` gives access to data of interest for the two programs, in particular the records `<assoc_data_u>` and `<assoc_data_p>`; these records, of type `<assoc_data>` (see `<mod_types.f90>`), contain all the informations on sources (their possible counterparts in the other catalog, their neighbors in the

11. The commented out `<, only : ...>` part is just to remind all the variables used.

same catalog, etc.) which are necessary to compute probabilities of association. Other data which may be used only by «example\_simul» are in «mod\_simul\_catalogs.f90»; those only for «example\_read» are in «mod\_read\_catalogs.f90».

The files «mod\_Aspects.f90», «mod\_simul\_catalogs.f90», «mod\_read\_catalog.f90» and «mod\_output\_prob.f90» also provide some procedures which we now describe.

#### a. Procedures defined in «mod\_Aspects.f90»

- «general\_preliminaries»: preliminaries required for computations under all assumptions. Computes the first part of «assoc\_data\_u» and «assoc\_data\_p»;
- «oto\_preliminaries»: additional preliminaries required for computations under  $H_{o:o}$  only. Computes the second part of «assoc\_data\_u» and «assoc\_data\_p»;
- «sto\_analysis»: iteration procedure converging to the maximum-likelihood estimate  $\hat{f}_{s:o}$  of  $f$  («sto\_f\_u»). Computes also  $\hat{f}'_{s:o}$  («sto\_f\_p») and the standard deviation of  $\hat{f}_{s:o}$  («std\_dev\_sto\_f\_u»);
- «ots\_analysis»: iteration procedure converging to the maximum-likelihood estimate  $\hat{f}'_{o:s}$  of  $f'$  («ots\_f\_p»). Computes also  $\hat{f}_{o:s}$  («ots\_f\_u») and the standard deviation of  $\hat{f}'_{o:s}$  («std\_dev\_ots\_f\_p»);
- «oto\_analysis»: iteration procedure converging to the maximum-likelihood estimate  $\hat{f}_{o:o}$  of  $f$  («oto\_f\_u»). Computes also  $\hat{f}'_{o:o}$  («oto\_f\_p») and the standard deviation of  $\hat{f}_{o:o}$  («std\_dev\_oto\_f\_u»);
- «func\_ln\_sto\_Lh»: log-likelihood  $\ln L_{s:o}$  for a given  $f$ ;
- «func\_ln\_ots\_Lh»: log-likelihood  $\ln L_{o:s}$  for a given  $f'$ ;
- «compute\_ln\_oto\_Lh»: procedure computing  $\ln L_{o:o}$  for a given  $f$ , a grid of equidistant values of  $f$ , or both;
- «func\_ln\_oto\_Lh\_alt»: alternative computation of the log-likelihood  $\ln L_{o:o}$  for a given  $f$ . Not recommended;
- «compute\_sto\_prob»: computes  $P_{s:o}(A_{i,j} | C \cap C')$  for a given  $f$  and for all  $(i, j) \in \llbracket 1, n \rrbracket \times \llbracket 1, n' \rrbracket \setminus \{(0, 0)\}$ ;
- «compute\_ots\_prob»: computes  $P_{o:s}(A_{i,j} | C \cap C')$  for a given  $f'$  and for all  $(i, j) \in \llbracket 1, n \rrbracket \times \llbracket 1, n' \rrbracket \setminus \{(0, 0)\}$ ;
- «compute\_oto\_prob»: computes  $P_{o:o}(A_{i,j} | C \cap C')$  for a given  $f$  and for all  $(i, j) \in \llbracket 1, n \rrbracket \times \llbracket 1, n' \rrbracket \setminus \{(0, 0)\}$ .

#### b. Procedures defined in «mod\_simul\_catalogs.f90»

- «simul\_catalogs»: creates twin mock catalogs;
- «write\_catalogs»: writes twin catalogs to output files;
- «seed\_format»: output format for the array of seeds used by the generator of random numbers.

#### c. Input/output procedures

Defined in «mod\_read\_catalog.f90»

- «read\_catalog»: reads a single catalog.

Defined in «mod\_output\_prob.f90»

- «output\_sto\_prob», «output\_ots\_prob», «output\_oto\_prob»: writes in files the probabilities of association to every source in  $K$  and  $K'$  of all its possible counterparts;
- «write\_prob»: writes in a file the probabilities of association to a single source of all its possible counterparts. It is called indirectly in «example\_read» through the «output\_\*t\*\_prob» procedures described above, but may also be called directly.

# Complements

## A. Efficient search for possible counterparts

The search procedure for possible counterparts described in § P-5.2 may be accelerated in the following way. For most  $M_i$ , one does not need to *test* for each  $M'_k$  whether  $\psi_{i,k} \leq R'$ . Let us write  $E_i$  the domain of right ascensions  $\alpha'$  out of which no point  $M'$  of declination  $\delta'$  and closer to  $M_i$  than distance  $R'$  may be found. The angular distance  $\psi(M_i, M')$  between  $M'$  and  $M_i$  is given (cf. Eq. P-A.15) by

$$\cos \psi(M_i, M') = \cos(\alpha' - \alpha_i) \cos \delta_i \cos \delta' + \sin \delta_i \sin \delta'. \quad (4)$$

If  $\delta_i \notin [-\pi/2 + R', \pi/2 - R']$ , then  $E_i = [0, 2\pi]$ . Else, the minimum of  $\cos(\alpha' - \alpha_i)$  under the constraint  $\cos \psi(M_i, M') \geq \cos R'$  is reached when  $\sin \delta' = \sin \delta_i / \cos R'$  and

$$\cos(\alpha' - \alpha_i) = \cos \Delta_i, \quad \text{where } \Delta_i = \arccos \frac{\sqrt{\cos^2 R' - \sin^2 \delta_i}}{\cos \delta_i}. \quad (5)$$

The domain of possible right ascensions is then given by

$$E_i = \begin{cases} [0, \alpha_i + \Delta_i - 2\pi] \cup [\alpha_i - \Delta_i, 2\pi] & \text{if } \alpha_i + \Delta_i > 2\pi, \\ [0, \alpha_i + \Delta_i] \cup [\alpha_i - \Delta_i + 2\pi, 2\pi] & \text{if } \alpha_i - \Delta_i < 0, \\ [\alpha_i - \Delta_i, \alpha_i + \Delta_i] & \text{otherwise.} \end{cases} \quad (6)$$

For a catalog  $K'$  ordered by increasing right ascension (if not, this is the first thing to do), one may easily find the subset of indices  $k$  for which  $\alpha'_k \in E_i$ . For instance, if  $E_i = [\alpha_i - \Delta_i, \alpha_i + \Delta_i]$ , one just has to find by dichotomy the indices  $k^-$  and  $k^+$  such that  $\alpha'_{k^- - 1} < \alpha_i - \Delta_i \leq \alpha'_{k^-}$  and  $\alpha'_{k^+} \leq \alpha_i + \Delta_i < \alpha'_{k^+ + 1}$ ; sums like  $\sum_{k=1; \psi_{i,k} \leq R'}^{n'}$  may then be replaced by  $\sum_{k=k^-; \psi_{i,k} \leq R'}^{k^+}$ .

Whatever the domain  $E_i$ , these sums may be further restricted to sources with a declination  $\delta'_k \in [\delta_i - R', \delta_i + R'] \cap [-\pi/2, \pi/2]$ .

This procedure is implemented in subroutine `<alpha_bounds>` of `<mod_Aspects.f90>`.

## B. Simulation of positions

We provide here some explanations on how subroutine `<position>` of file `<mod_simul_catalogs.f90>` simulates the observed position of a source from its true position (or the converse) and its positional uncertainty parameters.

Let  $M_0(\alpha_0, \delta_0)$  be the true position of a source,  $a$  ( $\ll \pi$  radians) and  $b$  be the semi-major and semi-minor axes of the positional uncertainty ellipse, and  $\vec{u}_a$  and  $\vec{u}_b$  be unit vectors along the major and minor axes ( $\vec{u}_a$  and  $\vec{u}_b$  are oriented so that  $(\vec{u}_a, \vec{u}_b, \vec{u}_{r_0})$  is a direct orthonormal basis).

For any vectors  $\vec{v}$  and  $\vec{w}$  perpendicular to  $\vec{u}_{r_0}$ , we denote by  $\angle(\vec{v}, \vec{w})^+$  the angle from  $\vec{v}$  to  $\vec{w}$  oriented counter-clockwise around  $\vec{u}_{r_0}$ , and by  $\angle(\vec{v}, \vec{w})^-$  the same angle oriented clockwise (i.e.,  $\angle(\vec{v}, \vec{w})^- = -\angle(\vec{v}, \vec{w})^+ = \angle(\vec{w}, \vec{v})^+$ ).

We want to simulate an observed position,  $M(\alpha, \delta)$ . First, define  $\vec{n} := \vec{u}_{r_0} \times \vec{u}_r / \|\vec{u}_{r_0} \times \vec{u}_r\|$ ,  $\vec{t} := \vec{n} \times \vec{u}_{r_0}$  (the basis  $(\vec{t}, \vec{n}, \vec{u}_{r_0})$  is therefore direct and orthonormal) and  $\psi := \angle(\vec{u}_{r_0}, \vec{u}_r)$ .

Let  $\beta_0 := \angle(\vec{u}_{\delta_0}, \vec{u}_a)^-$  and  $\beta := \angle(\vec{u}_\delta, \vec{u}_a)^-$  be the true and observed positional uncertainty angles, and define  $\gamma_0 := \angle(\vec{n}, \vec{u}_{\delta_0})^-$ ,  $\gamma := \angle(\vec{n}, \vec{u}_\delta)^-$  and  $\epsilon := \angle(\vec{u}_a, \vec{t})^+$  ( $\gamma$  and  $\beta$  are in the plane perpendicular to  $\vec{u}_r$ , not to  $\vec{u}_{r_0}$ , but one may consider here that  $\vec{u}_r \approx \vec{u}_{r_0}$ ; more rigorously, one may project the sphere on the tangent cylinder containing  $M_0$  and  $M$  and unroll this cylinder on a plane).

The following relations hold:

$$\gamma_0 + \beta_0 = \gamma + \beta = \angle(\vec{n}, \vec{u}_a)^-, \quad (7)$$

so

$$\begin{aligned} \gamma_0 + \beta_0 - \epsilon &= \gamma + \beta - \epsilon \\ &= \angle(\vec{n}, \vec{u}_a)^- - \angle(\vec{u}_a, \vec{t})^+ = \angle(\vec{n}, \vec{u}_a)^- + \angle(\vec{u}_a, \vec{t})^- = \angle(\vec{t}, \vec{n})^+ \\ &= \pi/2 \pmod{2\pi}; \end{aligned} \quad (8)$$

$$\cos \psi = \cos \delta_0 \cos \delta \cos(\alpha - \alpha_0) + \sin \delta_0 \sin \delta; \quad (9)$$

$$\cos \gamma_0 = \frac{\cos \delta \sin(\alpha - \alpha_0)}{\sin \psi}; \quad (10)$$

$$\sin \gamma_0 = \frac{\cos \delta_0 \sin \delta - \sin \delta_0 \cos \delta \cos(\alpha - \alpha_0)}{\sin \psi}. \quad (11)$$

(Cf. § P-A for Eqs. (9) to (11).)

One has

$$\overrightarrow{M_0 M} \approx \psi \vec{t} = \psi (\cos \epsilon \vec{u}_a + \sin \epsilon \vec{u}_b) = a r_1 \vec{u}_a + b r_2 \vec{u}_b, \quad (12)$$

where  $r_1$  and  $r_2$  are independent random numbers drawn from a normal distribution with mean 0 and standard deviation 1. Therefore,  $\psi \approx ([a r_1]^2 + [b r_2]^2)^{1/2}$  and, using the Fortran function  $\langle \text{atan2} \rangle$  to obtain a unique result in  $]-\pi, \pi]$ , one obtains  $\epsilon \approx \langle \text{atan2} \rangle(b r_2, a r_1)$ .

One may either draw  $\beta_0$  randomly and derive  $\alpha$ ,  $\delta$  and  $\beta$  (as in the code; § B.1), or draw  $\beta$  randomly and derive  $\alpha$  and  $\delta$  directly (§ B.2; not implemented). Note that in the second case, two positions may be valid solutions of the set of equations.

## 1. Determination of $\alpha$ , $\delta$ and $\beta$ from $\beta_0$ (and from $\alpha_0$ , $\delta_0$ , $\psi$ and $\epsilon$ )

Angle  $\gamma_0$  is first derived from Eq. (8),  $\beta_0$  and  $\epsilon$ .

Combining Eq. (11) and Eq. (9), one gets first

$$\sin \gamma_0 \sin \psi = \cos \delta_0 \sin \delta - \sin \delta_0 \frac{\cos \psi - \sin \delta_0 \sin \delta}{\cos \delta_0}, \quad (13)$$

then

$$\delta = \arcsin(\sin \gamma_0 \sin \psi \cos \delta_0 + \sin \delta_0 \cos \psi). \quad (14)$$

From Eq. (11) and Eq. (10), one obtains

$$\sin(\alpha - \alpha_0) = \frac{\cos \gamma_0 \sin \psi}{\cos \delta} \quad (15)$$

and

$$\cos(\alpha - \alpha_0) = \frac{\cos \delta_0 \sin \delta - \sin \gamma_0 \sin \psi}{\sin \delta_0 \cos \delta}. \quad (16)$$

Thus,

$$\alpha = \alpha_0 + \langle \text{atan2} \rangle(\sin[\alpha - \alpha_0], \cos[\alpha - \alpha_0]) \pmod{2\pi}. \quad (17)$$

Using  $\langle \text{atan2} \rangle$ , one derives  $\gamma$  from

$$\cos \gamma = \frac{\cos \delta_0 \sin(\alpha - \alpha_0)}{\sin \psi} \quad (18)$$

and

$$\sin \gamma = \frac{\cos \delta_0 \sin \delta \cos(\alpha - \alpha_0) - \sin \delta_0 \cos \delta}{\sin \psi}, \quad (19)$$

and then  $\beta$  from Eq. (8) and  $\epsilon$ .

## 2. Determination of $\alpha$ , $\delta$ from $\beta$ (and from $\alpha_0$ , $\delta_0$ , $\psi$ and $\epsilon$ )

Angle  $\gamma$  is first derived from Eq. (8),  $\beta$  and  $\epsilon$ .

From Eq. (18), one obtains

$$\alpha = \alpha^+ = \alpha_0 + \arcsin \frac{\cos \gamma \sin \psi}{\cos \delta_0} \pmod{2\pi} \quad (20)$$

or

$$\alpha = \alpha^- = \alpha_0 + \pi - \arcsin \frac{\cos \gamma \sin \psi}{\cos \delta_0} \pmod{2\pi}. \quad (21)$$

The combination  $\sin \delta_0 \times \text{Eq. (9)} + \cos \delta_0 \cos(\alpha^\pm - \alpha_0) \sin \psi \times \text{Eq. (19)}$  leads to

$$\sin \delta^\pm = \frac{\sin \delta_0 \cos \psi + \cos \delta_0 \cos(\alpha^\pm - \alpha_0) \sin \gamma \sin \psi}{1 - \cos^2 \gamma \sin^2 \psi}, \quad (22)$$

and  $\cos \delta_0 \cos(\alpha^\pm - \alpha_0) \times \text{Eq. (9)} - \sin \delta_0 \sin \psi \times \text{Eq. (19)}$  to

$$\cos \delta^\pm = \frac{\cos \psi \cos \delta_0 \cos(\alpha^\pm - \alpha_0) - \sin \gamma \sin \psi \sin \delta_0}{1 - \cos^2 \gamma \sin^2 \psi}. \quad (23)$$

Declinations  $\delta^+$  and  $\delta^-$  are then derived using  $\langle \text{atan2} \rangle$ . Values of  $\delta^\pm$  out of  $[-\pi/2, \pi/2]$  are excluded, but both may fall in this interval: one must arbitrarily select one of the positions  $(\alpha^+, \delta^+)$  and  $(\alpha^-, \delta^-)$ .

## C. Computation of $L_{o:o}$

### 1. Through integration of $\partial \ln L_{o:o} / \partial f$

The most efficient way to compute  $L_{o:o}$  is to integrate Eq. (P-80) with respect to  $f$ . This is done with the adaptative quadrature subroutine `<compute_ln_oto_Lh>` of `<mod_Aspects.f90>`. This procedure may compute  $\ln L_{o:o}$  for a single  $f$ , a grid of equidistant values of  $f$  starting at 0, or both.

The integration starts at  $f = 0$ . Subroutine `<compute_ln_oto_Lh>` first computes  $d(f) := \partial \ln L_{o:o} / \partial f$  (function `<drv_ln_oto_Lh>`) for a regular grid of values of  $f$ . Because  $d$  may vary a lot on a bin, especially near  $f = 0$ , the grid is then refined (procedure `<refine_grid>`): each bin  $[f_i, f_s]$  is recursively subdivided until

$$|d(f_i) + d(f_s) - 2d(f_m)| < \langle \text{epsilon\_ln\_oto\_Lh} \rangle \times (|d[f_i]| + |d[f_s]| + 2|d[f_m]|), \quad (24)$$

where  $f_m = (f_i + f_s)/2$  and `<epsilon\_ln\_oto\_Lh>` ( $> 0$  and  $\ll 1$ ) is a parameter defined in `<mod_constants.f90>` (cf. § VI.5). This ensures that the curvature of  $d$  in  $[f_i, f_s]$  is negligible and that the integration of  $d$  with the trapezoidal rule (i.e., interpolating  $d$  on the bin with a linear function) would provide an accurate value of  $\ln L_{o:o}(f_s) - \ln L_{o:o}(f_i)$  (typically, at most of the order of `<epsilon\_ln\_oto\_Lh>` in relative value).

Actually, instead of linear functions, we use cubic functions. The latter are interpolated on the values of  $d$  in the bin of interest and the two adjacent ones, following the procedure described in Steffen (1990) (function `<Steffen_integral>`). The final accuracy of  $\ln L_{o:o}$  should therefore be much better than with the trapezoidal rule.

### 2. Alternative method

The one-to-one likelihood may be computed in another way than from Eqs. (P-80) and (P-82) (cf. § P-4.2). To do this, we first define

$$\Lambda_i := P_{o:o} \left( \prod_{k=i}^n c_k \mid C' \cap \prod_{k=1}^{i-1} A_{k,0} \right). \quad (25)$$

One has

$$P_{o:o}(C \mid C') = \Lambda_1 \quad (26)$$

and, for any  $i \in \llbracket 1, n \rrbracket$ ,  $\Lambda_i$  may be computed as a function of  $\Lambda_{i+1}$  in the following way.

For  $\omega_1 = A_{i,0}$ ,  $\omega_2 = \prod_{k=i}^n c_k$  and  $\omega_3 = C' \cap \prod_{k=1}^{i-1} A_{k,0}$ , Eq. (P-3) gives

$$\Lambda_i = \frac{P_{o:o}(A_{i,0} \cap \prod_{k=i}^n c_k \mid C' \cap \prod_{k=1}^{i-1} A_{k,0})}{P_{o:o}(A_{i,0} \mid [\prod_{k=i}^n c_k] \cap C' \cap \prod_{k=1}^{i-1} A_{k,0})}. \quad (27)$$

Let us compute the numerator of Eq. (27). With  $\omega_1 = c_i$ ,  $\omega_2 = \prod_{k=i+1}^n c_k \cap A_{i,0}$  and  $\omega_3 = C' \cap \prod_{k=1}^{i-1} A_{k,0}$  in Eq. (P-3), one obtains

$$P_{o:o}(A_{i,0} \cap \prod_{k=i}^n c_k \mid C' \cap \prod_{k=1}^{i-1} A_{k,0}) = P_{o:o}(c_i \mid [\prod_{k=i+1}^n c_k] \cap C' \cap \prod_{k=1}^i A_{k,0}) P_{o:o}(\prod_{k=i+1}^n c_k \cap A_{i,0} \mid C' \cap \prod_{k=1}^{i-1} A_{k,0}). \quad (28)$$

The first factor in the right-hand side of Eq. (28) is simply

$$P_{o:o}(c_i \mid [\prod_{k=i+1}^n c_k] \cap C' \cap \prod_{k=1}^i A_{k,0}) = P_{o:o}(c_i \mid A_{i,0}) = \xi_{i,0} d^2 \vec{r}_i. \quad (29)$$

The second factor is

$$P_{o:o}(\prod_{k=i+1}^n c_k \cap A_{i,0} \mid C' \cap \prod_{k=1}^{i-1} A_{k,0}) = P_{o:o}(\prod_{k=i+1}^n c_k \mid C' \cap \prod_{k=1}^i A_{k,0}) P_{o:o}(A_{i,0} \mid C' \cap \prod_{k=1}^{i-1} A_{k,0}), \quad (30)$$

where we have used once again Eq. (P-3), with  $\omega_1 = \prod_{k=i+1}^n c_k$ ,  $\omega_2 = A_{i,0}$  and  $\omega_3 = C' \cap \prod_{k=1}^{i-1} A_{k,0}$ .

The right-most term in Eq. (30) is

$$P_{o:o}(A_{i,0} \mid C' \cap \prod_{k=1}^{i-1} A_{k,0}) = P_{o:o}(A_{i,0}) = 1 - f, \quad (31)$$

so, combining Eqs. (27), (28), (29), (30), (31) and (P-19), one obtains

$$\Lambda_i = \frac{\xi_{i,0} d^2 \vec{r}_i}{P_{o:o}(A_{i,0} \mid [\prod_{k=i}^n c_k] \cap C' \cap \prod_{k=1}^{i-1} A_{k,0})} \Lambda_{i+1}. \quad (32)$$

From Eq. (32), we get by iteration that

$$\Lambda_1 = \left( \prod_{i=1}^n \frac{\zeta_{i,0} d^2 \vec{r}_i}{P_{\text{o.o.}}[A_{i,0} | (\bigcap_{k=i}^n c_k) \cap C' \cap \bigcap_{k=1}^{i-1} A_{k,0}]} \right) \Lambda_{n+1} \quad (33)$$

and, since  $P_{\text{o.o.}}(C | C') = \Lambda_1$  and  $\Lambda_{n+1} = 1$ , that

$$P_{\text{o.o.}}(C | C') = \prod_{i=1}^n \frac{\zeta_{i,0} d^2 \vec{r}_i}{P_{\text{o.o.}}(A_{i,0} | [\bigcap_{k=i}^n c_k] \cap C' \cap \bigcap_{k=1}^{i-1} A_{k,0})}. \quad (34)$$

Because the event  $A_{i,0}$  does not depend on the coordinates  $\bigcap_{k=1}^{i-1} c_k$  of sources without counterpart,

$$P_{\text{o.o.}}(A_{i,0} | [\bigcap_{k=i}^n c_k] \cap C' \cap \bigcap_{k=1}^{i-1} A_{k,0}) = P_{\text{o.o.}}(A_{i,0} | C \cap C' \cap \bigcap_{k=1}^{i-1} A_{k,0}). \quad (35)$$

Finally, one obtains from Eqs. (34), (35), (P-31) and (P-13) that

$$L_{\text{o.o.}} = \left( \prod_{i=1}^n \frac{\zeta_{i,0}}{P_{\text{o.o.}}[A_{i,0} | C \cap C' \cap \bigcap_{k=1}^{i-1} A_{k,0}]} \right) \prod_{j=1}^{n'} \xi_{0,j}. \quad (36)$$

This formula is actually also valid for  $L_{\text{s.o.}}$  (with  $P_{\text{o.o.}}$  replaced by  $P_{\text{s.o.}}$ ), but is much less convenient than Eq. (P-32).

The terms  $P_{\text{o.o.}}(A_{i,0} | C \cap C' \cap \bigcap_{k=1}^{i-1} A_{k,0})$  in Eq. (36) can be computed in the same way as the probabilities  $P_{\text{o.o.}}(A_{i,j} | C \cap C')$  (cf. § P-5.4): to take into account the constraint  $\bigcap_{k=1}^{i-1} A_{k,0}$ , one may for instance restrict to  $j_k = 0$  the sums on  $j_k$  in Eq. (P-96), and this for all indices  $k$  such that  $\phi(k) < i$ .

This method is used in function `<func_ln_oto_Lh_alt>` of `<mod_Aspects.f90>`. The current implementation is however very inefficient and the subroutine `<compute_ln_oto_Lh>` should be preferred.

## D. One-to-one computations for $n > n'$

Although one always can define  $K$  and  $K'$  under assumption  $H_{\text{o.o.}}$  in such a way that  $n \leq n'$ , it is interesting to treat the case where  $n > n'$  to check the consistency of numerical calculations (cf. § P-5.5).

### 1. Probability of association

If  $n > n'$ , then  $n$  and  $f$  are replaced by  $n'$  and  $f'$  in Eq. (P-61). The denominator (Eq. (P-65)) of Eq. (P-4) becomes

$$P_{\text{o.o.}}(C | C') = \Xi \sum_{\substack{j_1=0 \\ j_1 \notin X_0}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \notin X_1}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin X_{n-1}}}^{n'} \frac{(n-q)!}{n!} f'^q (1-f')^{n'-q} \prod_{k=1}^n \xi_{k,j_k} = \Xi (1-f')^{n'-n} \sum_{\substack{j_1=0 \\ j_1 \notin X_0}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \notin X_1}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin X_{n-1}}}^{n'} \prod_{k=1}^n \eta'_{k,j_k}, \quad (37)$$

where

$$\eta'_{k,0} := (1-f') \xi_{k,0} \quad \text{and} \quad \eta'_{k,j_k} := \frac{f' \xi_{k,j_k}}{n - \#X_{k-1}} \quad \text{if } j_k \neq 0. \quad (38)$$

The numerator (Eq. (P-69)) is similarly modified:

$$P_{\text{o.o.}}(A_{i,j} \cap C | C') = \Xi (1-f')^{n'-n} \zeta'_{i,j} \sum_{\substack{j_1=0 \\ j_1 \notin X_0^*}}^{n'} \cdots \sum_{\substack{j_{i-1}=0 \\ j_{i-1} \notin X_{i-2}^*}}^{n'} \sum_{\substack{j_{i+1}=0 \\ j_{i+1} \notin X_i^*}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin X_{n-1}^*}}^{n'} \prod_{\substack{k=1 \\ k \neq i}}^n \eta'_{k,j_k}, \quad (39)$$

where

$$\zeta'_{i,0} := (1-f') \xi_{i,0} \quad \text{and} \quad \zeta'_{i,j} := \frac{f' \xi_{i,j}}{n} = \frac{f \xi_{i,j}}{n'} \quad \text{if } j \neq 0, \quad (40)$$

$$\eta'_{k,0}^* := (1-f') \xi_{k,0} \quad \text{and} \quad \eta'_{k,j_k}^* := \frac{f' \xi_{k,j_k}}{n - \#X_{k-1}^*} \quad \text{if } j_k \neq 0. \quad (41)$$

## 2. Expression of $\partial \ln L_{o:o}/\partial x_p$

Eq. (P-76) becomes

$$\begin{aligned} \frac{\partial P_{o:o}(C | C')}{\partial x_p} &= \Xi \frac{\partial([1 - f']^{n'-n})}{\partial x_p} \sum_{\substack{j_1=0 \\ j_1 \notin X_0}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \notin X_1}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin X_{n-1}}}^{n'} \prod_{k=1}^n \eta'_{k,j_k} \\ &+ \Xi (1 - f')^{n'-n} \sum_{\substack{j_1=0 \\ j_1 \notin X_0}}^{n'} \sum_{\substack{j_2=0 \\ j_2 \notin X_1}}^{n'} \cdots \sum_{\substack{j_n=0 \\ j_n \notin X_{n-1}}}^{n'} \sum_{i=1}^n \frac{\partial \ln \eta'_{i,j_i}}{\partial x_p} \prod_{k=1}^n \eta'_{k,j_k}, \end{aligned} \quad (42)$$

so

$$\frac{\partial \ln L_{o:o}}{\partial x_p} = (n' - n) \frac{\partial \ln(1 - f')}{\partial x_p} + \sum_{i=1}^n \sum_{j=0}^{n'} \frac{\partial \ln \zeta'_{i,j}}{\partial x_p} P_{o:o}(A_{i,j} | C \cap C'). \quad (43)$$

For  $x_p \neq f$ , one recovers Eq. (P-79) with  $\zeta'$  instead of  $\zeta$ .

For  $x_p = f$  ( $= n' f' / n$ ), Eq. (P-80) becomes

$$\frac{\partial \ln L_{o:o}}{\partial f} = \frac{n(1 - f) - \sum_{i=1}^n P_{o:o}(A_{i,0} | C \cap C')}{f(1 - f)}. \quad (44)$$

The numerator being the same, Eq. (P-81) still holds.

## 3. Alternative expression of the likelihood

The alternative expression of the likelihood given by Eq. (36) becomes

$$L_{o:o} = (1 - f')^{n'-n} \left( \prod_{i=1}^n \frac{\zeta'_{i,0}}{P_{o:o}[A_{i,0} | C \cap C' \cap \bigcap_{k=1}^{i-1} A_{k,0}]} \right) \prod_{j=1}^{n'} \xi_{0,j}, \quad (45)$$

where  $P_{o:o}(A_{i,0} | C \cap C' \cap \bigcap_{k=1}^{i-1} A_{k,0})$  is computed as detailed in § P-5.4.3 from Eq. (P-96), with  $\zeta$  replaced by  $\zeta'$  and with  $f'$  and  $n$  instead of  $f$  and  $n'$  in the expressions of  $\tilde{\eta}$  and  $\tilde{\eta}^*$ .

## E. One-to-several results

The one-to-several assumption is fully symmetrical to  $H_{s:o}$ , and all results derived under  $H_{o:s}$  may be obtained from § P-3 by swapping  $K$  and  $K'$ . We give them here for convenience.

The probabilities of association are

$$P_{o:s}(A_{i,j} | C \cap C') = \begin{cases} \frac{f' \xi_{i,j}}{(1 - f') n \xi_{0,j} + f' \sum_{k=1}^n \xi_{k,j}} & \text{if } i \neq 0, \\ \frac{(1 - f') n \xi_{0,i}}{(1 - f') n \xi_{0,j} + f' \sum_{k=1}^n \xi_{k,j}} & \text{if } i = 0 \end{cases} \quad (46)$$

for  $j \neq 0$  (cf. Eq. (P-24)), and

$$P_{o:s}(A_{i,0} | C \cap C') = \prod_{j=1}^{n'} (1 - P_{o:s}[A_{i,j} | C \cap C']) \quad (\text{cf. Eq. (P-26)}). \quad (47)$$

The overall likelihood is

$$L_{o:s} = \left( \prod_{i=1}^n \xi_{i,0} \right) \prod_{j=1}^{n'} \left( [1 - f'] \xi_{0,j} + \frac{f'}{n} \sum_{k=1}^n \xi_{k,j} \right) \quad (\text{cf. Eq. (P-32)}). \quad (48)$$

A maximum likelihood estimator of  $f'$  is

$$\hat{f}'_{o:s} = 1 - \frac{1}{n'} \sum_{j=1}^{n'} \hat{P}_{o:s}(A_{0,j} | C \cap C') \quad (\text{cf. Eq. (P-39)}), \quad (49)$$

where  $\hat{P}_{o:s}$  is the value of  $P_{o:s}$  at  $f' = \hat{f}'_{o:s}$ .

An estimator of  $f$  is

$$\hat{f}_{o:s} = 1 - \frac{1}{n} \sum_{i=1}^n \hat{P}_{o:s}(A_{i,0} | C \cap C') \quad (\text{cf. Eq. (P-42)}). \quad (50)$$

## F. Tedious several-to-one calculations

### 1. Expression of $\partial^2 \ln L_{s:o} / \partial f^2$

We prove here Eq. (P-41), and thus that  $L_{s:o}$  is convex and has only one maximum at  $f = \hat{f}_{s:o}$  (cf. § P-3.2.2). Deriving Eq. (P-38), one obtains

$$\begin{aligned} \frac{\partial^2 \ln L_{s:o}}{\partial f^2} &= -\frac{1}{f^2(1-f)^2} \left( n[1-f]^2 + f[1-f] \frac{\partial \sum_{i=1}^n P_{s:o}[A_{i,0} | C \cap C']}{\partial f} + [2f-1] \sum_{i=1}^n P_{s:o}[A_{i,0} | C \cap C'] \right) \\ &= -\frac{1}{f^2(1-f)^2} \sum_{i=1}^n \left( [1-f]^2 + f[1-f] \frac{\partial P_{s:o}[A_{i,0} | C \cap C']}{\partial f} + [2f-1] P_{s:o}[A_{i,0} | C \cap C'] \right). \end{aligned} \quad (51)$$

One has

$$\begin{aligned} f(1-f) \frac{\partial P_{s:o}(A_{i,0} | C \cap C')}{\partial f} &= f(1-f) \frac{-n' \xi_{i,0} (1-f) n' \xi_{i,0} + f \sum_{j=1}^{n'} \xi_{i,j} - (1-f) n' \xi_{i,0} (-n' \xi_{i,0} + \sum_{j=1}^{n'} \xi_{i,j})}{([1-f] n' \xi_{i,0} + f \sum_{j=1}^{n'} \xi_{i,j})^2} \\ &= -\frac{(1-f) n' \xi_{i,0}}{(1-f) n' \xi_{i,0} + f \sum_{j=1}^{n'} \xi_{i,j}} \frac{f \sum_{j=1}^{n'} \xi_{i,j}}{(1-f) n' \xi_{i,0} + f \sum_{j=1}^{n'} \xi_{i,j}} \\ &= -P_{s:o}(A_{i,0} | C \cap C') \sum_{j=1}^{n'} P_{s:o}(A_{i,j} | C \cap C') \\ &= -P_{s:o}(A_{i,0} | C \cap C') (1 - P_{s:o}[A_{i,0} | C \cap C']), \end{aligned} \quad (52)$$

so

$$\begin{aligned} (1-f)^2 + f(1-f) \frac{\partial P_{s:o}(A_{i,0} | C \cap C')}{\partial f} + (2f-1) P_{s:o}(A_{i,0} | C \cap C') \\ &= (1-f)^2 - P_{s:o}(A_{i,0} | C \cap C') (1 - P_{s:o}[A_{i,0} | C \cap C']) + (2f-1) P_{s:o}(A_{i,0} | C \cap C') \\ &= (1-f)^2 - 2(1-f) P_{s:o}(A_{i,0} | C \cap C') + P_{s:o}(A_{i,0} | C \cap C')^2 \\ &= ([1-f] - P_{s:o}[A_{i,0} | C \cap C'])^2. \end{aligned} \quad (53)$$

Equation (P-41) follows immediately from Eqs. (51) and (53).

### 2. Analytic expression of $\hat{\partial}^2 \ln L_{s:o} / (\hat{\partial} x_p \hat{\partial} x_q)$

Deriving Eq. (P-74), one obtains

$$\frac{\partial^2 \ln L}{\partial x_p \partial x_q} = \frac{1}{P(C | C')} \frac{\partial^2 P(C | C')}{\partial x_p \partial x_q} - \frac{1}{P^2(C | C')} \frac{\partial P(C | C')}{\partial x_p} \frac{\partial P(C | C')}{\partial x_q}, \quad (54)$$

and, because of Eqs. (P-74) and (P-28),

$$\frac{\hat{\partial}^2 \ln L}{\hat{\partial} x_p \hat{\partial} x_q} = \frac{1}{\hat{P}(C | C')} \frac{\hat{\partial}^2 P(C | C')}{\hat{\partial} x_p \hat{\partial} x_q}. \quad (55)$$

From Eqs. (P-33), (P-74) and (P-4), one gets

$$\frac{\partial^2 P_{s:o}(C | C')}{\partial x_p \partial x_q} = \sum_{i=1}^n \sum_{j=0}^{n'} \frac{\partial^2 \ln \zeta_{i,j}}{\partial x_p \partial x_q} P_{s:o}(A_{i,j} \cap C | C') + \sum_{i=1}^n \sum_{j=0}^{n'} \frac{\partial \ln \zeta_{i,j}}{\partial x_p} \frac{\partial P_{s:o}(A_{i,j} \cap C | C')}{\partial x_q}. \quad (56)$$

Using Eqs. (P-22) and (P-75) with  $h_k = \sum_{j_k=0}^{n'} \zeta_{k,j_k}$  and  $\Upsilon = \llbracket 1, n \rrbracket \setminus \{i\}$ , the right-most term above becomes

$$\begin{aligned} \frac{\partial P_{s:o}(A_{i,j} \cap C | C')}{\partial x_q} &= \Xi \frac{\partial \zeta_{i,j}}{\partial x_q} \prod_{\substack{k=1 \\ k \neq i}}^n \sum_{j_k=0}^{n'} \zeta_{k,j_k} + \Xi \zeta_{i,j} \sum_{\substack{\ell=1 \\ \ell \neq i}}^n \frac{\partial \sum_{j_\ell=0}^{n'} \zeta_{\ell,j_\ell}}{\partial x_q} \prod_{\substack{k=1 \\ k \notin \{i,\ell\}}}^n \sum_{j_k=0}^{n'} \zeta_{k,j_k} \\ &= \Xi \frac{\partial \ln \zeta_{i,j}}{\partial x_q} \zeta_{i,j} \prod_{\substack{k=1 \\ k \neq i}}^n \sum_{j_k=0}^{n'} \zeta_{k,j_k} + \Xi \frac{\zeta_{i,j}}{\sum_{j_i=0}^{n'} \zeta_{i,j_i}} \sum_{\substack{\ell=1 \\ \ell \neq i}}^n \sum_{j_\ell=0}^{n'} \frac{\partial \ln \zeta_{\ell,j_\ell}}{\partial x_q} \zeta_{\ell,j_\ell} \prod_{\substack{k=1 \\ k \neq \ell}}^n \sum_{j_k=0}^{n'} \zeta_{k,j_k} \\ &= \frac{\partial \ln \zeta_{i,j}}{\partial x_q} P_{s:o}(A_{i,j} \cap C | C') + P_{s:o}(A_{i,j} | C \cap C') \sum_{\substack{\ell=1 \\ \ell \neq i}}^n \sum_{j_\ell=0}^{n'} \frac{\partial \ln \zeta_{\ell,j_\ell}}{\partial x_q} P_{s:o}(A_{\ell,j_\ell} \cap C | C'). \end{aligned} \quad (57)$$

For  $\vec{x} = \hat{x}_{s,o}$ ,

$$\begin{aligned} \sum_{\substack{\ell=1 \\ \ell \neq i}}^n \sum_{j_\ell=0}^{n'} \frac{\partial \ln \zeta_{\ell, j_\ell}}{\hat{\partial} x_q} \hat{P}_{s:o}(A_{\ell, j_\ell} \cap C | C') &= \sum_{\ell=1}^n \sum_{j_\ell=0}^{n'} \frac{\partial \ln \zeta_{\ell, j_\ell}}{\hat{\partial} x_q} \hat{P}_{s:o}(A_{\ell, j_\ell} \cap C | C') - \sum_{j_i=0}^{n'} \frac{\partial \ln \zeta_{i, j_i}}{\hat{\partial} x_q} \hat{P}_{s:o}(A_{i, j_i} \cap C | C') \\ &= - \sum_{k=0}^{n'} \frac{\partial \ln \zeta_{i, k}}{\hat{\partial} x_q} \hat{P}_{s:o}(A_{i, k} \cap C | C') \end{aligned} \quad (58)$$

since the first term on the right-hand side of the first line is zero from Eqs. (P-33) and (P-28). Finally, combining Eqs. (56), (57), (58) and dividing by  $\hat{P}_{s:o}(C | C')$ , one obtains from Eqs. (55) and (P-4) that

$$\frac{\partial^2 \ln L_{s:o}}{\hat{\partial} x_p \hat{\partial} x_q} = \sum_{i=1}^n \sum_{j=0}^{n'} \left( \frac{\partial^2 \ln \zeta_{i, j}}{\hat{\partial} x_p \hat{\partial} x_q} + \frac{\partial \ln \zeta_{i, j}}{\hat{\partial} x_p} \left[ \frac{\partial \ln \zeta_{i, j}}{\hat{\partial} x_q} - \sum_{k=0}^{n'} \frac{\partial \ln \zeta_{i, k}}{\hat{\partial} x_q} \hat{P}_{s:o}(A_{i, k} | C \cap C') \right] \right) \hat{P}_{s:o}(A_{i, j} | C \cap C'). \quad (59)$$

For  $x_p = x_q = f$ , one recovers Eq. (P-41) at  $f = \hat{f}_{s:o}$ . For other unknown parameters, a numeric computation might be simpler... Whatever the method, one can then build the covariance matrix of  $\hat{x}_{s,o}$  and derive the uncertainties on the unknown parameters from it (cf. Eq. (P-34) and § P-3.2.1).

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