Systematic errors in GAIA's radial velocity measurements.

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1 Introduction.

This report is intended to contribute to the discussion on how to optimize the accuracy of RV measurements with GAIA's spectrometer. It is a fairly loose collection of questions, remarks, suggestions and a few modest results to which, hopefully, much will be added by other members of the RVS-WG during the coming weeks and months.

It is strictly limited to *systematic errors* because the *random error* budget has already been established satisfactorily in the CTSR. Furthermore it is limited to errors in the radial velocity because, to some extent, systematic errors are proper to the application the data are used for. E.g., an asymmetric deformation of spectral features may not be very harmful for the determination of atmospheric parameters but it may well cause a significant bias in the RV. Therefore, potential problems with each specific application of the spectrometer's data, had better be identified by those who are experienced in that application.

Systematic errors may be introduced by almost every step in the processes of data-acquisition, data reduction and Doppler-shift measurement. To name but a few problems which have already been discussed in connection with ground-based spectrographs: diverse optical aberrations (and even poor focusing) causing the PSF to be asymmetric and variable across the spectrum, non-random sensitivity variations over the CCD, intra-pixel sensitivity variations (becoming more relevant as the pixel size exceeds the size of typical spectral features), instability of the wavelength calibration, insufficient knowledge about the overall instrumental response and in particular of the spectrograph's blaze profile (hampering the rectification of the spectra), spectral differences between object and template leading to a 'mismatch error' in the Doppler-shift, etc.

Obviously we should try and establish a complete census of all potential sources of systematic error. Unfortunately this is extremely difficult because, apart from a number of more general and well-known effects like those mentioned above, most systematic errors are specific for each telescope-spectrograph-detector-software combination. Some may be suspected from the design and hence studied thoroughly, some will hopefully show up in dedicated test exposures, some may show up only when it is too late (i.e. causing science spectra to be irreparably degraded) and some may not show up at all, possibly falsifying certain scientific conclusions based upon them.

However, it is not all doom and gloom. From the way the preparation of the final concept design is being managed and the working groups have been organized, it is clear that there will be maximal openness towards – and involvement from the scientific community. This should give us a fighting chance to get things right in the end. And if we don't we'll only have ourselves to blame.

In Section 2 we make some general remarks on potential sources of systematic error in the hardware, the data-reduction software and the RV-measurement procedure respectively, insofar as they can be conceived on the basis of the information available at present which is essentially the CTSR and, for a few particular details, the older document GAIA/MMS/TN/037.97, Sect.5 (hereinafter referred to as G98) which was distributed at the Nov.'98 workshop in

Leiden. As a consequence some technical aspects are not entirely clear and some may be missing altogether. Any comments, criticisms, corrections and additions to this section will therefore be most welcome! Obviously, for a comprehensive picture of any bias resulting from the algorithms used for data-reduction and RV-measurement we have to await their development and test results, but for the present at least we can make a start with what we presently know.

Section 3 presents a preliminary study of two software-related error sources (both well-known and probably harmless in this case) and a hardware-related one which is specific for the GAIA configuration and which could cause quasi-periodic errors of up to 3 $\mathrm{km\,s^{-1}}$. Section 4 offers some provisional conclusions.

2 Provisional survey of potential sources of systematic error.

2.1 Hardware.

2.1.1 General remarks.

The points made below concern only those error sources whose effect is not (or not completely) described by the variation of the PSF with wavelength and position in the spectrometer's focal plane, i.e. in the whole of the spectrometric instrument we consider only the dispersive element and the detector. Any other problems had better be looked at when realistic models for the PSF have become available.

In the present stage inevitably we have to rely on simulations to study the performance of the instrument and to assess the accuracy of the results. However, it would be highly desirable to repeat and double-check all tests, using the actual instruments and software which will operate during the mission. Ideally this would be done after a complete assembly of the instrument, e.g. with the spectro-telescope mounted on a turning table and illuminated by a tunable source through a grid of pin-holes. This could provide us with a data-base which relates a sufficiently fine grid of incident directions and of wavelengths, to the *measured* position of their image in the FOV. Also we could obtain a digital representaton of the *observed* PSF as a function of position in the FOV and of wavelength. In particular we could then assess how realistic were the simulations upon which, meanwhile, the development of data-reduction software will have been based, and it might lead to further improvements to the latter or allow us to derive a posteriori corrections.

Several objections against such tests have been voiced:

- If we are sufficiently careful and meticulous with the simulations, "real-life" tests are redundant;
- actually the conditions of extreme mechanical and thermal stability under which the satellite will operate simply cannot be reproduced on earth so the test results might be irrelevant or even misleading;
- demanding tests which were not implied by the original specifications for the instrument may cause a delay for the mission as well as a considerable increase of the costs.

The first argument may be valid in theory but recent experience with comparably complicated instruments has demonstrated that human failure just cannot be ruled out. The second argument is in fact correct regarding *some*, but by no means *all* potential sources of systematic error: it should be considered for each case individually. The third argument is undoubtedly serious: we cannot jeopardize the whole mission by being extremely cautious about one aspect of it; however, much of this problem might be avoided by formulating the specifications for manufacture in a way which more directly targets the elimination of potential error sources or the availability of sufficient information to correct for their effect.

The latter would be straightforward if all of the hardware and data-reduction software related to spectroscopy, were to be produced by a single manufacturer. Then one could impose a "benchmark" on the image quality of spectra (e.g. specifying a limited set of bright sources which mimick stellar spectra, to illuminate the spectro telescope from the whole range of angles which will occur in practice, requiring that for a given source all these spectra are *consistent*, i.e. that any differences in the features as recorded during such a test exposure (apart from those caused by sampling[1] or by what little noise that might be inevitable even in a laboratory experiment) are not only well understood but that the manufacturer also provides the algorithms (correction factors, transformations, ...) necessary to eliminate the differences or at least to reproduce these different appearances from the true spectrum of the source considered, within a specified margin of tolerance.

While this ideal situation cannot be realized we can at least try and devise specific tests and measurements for each component, to be done by the manufacturer, providing a comprehensive picture of its actual performance as well as detailed information which could help us to understand and correct any problems arising later. A few examples are given below.

2.1.2 The dispersive element.

With any grating-based dispersive element the following phenomena demand attention (see e.g. Loewen 1970):

- *grating ghosts and satellites*: this is a straightforward matter of manufacturing quality and their absence should be required explicitly in the design specifications;
- *far scatter*: since very bright objects may be imaged alongside very weak ones we need to pay special attention to the (diffuse) stray light which is caused by inevitable small defects in the smoothness of the grating's facets, by edge-effects at each facet etc.; it can be measured and characterized but we shall have to ask for this information explicitly, since it is seldom (if at all) relevant for ground-based spectrographs;
- *variable efficiency*: in general the transmission coefficient of the dispersive element depends on the wavelength and on the polarization of the incident light; this dependence should be measured and communicated in digital form to the users of the data; could we include it in the simulations, using a provisional model for it?
- *blazing*: the blaze profile of the grating must be scrutinized very carefully; in principle it should be perfectly predictable but (apparent) deviations from its theoretical shape have been known to occur; if that is the case these should be detected and measured in detail;

Proper to the RVS configuration, from Sect. 3.5.2 of the CTSR the following phenomena emerge as distorting the image in the FOV and/or affecting the resolution:

- *Slit curvature* (p.166) by which is meant presumably the *across-scan motion* mentioned on p.167 and likewise the *star-line curvature* detailed in G98; we shall henceforth refer to it by the latter name which is the least confusing since there is no slit involved and it has nothing to do with the across-scan motion caused by the scanning law. A prelimnary study of its effect is presented in Sect. 3.2.3, where we argue that it may cause RV errors of up to 3 km/sec regardless of the stars' brightness or spectral type.
- *Anamorphose*: if the effect is merely as described on p.167 then it should not cause any error in the Doppler-shift measurement; however, it would be wise to check that in practice no complications arise like a misalignment between the axes defining the anamorphose and the rows & columns of the CCD.

[1] these can be avoided, with an accuracy dictated by the scientific requirements, by comparing only the spectra for which a given wavelength is imaged in a different area but on the same sub-pixel position.

- *A trapezium-like distortion caused by the telescope optics ...*: if this means (as the text seems to suggest) that a perfect square at infinity would be imaged as a trapezium if the dispersive element were removed, then it would not affect shape of any spectrum but it would mean that a spectrum situated at the short side of the trapezium would be exposed on the FOV for a slightly longer time than a spectrum situated at the longer side. This would cause no harm in itself, but actually the proposed remedy *different sequencing for the three CCDs covering the FOV* might do so, for a spectrum which straddles two adjoining chips. But perhaps I misunderstand the text completely, so could we have more details from the optics people?

- *Dispersive elements cause a rotation of the spectrum during the motion of a star across the CCD*: the text on p. 168 seems to suggest that after correction there is a residual rotation of $-4^{\circ}.1$ to $+4^{\circ}.1$. This seems very large and, if true, it would certainly require non-trivial on-board transformation and rebinning to arrive at the final format of 3×310 pixels in which the spectrum should be transmitted to the ground. But again, this may be but conjecture and the designers of the spectrometer will be able to clarify the situation.

2.1.3 The CCD.

First of all, in the document RVS-CoCo-001 I suggest to quote the actual value for the dark current rather than just stating that it is "negligible". In TDI mode it will contribute on average only 1.2 e^{-}/px after integration. This is very little indeed, but the noise associated with it must also be estimated at 1 e^{-}/px, which is perhaps not quite negligible, in comparison with the read-out noise for instance.

A comprehensive survey of potential problems occurring with a CCD is given by McLean 1997, who also suggests simple tests to detect them; undoubtedly the people who will formulate the quality specifications for the detector are already familiar with this and similar work, so we need not go into all details here. However, from recent experience with some of the the devices installed at ESO, we believe it would be helpful to demand of the manufacturer:

- dark-current frames recorded after short and long periods;

- many bias frames (recorded both in ordinary mode and in TDI mode);

- a detailed map of the CCD's response at different wavelengths, showing the pixel-to-pixel sensitivity variations, bad pixels, traps and any larger-scale blemishes.

- detailed information on the intra-pixel sensitivity variation: we need the sensitivity as a function of position within a pixel with sufficient resolution to enable us to convolve it with the PSF.

Apart from that it would be useful (and not too costly I think) to record a similar set of bias frames once the CCD has been installed in the satellite, to check that it still behaves correctly in its operational environment (see e.g. De Cuyper and Hensberge 2000, who detected periodic read-out patterns probably caused by "cross-talk" with surrounding electronic components).

Concern about the degradation of CTE due to radiation damage in space, has already been voiced in the CTSR, and obviously some provision will have to be made to monitor it at regular intervals. So I wonder if one could extend this facility to recreate, at the same time, dark-current frames, bias frames and response frames so that any changes in the detector's condition can be seen in more detail?

2.1.4 Wavelength calibration.

Apart from the general principle that the position (in the FOV) of a particular wavelength of a given star will be predicted from the position of that object as determined by the astrometric observations, we do not know yet how it will be done, so this topic has to be deferred.

2.2 Data-reduction software.

This topic also has to be deferred until we know more about potential stray light, the extent to which sky-contamination can be avoided, contamination by neighbouring bright sources can be modeled etc.

Nevertheless, right now I would venture a remark on the matter of *optimal extraction* of spectra, which has been mentioned in the CTSR and in RVS-CoCo-001. The algorithm (Horne 1986) requires a virtually exact knowledge of the across-order intensity distribution, which may be very difficult to obtain with the present instrument: even if we manage to predict it from the real PSF, taking account of TDI, image distortions etc., CTE degradation may cause quasi-random deviations from this model. And if the across-order intensity distribution is not correct, the algorithm may introduce a bias in the extracted values. Furthermore, Hensberge and David (2001) demonstrated that the maximal gain in S/N (i.e. a factor of about 1.7) is attained only under very specific conditions on the across-order profile and on the extraction slit, and it is not clear whether these conditions are met here. Therefore I would conclude that 'optimal extraction' may not be advisable for the RVS spectra and that, if it is implemented, a plain unweighted extraction should be available also.

2.3 Doppler-shift measurement procedure.

As matters stand, the method of cross-correlation, as proposed in the CTSR, seems to be the best option. With this method, the following points require special attention:

- *the choice of templates*: masks, synthetic spectra or observed spectra? Although in recent years there has been a growing insight into the systematic discrepancies between the results obtained with masks and those obtained with synthetic spectra, the matter is still not completely resolved even for late-type spectra; and for early-type spectra, masks just don't work. Unless the template spectrum is intrisically (i.e. apart from a Doppler shift) identical to the object spectrum, there is always a risk of introducing a bias. This problem is far from being resolved, and presently the most sensible attitude is probably to provide for the adoption of all three options and for numerous checks of consistency between their respective results.

- *centroiding the correlation peak*: we need the position of the actual maximum of the correlation function, which means we have to interpolate between the pixel positions upon which the correlation function has been sampled; even if we ignore the effect of noise in this step, this involves two potential error sources:
  - discretization effect: even for a symmetrical, noiseless function $f(x)$ the position of its maximum generally cannot be recovered exactly from a sampled representation unless one can use $f(x)$ itself as the interpolating function; the resulting errors are usually very small but just to make sure, in Sect.3.2 we made an estimate of what they could amount to with GAIA's spectra;
  - asymmetry: if object and template are not intrinsically identical, the correlation function is asymmetrical and the actual technique used for the interpolation, should be scrutinized; in many cases one still gets satisfactory results by simply fitting a gaussian to the part above half-maximum, and this is the way it was done in the simulations below; but as the asymmetry gets more severe, obviously this

technique must fail; viable alternatives are still being studied but so far exhibit severe drawbacks like making the measurement much more sensitive to noise or requiring some form of manual intervention;

- *the end-points of the spectra*: it is well-known (see e.g. CTSR, p.265) that the choice of the boundaries of the wavelength-range over which the cross-correlation is done, may introduce a bias; generally this can be avoided when spectra are treated individually with visual inspection and manual intervention, but in automated measurements one should carefully assess the potential amount of bias; as an example, in Sect.3.2.2 we have estimated this *boundary error* for the solar spectrum with different amounts of line-broadening, but the actual magnitude of the error also depends of the nature of the spectrum so these simulations will be repeated in due course for all spectra which have been made available recently by the Padova-Asiago Group.

- *calculation of the corrrelation function*: by Fourier Transform (fast) or by direct summation (slow)? But calculation speed is not the only issue here: since we only have a finite part of the spectrum, both methods tamper with the information to some extent, so both may bias the RV; we have not yet studied the potential magnitude of this bias for the case of GAIA, but in the (unlikely) case that the bias from both methods would turn out to be significant for some applications, we might take advantage of the fact that at least their respective bias will be *different*, so at present we should not yet commit ourselves to either of these methods.

- *preparation of the spectra*: after their extraction from the CCD-image, wavelength-calibration and rebinning to samples with constant step-size in log(wavelength), a spectrum may be subjected to several further manipulations (rectification, filtering, end-masking, zero-padding, ...) before it is fed to a cross-correlator. The potential bias introduced by each of these steps cannot be discussed a priori and independently of the data to which they will be applied. As a rule it would be best simply to avoid such manipulations, except for rectification which is usually indispensible to avoid bias caused by the variation of the (pseudo-)continuum of object and/or template. Depending on which method of cross-correlation will be adopted, a dedicated study of (some of) these effects will be made later on.

3 Simulation of some systematic errors.

3.1 Experimental set-up.

In order to obtain a crude simulation of what a typical late-type spectrum might look like as observed by GAIA, we started from the digital solar atlas by Delbouille et al.(1973) in the wavelength range 847-870nm[2]. This was broadened with 6 different values for an additional rotation velocity (5, 10, 20, 40, 80 and 160 $\mathrm{km\,s^{-1}}$), then convolved with different models for the effective 1-dimensional PSF (hereinafter EPSF, describing the combined effects of optical distortion, TDI and unweighted spectrum extraction) and finally rebinned to GAIA's pixels eightfold, each version shifted over 1/8th of a pixel with respect to the previous one.

The only kind of optical distortion considered here is *star-line curvature*, introduced in Sect.2.1.2; it was singled out for the following two reasons: (i) it is an inevitable phenomenon which the present design of the dispersive element seems to have reduced already as much as it is technically possible and (ii) its effect may turn out to be a limiting factor for some of

[2]These simulations were done before June; therefore the libraries of spectra from the Padova-Asiago Group were not yet available so that only the solar spectrum was used, being a typical late-type one. For the same reason the wavelength range was chosen as in G98 and is therefore slightly different from the one recommended in RVS-CoCo-001. However, although proper checks will be done afterwards, there is little doubt that the conclusions on the particular errors considered here, are valid nonetheless.

the applications of the RVS-data. Star-line curvature makes the EPSF slightly asymmetric in a way which depends both on the wavelength and on the position in the FOV. This variable asymmetry is propagated into the spectral features. As a result, spectra of the same object recorded at different positions in the FOV are not entirely consistent, and intrinsic spectral differences, even between objects recorded at the same position, may be modified. The resulting potential bias in Doppler-shift measurements belongs to the broad collection of '*spectrum-mismatch errors*', but to avoid any confusion with other items in this collection (whether or not proper to the RVS) hereinafter we shall use the terms *SLC-mismatch* for the spectrum-mismatch caused by star-line curvature and *SLC-mismatch error* for the resulting bias.

Models for the EPSF were obtained as follows. Lacking complete and digitized knowledge about the shape of the *local* PSF in the FOV, provisionally we used a gaussian with $\sigma = 1$ pixel. The distortion of the image by star-line curvature during TDI was simulated by averaging (along a column of the CCD) the contributions from this gaussian profile centered on 41 different points of a parabola touching the column in the middle. The parameters of the parabolae were read from G98, Figure 5.3/3, for three different across-scan locations of the spectrum in the FOV, conveniently labeled -.5, 0, +.5 as in the said figure. We also made an EPSF model not affected by the star-line curvature to see what errors can be expected in a cross-correlation with a non-GAIA template. For convenience in the following discussion we rank the 4 EPSF models so that the non-distorted (or symmetrical) one is first and the others follow in ascending order according to their FOV location.

Including also the non-broadened solar spectrum we thus have simulated 28 spectra such as could appear in radial-velocity measurements based on GAIA's observations; 7 of these emulate an 'external' spectrum with which one from GAIA is to be cross-correlated. We correlated only couples of spectra with the same broadening so, altogether we have 70 cases, among which 28 couples of *identical* spectra which were used in particular to separate the SLC error from the other ones).

For each couple thus defined, we considered the unshifted version of the lowest ranking member as the template, and cross-correllated it with each of the 8 versions (i.e. shifted over a pixel fraction) of the other one. For the wavelength region over which the cross-correlation was done we used three possible choices, differing by their redward boundary, notably (1) [847.7, 864.1], (2) [847.7, 868.5] and (3) [847.7, 869.6]. The first of these was a 'careful' choice such as one would make when handling spectra individually, while the other two are such as could occur in an automated procedure which does not allow for individual checks (i.e. they are suitable for some spectra but not quite so for other ones, in particular fast rotators).

The position of the maximum of the CC function was obtained by fitting a Gaussian to it twice, over 7 and 8 pixels respectively, except with the fastest rotators (160 $\mathrm{km\,s^{-1}}$) where we had to use 9 and 10 pixels for the fits to succeed [3]. The two-fold fit is required for a reduction of the discretization error as proposed by David & Verschueren (1995). Finally the error in the position was obtained by subtracting the shift applied to the 'object spectrum' from the fitted position of the gaussian.

3.2 Results.

3.2.1 Discretization error.

Fig. 1 shows a typical example of the total error versus sub-pixel position, for a couple of typical cases as described above. The errors vary only weakly with the sub-pixel position (indicating that the discretization error has in fact been reduced successfully) and the residual variation turns out to be quite insensitive to the choice of the wavelength boundaries.

[3] the numbers of pixels used here are actually larger than they should be in a careful treatment, and are necessitated only by the rather unfortunate way in which gaussian centroiding has been implemented in MIDAS

Therefore, for each couple we simply took the largest of the three PTV amplitudes as an estimate for the residual discretization error.

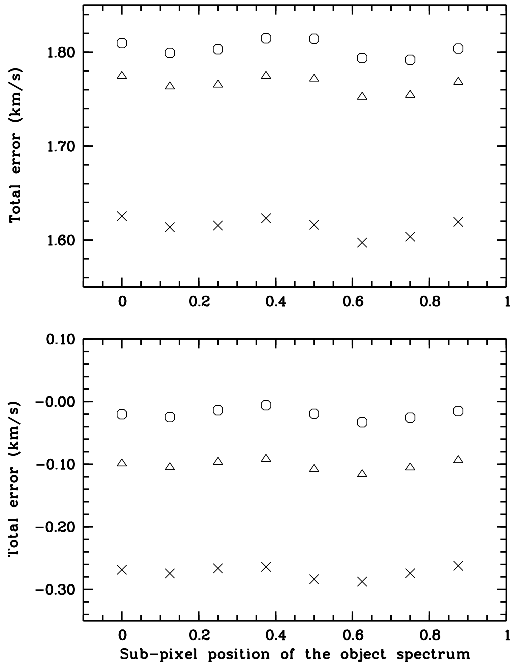

Figure 1: The 'Doppler-shift error' as a function of sub-pixel position. In the lower frame the object and the template are identical (solar spectrum) up to a shift of $n/8$, $n = 0, 1, \dots 7$. In the upper frame the template is the solar spectrum recorded at FOV position 0.0 while the object is the same, recorded at position 0.5. Circles, triangles and crosses correspond respectively to the wavelength regions 1, 2 and 3 used in the cross-correlation.

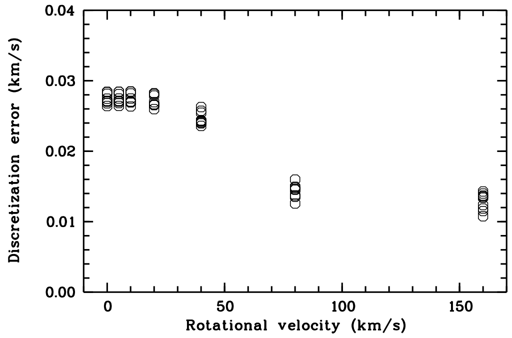

Figure 2: The residual discretization error as a function of rotational broadening.

The resulting estimates are shown in Fig. 2: the relatively small spread of the errors at any given rotational velocity indicates that they are not very sensitive to the SLC-mismatch within a couple, and (as expected) they decrease with increased broadening. Anyway, they remain well below the $0.1\,\mathrm{km\,s^{-1}}$ level and should therefore not harm any of the projected applications of GAIA's RVS.

3.2.2 Boundary error.

Averaging the 'total error' (illustrated in Fig. 1) for each couple over the sub-pixel position of the object, yields three quantities the *range* of which should be a reasonable estimate of the potential boundary error. The results are shown in Fig. 3. The boundary errors are clearly above the $0.1\,\mathrm{km\,s^{-1}}$ level, increasing considerably with increased rotational broad-

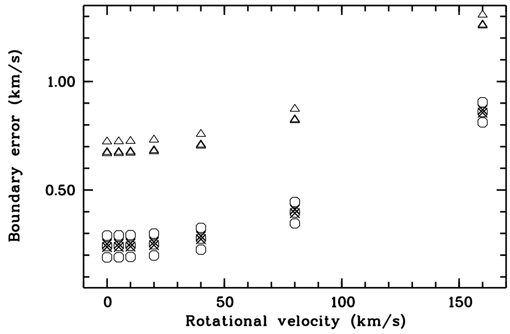

Figure 3: The boundary error as a function of rotational broadening. Crosses: identical EPSF for template and object (i.e. no SLC-mismatch); circles: asymmetric (and different) EPSF for both spectra; triangles: template obtained with the symmetrical EPSF, object with an asymmetrical one.

ening. However, as pointed out above, these estimates are based on experiments in which (deliberately) not all CC boundaries were chosen carefully, and Fig. 1 shows that they can be reduced considerably by a proper choice of the boundaries.

3.2.3 SLC-mismatch error.

For the couples of spectra created with different models for the EPSF, we subtracted from each 'total error' the corresponding value obtained without SLC-mismatch, to isolate the contribution due to the star-line curvature. The results shown in Fig. 4 demonstrate that this kind of error may rise well above the $1\,\mathrm{km\,s^{-1}}$ level and that their magnitude is nowise diminished by using a non-deformed spectrum as the template. All symbols corresponding to couples in which object and template have the same EPSF, coincide almost perfectly. This indicates that the contribution from other error sources was indeed removed successfully and that the effects do not depend on the rotational velocity of the observed stars. The latter may indicate that the *importance* of this error source does not depend very much on the nature of the spectra involved.

The error appears to be very sensitive to the actual nature of the SLC-mismatch but, unfortunately, there seems to be no straightforward correlation between the actual error and the parameters characterizing the curvature of the scan lines. This complication is not unexpected since the curvature changes with the wavelength as well as with the FOV position so that different parts of the spectrum respond in a different way to a change in the FOV position. Whether or not this implies that the actual value of the error also depends strongly on the spectral type, is a question which can now be investigated using the spectra provided by the Padova-Asiago Group.

Anyway, as a consequence of the scanning law, a Doppler-shift bias which depends on the location of the spectra in the FOV might easily be misinterpreted as a (quasi-)periodical RV-variability, so it is important that we study this effect in full detail.

4 Conclusions.

In view of the accuracy requirements imposed on radial-velocity measurements based on spectra from GAIA's RVS, we may formulate the following provisional conclusions:

- In general:

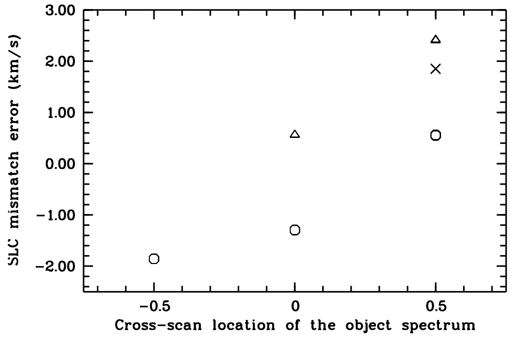

Figure 4: Errors due to the star-line curvature as a function of the position of the object in the FOV. Circles: template obtained with symmetrical EPSF; triangles: template from position -0.5; Crosses: template from position 0.0.

  - the effect of several error sources already known or suspected, still needs to be assessed for the specific case of GAIA's RVS;
  - at any stage in the design or the construction it is important to be alert to the risk of systematic errors; the astrometry people provide a shining example in this respect;
  - an extra effort is needed to devise suitable operational tests which it is feasible to perform both during construction and after the instrument has been assembled.

- as a result of the simulations reported here:
  - discretization errors are negligible if the correction proposed by David & Verschueren (1995) is applied;
  - boundary errors may be harmful occasionally, at least to the most sensitive applications projected for GAIA (i.e. detection of extra-terrestrial planets), but they can be reduced by manual intervention if necessary.
  - star-line curvature may cause SLC-mismatch even between different spectra of the same object, which may introduce a systematic error of the order of several $\mathrm{km\,s^{-1}}$ in the radial velocity; it is not yet clear whether it will be possible to correct this error in any way, so it may turn out to be a limiting factor to the final accuracy which can be achieved.

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