Fine Guidance Sensor Instrument Report

THE ST ScI TRANSFER FUNCTION MODE
DATA REDUCTION PACKAGE

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I. SUMMARY

The purpose of this Instrument Report is to describe the strategy and the basic algorithms that have been implemented in the ST ScI Fine Guidance Sensor Transfer Function Mode Reduction Package. The Transfer Function Mode Reduction Package software is used for the analysis of Science Verification data, Instrument Scientist Calibration data, and General Observer scientific data. At present, the Transfer Function Mode Reduction Package (TFMRP) is the principal tool to be used for all double star data analysis. References to the actual code are included throughout this report. However, the emphasis is on the techniques so this Instrument Report can serve as the basic reference for the SDAS personnel who will actually implement the package in the STSDAS/IRAF environment. Future General Observers will have access to this Report and a new Fine Guidance Sensor (FGS) Instrument Handbook will also include information that General Observers will need to know regarding the Institute's ability to help them with their FGS data analysis. A detailed description of the code and its usage is given in [6].

The present version of the ST ScI TFMRP is designed to do two main things: (1) To calibrate FGS Single Star transfer functions by using calibration data taken on selected single stars. Appropriate Calibration Data Base System (CDBS) tables will be populated (or modified) as a result of these calibration observations and the associated data reduction; (2) To analyze FGS transfer function observations on double stars. The analysis of triple stars and extended objects (i.e., angular diameter measurements or measurements of nebular objects) will be discussed in a future Instrument Report. The calibration data for them will be acquired during the Cycle 1 Instrument Scientist calibration observations. The basic transfer function calibration effort consists of a '19 Points of Light' measurement in the prime FGS, the one in radial bay #3.
II. INTRODUCTORY NOTES

In the following we will assume that the reader has some knowledge of the FGS as an astrometric instrument and in particular with the TRANSfer function astrometric Mode. The reader can find detailed descriptions of the FGS modes of operation in several HST project documents and journal articles. To guide the reader to this literature, a complete list of the relevant documents and papers is given in the references at the end of this Report.

We also assume that the FGS TRANS Mode data are retrieved from the DMF/DADS system through Retlist and decoded using the ST ScI AEDP unpacking software [5].

When running in calibration mode, the TFMRP will produce data for the CDBS or the PDB (Project Data Base) databases (Fig. 1). For example, as the mis-figured primary mirror has induced field dependent aberrations (as seen by the FGSs), it is now imperative to calibrate the Single Star transfer function all across the FGS field of view (hence the ‘19 Points of Light’ observations referred to above). As shown in Fig. 1, the present version of the TFMRP includes data rectification, data smoothing, and double star measurement. The latter is primarily based on a correlation technique.

In the next three sections each step will be illustrated and a brief discussion of the relevant algorithms given.
III. DATA RECTIFICATION

Data rectification is comprised of four main corrections, namely the encoder readings corrections, the photomultiplier tube (PMT) mismatch corrections, the differential velocity aberration correction, and the minimization of the spacecraft jitter.

The encoder readings correction refers to the application of a look-up table which contains a set of values representing the systematic shifts of the encoder readings as a function of encoder position. These systematic corrections were determined by measurement during on-ground testing. They are to be delivered by Perkin-Elmer Corp. (now Hughes Danbury Optical Systems). Both the sign and the amplitudes of these effects are important, for being systematic errors, applying them with the incorrect parity will double them. The correct table is still not in the CDBS. More information on the nature and the detection of the encoder corrections can be found in the Astrometry Handbook [1].

The FGS Transfer Function is usually written as $S = (A - B)/(A + B)$ where $A$ and $B$ are the photomultiplier counts from the two photomultiplier tubes per axis. (Acquiring the photomultiplier counts by moving the FGS instantaneous field-of-view across the scientific target is referred to as scanning the target so sometimes the transfer function is called a transfer scan.) There are two axes per FGS (arranged by a polarizing beam splitter); the subscript $x$ or $y$ is added to $S$ in order to specify which axis is meant. Similarly, an $x$ or $y$ subscript is attached to $A$ and $B$ when clarity is needed. The PMT counts vary in a regular fashion with the angular distance between the current location of the center of the FGS instantaneous field-of-view and the interferometer null (which is roughly aligned with the optical axis of the HST). To concretely fix ideas, a set of transfer functions, as expected before launch, is given in Fig. 2. The zero noise, ideal equation for the transfer function, as illustrated in Fig. 2, predicts that $S$ will vanish when the instantaneous field-of-view is far away from the optical axis (say $> 0.1$ arcsec). In practice, this condition is rarely realized because $A$ and $B$ are never equal far from the null (or even exactly at it) as a consequence of mismatch in the responsitivity or sensitivity of the two photomultiplier tubes. Thus, a
PMT mismatch correction is necessary. It consists of the computation of the mean value of $A - B$ far from the null (say $\Delta ab$). The revised version of $S$ takes the form

$$S = (A - B - \Delta ab)/(A + B).$$

This mismatch correction is applied in the subroutine MAKE_SCURVE.

The differential velocity aberration correction includes the reduction of the observed line of sight to the solar system barycenter in a reference frame of fixed orientation (e.g., J2000.0). It includes the motion of the HST spacecraft about the center of mass of the Earth, the motion of the center of mass of the Earth about the Earth-Moon barycenter, and finally the motion of the Earth-Moon barycenter about the solar system barycenter. (The intermediary of going to the heliocenter is unnecessary.) Differential velocity aberration plays a much bigger role in the reduction of POSitional Mode data than it does in the reduction of TRANSfer Mode data so it is discussed in the POS Mode Instrument Report [8].

The minimization, and hopefully complete removal, of the solar-array induced jitter will be a major task during data rectification. Since all FGS data should be taken in the 32 Kbit telemetry mode, we will have the maximum amount of information, from the Guide Stars, with which to accomplish this. An algorithm for jitter removal does exist but further investigation is needed to determine if it is sufficient. The current approach is that of executing multiple scans while taking science data in TRANS Mode. In this way, jitter corrupted scans can be easily identified (by comparison to the others) and removed from the set which will then be processed through this pipeline. Actual observational data provides an estimate of an average of 2-3 (unusable) jitter corrupted scans out of 10.
IV. DATA SMOOTHING

In this section we discuss the data smoothing technique which is applied to the transfer function data after rectification. The idea here is to fit the raw data in such a way that all the essential features in the transfer function are preserved in a noiseless (or at least a higher signal-to-noise) version. A cubic-spline fit might be deemed appropriate for this; we decided instead to use a piece-wise polynomial fit for two reasons. First, as this technique is close to the spline approach, we expected analogous performance (see Fig. 3). Second, a polynomial representation of the smoothed transfer function makes it possible to compute the correlation integral (used during double star measurement) analytically (see Eq. (3) §V). In the next two sub-sections we will detail our approach to fitting the $S$ curve.

a) Functional Fitting

Having obtained the experimental curve (dotted curve in Fig. 3), which is a function of the instrumentally and scientifically corrected star selector encoder angle readings, we fit it piecewise to low-order polynomials. The fits are executed via a constrained, non-equally weighted, least squares algorithm. Since this is a photon (i.e., Poisson) process we know the standard deviations of each value of $S$. Hence, we can reliably determine weights. The polynomials (we allow linear, quadratic, and cubic) are forced to obey continuity conditions at their joining points. In addition, depending on the degree of the polynomial, we may also demand differentiability and even a higher order of smoothness (all enforced by Lagrange multipliers at the joining points).

There are two refinements to this procedure. One is that the choice of the mean width of the intervals is governed by a minimum number of pairs of photomultiplier counts per interval constraint. The other is that the upper limit for a particular interval’s width is governed by the local curvature. The analytical details are in the next subsection. The piecewise linear continuous fit to the data is shown in Fig. 3.
b) Analytical Details

Define $H(x)$ to be the usual Heaviside function,

$$H(x) = \begin{cases} 
1 & x \geq 0 \\
0 & x < 0.
\end{cases}$$

So, if $a < b$ then $h(x; a, b) = H(x - a)H(b - x)$ has the properties

$$h(x; a, b) = \begin{cases} 
0 & x < a \\
1 & x \in [a, b] \\
0 & x > b.
\end{cases}$$

Next define $N$ joints (or knots in spline terminology) $z_1, z_2, \ldots, z_N$. The joints are where we will enforce continuity, smoothness, and so on. We also need the general polynomial $P_d(x)$ of degree $d$; viz.

$$P(x) = a + bx + cx^2 + \cdots + qx^d.$$ 

As we shall need one $d$'th order polynomial per interval (the boundaries of the intervals are defined by the set of joint locations $\{z_n\}$), we will use a double indexing scheme for the coefficients in $P = P_n$ ($n = 0, 1, 2, \ldots, N$)

$$P_n(x) = a_{n0} + a_{n1}x + a_{n2}x^2 + \cdots + a_{nd}x^d$$

$P_n$ is defined everywhere $[i.e., x \in (-\infty, \infty)]$ but will only be used on $[z_n, z_{n+1}]$.

We want to represent a function $F(x)$ on $x \in [x_{\text{min}}, x_{\text{max}}]$, where $x_{\text{min}} = z_1$ and $x_{\text{max}} = z_N$, by a linear combination of $N - 1$ $d$'th order polynomials $\{P_n\}$ which obey various boundary conditions at $\{z_n\}$. Thus, we write

$$F(x) = \sum_{n=1}^{N-1} h(x; z_n, z_{n+1})P_n(x)$$

where, were we only enforcing continuity at the $N - 2$ interior points $\{z_n\}$ one would have the constraints

$$P_n(z_{n+1}) = P_{n+1}(z_{n+1}); \quad n = 1, \cdots, N - 2.$$
We also want the determination of the \( \{a_{nm}\} \) to rest on least squares given that we have measured \( F(x) \) at \( x_{min} = x_1, x_2, \ldots, x_L = x_{max} \). Thus, we form

\[
R_c = \sum_{\ell=1}^{L} w_{\ell} [F(x_{\ell}) - \sum_{n=1}^{N-1} h(x_{\ell}; z_n, z_{n+1}) P_n(x_{\ell})]^2 - \sum_{n=1}^{N-2} \lambda_{n+1} [P_n(z_{n+1}) - P_{n+1}(z_{n+1})]
\]

and minimize \( R_c \) with respect to the \( (N-1)d \) values of \( \{a_{nm}\} \) and the \( N - 2 \) Lagrange multipliers \( \{\lambda_n\} \). (In practice, we do not solve for the Lagrange multipliers in the formal way but instead enforce the constraint conditions as additional equations of observation with extremely high weights; the relative weights are typically \( 10^6 \) to 1.) The weights \( w_{\ell} \) are the photon-noise implied weights of the Transfer Function from Eq. (1). There is a point of subtlety for \( A \) and \( B \) are anti-correlated; thus

\[
\sigma_S = (\sqrt{A} + \sqrt{B})/ < A + B >, \quad w_S = 1/\sigma_S^2
\]

in the notation of Eq. (1).

The extension to incorporate smoothness at the joints is accomplished by minimizing \( R_s \) instead of \( R_c \);

\[
R_s = R_c - \sum_{n=1}^{N-2} \Lambda_{n+1} [P'_n(z_{n+1}) - P'_{n+1}(z_{n+1})]
\]

where \( P'_n(z_k) \) means \( \frac{dP_n(x)}{dx} \big|_{x=z_k} \).

The constrained piece-wise least squares fit to the rectified \( S \) curve data is performed with a call to the subroutine SCURVE\_INTERP.
V. DOUBLE STAR MEASUREMENT

a) The Calculation of the Parameters of a Binary Star

Double star measurement refers, in the present version of the code, mainly to the determination of the parameters of double stars. It includes, at the moment, two different (although interconnected) functions, namely (1) the co-adding of several scans on the same scientific target and (2) the determination of the two separations ($dx$ and $dy$), the magnitude difference between the primary and the secondary components ($\Delta m$), and, ultimately, the computation of the position angle (PA) of double stars. In §V.b below, we will discuss the determination of $dx$, $dy$, and $\Delta m$, and then the simpler problem of co-adding scans. The computation of PA is detailed in §V.c.

b) Algorithm Details

Assume that we know the form of the ‘Single Star’ transfer function, that is the reference transfer function for this place in this FGS. The hypothesis is that the incoming light from two different sources, close by on the celestial sphere, is incoherent and the application of the superposition principle yields the expected Double Star transfer function, $D(x)$ in the form of a linear combination of two single star transfer functions $S$, viz.

$$D(x) = A(\Delta m)[S(x + x_0) + B(\Delta m)S(x + x_0 + dx)]$$

(and its analog for the $y$-axis), where the second single star transfer function $S(x + dx)$ is identical to the first but displaced along the $X$-axis by an additional amount $dx$, the projected double star separation. The shared shift of $x_0$ in the single star reference transfer function is to correct for an arbitrary translation between the reference star transfer function and those of the double star under study. $A(\Delta m)$ is an overall normalization factor. $B(\Delta m)$ represents the intensity ratio between the primary and the secondary stars comprising the double. Both of these factors depend on the apparent magnitude difference between the two stars, $\Delta m$. 
The model just described is fitted to the observed transfer function curve and the parameters \( dx \) and \( \Delta m \) derived. It is worth noting here that two independent estimates of \( \Delta m \) are potentially available, one from each FGS axis.

In practice, a grid of models is generated by varying \( dx \) and \( \Delta m \). Each model is cross-correlated with the observed transfer function by computing the correlation integral

\[
C = \int D(t - u)S(t)dt.
\]  

The template function \( D \) is being cross-correlated with the actual Koester's prism fringe visibility function \( S \). The sought-for value of \( u \), which maximizes the correlation integral \( C \), represents the shift along this axis between the two functions. The optimum value will be denoted by \( u_0 \).

The best-fit model is chosen as the one with parameters which minimize the sum of the squares of the differences between the theoretical model in \( D \) and observed values in \( S \), viz.

\[
\int [D(t - u_0) - S(t)]^2 dt = \text{minimum}.
\]

This approach was preferred to the direct application of a least squares-like scheme for its robustness—in relation to the range of narrow separations (from 100 mas down to about 10 mas) where the astrometer FGS will make its most interesting detections—and the independent difficulty of giving sufficiently accurate initial guesses for \( dx \) and \( \Delta m \). However, if felt necessary, the accuracy of the fit can be improved, now using the answers from the correlation technique as initial guesses for a final least squares adjustment. Indeed, all possible options of correlation/least squares fitting are supported.

As discussed in §IV, before running the cross-correlation process, the photon noise in the observed transfer function is smoothed via a piece-wise low-order polynomial fit. Continuity is imposed at the bin boundaries up to a specified level (i.e., continuity, first derivatives continuous, or second derivatives continuous). This polynomial smoothing increases the resolution of the subsequent cross-correlation and makes it possible to compute the correlation integral \( C \), as well as the sum of squares to be minimized, \textit{analytically}. 
While not described in detail herein, there is a completely separate least squares version of this process (see the Franz et al. paper [10].), and a Fourier technique has also proven applicable (J. Hershey, in press).

b.1) Shifting the Transfer Functions

At this stage of the data processing the transfer functions from the different scans have been transformed into piece-wise continuous polynomials of a given degree. As explained above, owing to spacecraft motions, the template transfer function \( D \) and the actual transfer function \( S \) are not taken at the same location of the FGS \( x \) or \( y \) axes. To avoid stepping too many times through the loop in \( x_0 \) [see Eq. (2)], a coarse centering of \( D(x) \) with respect to the observed \( S(x) \) is first performed in the following fashion. First, we compute the distance of \( D(x) \) to \( S(x) \) as

\[
\Delta x = x_s - x_d,
\]

where \( x_s \) and \( x_d \) are the reference points defined by

\[
x_s = (x_{s,max} - x_{s,min})/2
\]

and similarly with a \( d \) subscript. To shift \( D(x) \) closer to \( S(x) \) we apply the translation

\[
x_d' = x_d + \Delta x,
\]

to the template curve \( D(x) \). This transformation requires that the coefficients of the polynomial representing the template be transformed accordingly. The new coefficients as a function of the old are given in Appendix 1.

b.2) Creating a Double Star Template

The actual formula used to generate a Double Star (D) template is [see also Eq. (2)]

\[
D(x) = \frac{R(x) + 10(-0.4\Delta m)R(x + dx)}{1 + 10(-0.4\Delta m)},
\]

(7)
where $R(x)$ is a single star transfer function taken as close as possible, within the FGS field-of-view, to the FGS location of the scientific observation $S(x)$. Naturally, a formula analogous to Eq. (7) applies for the $y$ axis.

Once $dx$ is fixed we can shift $R(x)$ to the new location $x + dx$. This will serve to represent the transfer function of the ‘secondary’ star (of course the assignment of primary vs. secondary is just a matter of convention) of the template double along the $x$ axis. Note though, the apparent magnitude difference has not yet been taken into account. Given $\Delta m$, Eq. (7) takes into account the contribution of the secondary star to the total intensity.

b.3) The Calculation of the Integrals

The heart of the subroutine CORR_TRANSF that correlates the observed scan and the current template (i.e., given $\Delta m$ and $dx$) finds the $x_0$ value that best correlates the two transfer functions, now represented by polynomials, according to Eq. (3). This integral can be evaluated analytically because of the simple, analytical representation we have developed for the smoothed transfer function; see Appendix 2. Similar comments apply to the minimization integral in Eq. (4); see Appendix 3.

b.4) Co-Adding Different Scans

Co-adding Transfer Scans refers to adding together multiple scans, taken on the same scientific target. This would be done to improve the signal-to-noise ratio both for fainter targets and as a primitive jitter smoothing technique. Since the coordinate system in which the transfer scans are acquired is not rigidly fixed, we need to determine the translation that has occurred between successive scans. This is represented by the parameter $x_0$ in the above equations. Thus, in a sense, we want to best fit one of the many scans acquired on a scientific target not with a single star reference transfer function, but with that scan of this target labeled the ‘reference’ scan. The procedure to do so is identical to that for fitting a binary star, only this is a one-parameter problem not a three-parameter problem (i.e., no need for $dx$ nor $\Delta m$). The same software that was just described can, therefore,
be used for this simpler purpose by constraining the values of these parameters. This is what we do. Suppose we want to co-add a set of scans taken on a single star. Subroutine CORR_TRANSF is then used with both \( dx \) and \( \Delta m \) set to zero. Suppose also that one of the scans is chosen as the reference (ref). Then, we first coarse shift the remaining ones to the reference scan as described in §V.b.1. Let us call \( shift_i = x_{si} - x_{ref} \) the computed displacement on the X axis of the i’th scan from the reference. Here, \( x_{si} = (x_{i,max} - x_{i,min})/2 \) and \( x_{ref} = (x_{ref,max} - x_{ref,min})/2 \). The residual shift, \( x0max \), is calculated from the implementation of Eq. (3) discussed in §V.b.3. Then, before co-adding the i’th scan to the reference one, the following transformation is applied to the X (Y) coordinate of the i’th scan

\[
x' = x + shift_i - x0max_i
\]

The formula given in Eq. (8) has been proven effective to better than 5 milli-second of arc.

Of course, the co-adding scheme can be different (for example, we can co-add the reference and one of the remaining scans, define the result as the new reference and repeat the co-adding step with another of the remaining scans) but Eq. (8) remains the basic transformation to be applied to the scan that is currently being co-added.

c) The Computation of the Position Angle

The computation of the position angle (PA) is done in a completely differential way. As discussed above, the double star measurement outputs \( dx \) and \( dy \), the separations between the two stars, along the interferometer X and Y axes. These quantities are expressed in the FGS image space in seconds of arc on the sky (demagnified). Both \( dx \) and \( dy \) are very much less than one arc second. We assume that differential optical distortions can be disregarded over such a small scale length. Thus, to transform \( dx \) and \( dy \) (considered as a plane vector with origin at the primary component of the double) into the V2–V3 plane we have to only account for the relative orientation of the two frames by using the most recent (on-flight calibrated) alignment matrices. The distortion correction tables are not applied.
The present version of the code uses the pre-launch transformations matrices, i.e.

\[ V_2 = -Y, \quad V_3 = X \quad \text{(FGS 1)} \]
\[ V_2 = X, \quad V_3 = Y \quad \text{(FGS 2)} \]
\[ V_2 = Y, \quad V_3 = -X \quad \text{(FGS 3)} \]

We have adopted the definition of the \( V_2 \)-\( V_3 \) plane as given in [2] Bradley et al. (1991, see their Fig. 1). The use of real alignment matrices will result in a small coupling of the reference axes and it requires the component \( dz \) defined as \( \sqrt{1 - (dz^2 + dy^2)} \).

Once in the \( V_2 \)-\( V_3 \) plane, knowledge of the spacecraft orientation (attitude) with respect to a reference equatorial North (i.e., at a specified epoch and equinox) gives the position angle of the double. The formula is, with all quantities in degrees,

\[ PA = 360 - \text{ANGV3} + \arctan(V2/V3). \quad (9) \]

\text{ANGV3} specifies the orientation of the \( V_3 \) axis as defined by the angle from the North counted positive through West (see Fig. 4). This quantity is given with quite good accuracy (of the order of 0.5 deg) in the FGS AEDP header files. As shown in Fig. 4,

\[ \text{PAV3} = 360 - \text{ANGV3} \] is the position angle (in the astronomical sense, i.e. the angle is counted positive from North towards the East) of the spacecraft \( V_3 \) axis. The reference equatorial North is that at equinox J2000.0 and epoch of the date. Eq. (9) is implemented in the subroutine POS\_ANGLE.

Notice that the position angle given in Eq. (9) would only be exact if the location of the double observed in the FGS 3 pickle coincides with the \( V_1 \) axis. Of course, this will never be the case as the pickle is some 10' away from the \( V_1 \) axis. However, Eq. (9) is appropriate for most applications. The exact expression for \( PA \) will be given in a forthcoming memo.
FGS-RELATED REFERENCES

Appendix 1

Transformation of the polynomial coefficients

Let $P_i(x)$ be the polynomial representing the smoothed TF (actual or template) in the i’th bin $x_i \leq x \leq x_{i+1}$. The degree of this polynomial is $\text{ndeg}$ (the degree of the polynomial does not change from bin to bin). Let us write $P_i(x)$ as

\begin{equation}
P_i(x) = \sum_{\ell=0}^{\text{ndeg}} a_{\ell}^{(i)} x^{\ell}.
\end{equation}

Next, we apply the transformation

\[ x' = x + xt \]

to Eq. (1.1), which gives

\[ P_i(x') = \sum_{\ell=0}^{\text{ndeg}} a_{\ell}^{(i)} (x' - xt)^{\ell}. \]

After expanding the expression $(x' - xt)^{\ell}$, and assuming that $\text{ndeg}=3$ (the highest degree we consider for the fitting polynomials), we obtain the final expression

\begin{equation}
P_i(x') = a_{0}^{(i)} c_{0} + a_{1}^{(i)} c_{1}(-xt) + a_{2}^{(i)} c_{2}(-xt)^{2}
+ a_{3}^{(i)} c_{3}(-xt)^{3}
+ \{a_{1}^{(i)} c_{0} + a_{2}^{(i)} c_{1}(-xt) + a_{3}^{(i)} c_{2}(-xt)^{2}\} x'
+ \{a_{2}^{(i)} c_{0} + a_{3}^{(i)} c_{1}(-xt)\} x^{2}
+ a_{3}^{(i)} c_{3} x^{3}.
\end{equation}

From Eq. (1.2) we can derive the table of transformation for the coefficients, i.e.

\begin{align}
a_{0i}' &= \sum_{\ell=0}^{\text{ndeg}} a_{\ell}^{(i)} c_{\ell}(-xt)^{\ell} \\
a_{1i}' &= \sum_{\ell=1}^{\text{ndeg}} a_{\ell}^{(i)} c_{\ell-1}(-xt)^{\ell-1} \\
a_{2i}' &= \sum_{\ell=2}^{\text{ndeg}} a_{\ell}^{(i)} c_{\ell-2}(-xt)^{\ell-2} \\
a_{3i}' &= \sum_{\ell=3}^{\text{ndeg}} a_{\ell}^{(i)} c_{\ell-3}(-xt)^{\ell-3},
\end{align}

where $\text{ndeg} = 3$ and $c_{k}^{\ell} = \frac{\text{m}}{k!(\ell-k)!}$. Eqs. (1.3) have been implemented in the subroutine SHIFT_DT.
Appendix 2

Direct approach to correlating FGS Transfer Scans.

Consider the fundamental relation

\[(2.1) \quad C(x_0) = \int_{-\infty}^{+\infty} S(x)D(x + x_0)dx.\]

We seek the \(x_0\) that maximize the expression (2.1), where \(S(x)\) is the observed TF scan. We can write it as

\[(2.2) \quad C(x_0) = \int_{x_{\text{min}}}^{x_{\text{max}}} S(x)D(x + x_0)dx\]

where \([x_{\text{max}} - x_{\text{min}}]\) is the size of the correlation window, i.e. the region where both \(S\) and \(D\) are different from zero. Since both the actual (observed) scan \(S\) and the template \(D\) are piecewise polynomials, we can write

\[(2.3) \quad C(x_0) = \sum_{j=1}^{n_{\text{bin}}} \int_{x_{j-1}}^{x_j} S_j(x)D(x + x_0)dx\]

where \(x_0 = x_{\text{min}}\) and \(x_{n_{\text{bin}}} = x_{\text{max}}\), and \(n_{\text{bin}}\) is the number of bins of the piecewise polynomial \(S\). (Indeed, \(x_0\) should be defined as \(x_0 = \text{min}\{x_{\text{min}}, \text{abscissa of left limit of the first bin of } S\}\). The same holds for \(x_{n_{\text{bin}}}\).

Now, given the bin \([x_{j-1}, x_j]\), we consider the segment \([x_{j-1} + x_0, x_j + x_0]\). Then, perform the change of variable

\[x + x_0 = x', dx' = dx\]

and substitute into Eq. (2.3). This gives

\[(2.4) \quad C(x_0) = \sum_{j=1}^{n_{\text{bin}}} \int_{x_{j-1} + x_0}^{x_j + x_0} S_j(x' - x_0)D(x')dx'.\]

To understand Eq. (2.4), let us think about the process of finding all the template bins in the region \([x_{j-1} + x_0, x_j + x_0]\). Suppose there are \(n_{\text{bin}}\) of such bins. Then Eq. (2.4) can be rewritten as

\[(2.5) \quad C(x_0) = \sum_{j=1}^{n_{\text{bin}}} \sum_{k=1}^{n_{\text{bin}}} \int_{y_{j-1}}^{y_j} S_j(x' - x_0)D_k(x')dx'.\]
Eq. (2.5) makes it explicit that $S_j$ and $D_k$ are the actual polynomials representing the observed $S$ curve in the bin $[x_{j-1}, x_j]$ and the template $D$ in the bin $[y_{k-1}, y_k]$, respectively. Here, $y_k$ and $y_{k-1}$ are the limits of the k’th template bin within $y_0 = x_{j-1} + x_0$ and $y_{\text{bin}j} = x_j + x_0$ [see Eq. (2.4)]. Both $S_j$ and $D_k$ are polynomials, thus

$$
S_j(x' - x_0)D_k(x') = \sum_{\ell=0}^{\text{degs}} \sum_{m=0}^{\text{degd}} a_{\ell+1,j} a_{m+1,k} (x' - x_0)^\ell a_{m+1,k}(x')^m.
$$

Considering that

$$(a + b)^n = \sum_{p=0}^{n} c_p^n a^{n-p} b^p
$$

$$
c_p^n = \frac{n!}{p!(n-p)!}
$$

it follows that

$$
(x' - x_0)^\ell = \sum_{p=0}^{\ell} c_p^{\ell} x^{\ell-p}(-x_0)^p.
$$

Hence, inserting Eq. (2.7) into Eq. (2.6),

$$
c(x_0) = \sum_{j=1}^{n_{\text{bin}}} \sum_{k=1}^{n_{\text{bin}} j \text{ ndegs ndegd}} \sum_{\ell=0}^{\text{degs}} \sum_{m=0}^{\text{degd}} \int_{y_{k-1}}^{y_k} A_{\ell+1,j} a_{m+1,k} x^m \left( \sum_{p=0}^{\ell} c_p^{\ell} x^{\ell-p}(-x_0)^p \right) dx',
$$

where $\text{degs}$ is the degree of the polynomial $S$ and $\text{degd}$ is the degree of the polynomial $D$.

Note: If $x_0 = 0$ we have to resolve the form $0^0$ coming from the term $(-x_0)^p$ in Eq. (2.8). Since that comes from the expression for $(a+b)^n$, when $x_0 = 0$ it means that $(x' - x_0)^\ell = x'$, and Eq. (2.8) becomes

$$
\int_{y_{k-1}}^{y_k} A_{\ell+1,j} a_{m+1,k} x^m x' dx'.
$$

We can now solve the integrals in Eq. (2.8) or Eq. (2.8a) as follows

$$
= A_{\ell+1,j} a_{m+1,k} \left[ \sum_{p=0}^{\ell} c_p^{\ell} x^{\ell-p}(-x_0)^p \right] dx
$$

$$
= a_{\ell+1,j} a_{m+1,k} \left( \frac{\ell}{m + \ell - p + 1} \right) \left[ \frac{y_{k}^{m+\ell-p+1} - (m+\ell-p+1)}{y_{k-1}^{m+\ell-p+1} - (m+\ell-p+1)} \right];
$$

which, substituted into Eq. (2.8), finally gives

$$
\sum_{j=1}^{n_{\text{bin}}} \sum_{k=1}^{n_{\text{bin}}} \sum_{\ell=0}^{\text{degs}} \sum_{m=0}^{\text{degd}} a_{\ell+1,j} a_{m+1,k} \left[ \sum_{p=0}^{\ell} c_p^{\ell} x^{\ell-p}(-x_0)^p \right] \left( \frac{y_{k}^{m+\ell-p+1} - (m+\ell-p+1)}{y_{k-1}^{m+\ell-p+1} - (m+\ell-p+1)} \right).
$$
Appendix 3

The computation of the integral in Eq. (3) of §V.b

Let us assume that

\[ f(x) = \sum_{i=1}^{ns} a_i x^{(i-1)} \]

and

\[ g(x) = \sum_{i=1}^{nd} b_i x^{(i-1)} \]

are, respectively, the actual TF scan and the template polynomials in one of the template bins \([d_2 - d_1]\). Then,

\[
\int_{d_1}^{d_2} [f(x) - g(x)]^2 \, dx = \int_{d_1}^{d_2} f(x)^2 \, dx + \int_{d_1}^{d_2} g(x)^2 \, dx - 2 \int_{d_1}^{d_2} f(x)g(x) \, dx. \tag{3.1}
\]

The various terms on the right hand side of Eq. (3.1) are (after a little algebra)

\[
f^2(x) = \sum_{i=1}^{2ns-1} \left( \sum_{\ell=1}^{i} a_\ell a_{i-\ell+1} \right) x^{(i-1)}
\]

\[
g^2(x) = \sum_{i=1}^{2nd-1} \left( \sum_{\ell=1}^{i} b_\ell b_{i-\ell+1} \right) x^{(i-1)}
\]

\[
(3.2)
\]

\[
f(x)g(x) = \sum_{i=1}^{ns} a_i x^{i-1} \sum_{i=1}^{nd} b_i x^{(i-1)} = \sum_{i=1}^{ns+nd-1} c_i x^{(i-1)}
\]

\[
\quad = \sum_{i=1}^{ns+nd-1} \left( \sum_{\ell=1}^{i} a_\ell b_{i-\ell+1} \right) x^{(i-1)}
\]

given that

\[ a_k = 0 \quad \forall \ k \in [ns + 1, \max(ns + nd - 1, 2ns - 1)] \]

and

\[ b_k = 0 \quad \forall \ k \in [nd + 1, \max(nd + ns - 1, 2nd - 1)] \]

we finally have

\[
\int_{d_1}^{d_2} [f(x) - g(x)]^2 \, dx = \sum_{i=1}^{2ns-1} x^{(i-1)} \sum_{\ell=1}^{i} a_\ell a_{i-\ell+1} \left[ d_2 - d_1 \right] + \sum_{i=1}^{2nd-1} x^{(i-1)} \sum_{\ell=1}^{i} b_\ell b_{i-\ell+1} \left[ d_2 - d_1 \right] - 2 \sum_{i=1}^{ns+nd-1} x^{(i-1)} \sum_{\ell=1}^{i} a_\ell b_{i-\ell+1} \left[ d_2 - d_1 \right].
\]