Response to Referee #2

Manuscript "Integrating uncertainty propagation in GNSS radio occultation retrieval: from excess phase to atmospheric bending angle profiles"

by Jakob Schwarz, Gottfried Kirchengast, and Marc Schwaerz,
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We thank the reviewer very much for the constructive feedback to our manuscript. We carefully considered all comments and revised the manuscript accounting for most of them. Our point-by-point responses to the comments are given below.

Comments by the reviewer are cited black upright*, our responses are* *blue italic*. *(line numbers used in our responses refer to the original AMT Discussions paper and text updates in the revised manuscript are quoted below with* *yellow highlighting*)

General Comments

As most of remote sensing techniques, uncertainty analysis is essential to quantify the retrieval credibility in a GNSS-RO system. This article describes the uncertainty propagation of GNSS-RO with step by step approach. From excess phase to bending angle, the propagation process of both random and systematic uncertainties at each step are introduced in details. While the description of the uncertainty propagation is nearly complete and the validation results are very impressive, I recommend this article published after minor revision on several issues:

1. The "**estimated system uncertainty" is not well-defined** and needs more explanation.

What are the sources of the system uncertainty in excess phase? Why can we model it with eq. 8? Are these estimated system uncertainty totally uncorrelated with random uncertainties in each step so that we **can treat them separately**? What if the bias actually comes from the signal randomness (e.g. the bending angle bias caused by signal noise as depicted by [Sokolovskiy et al., 2010])? Should we count it as system uncertainty or random uncertainty?

We see two aspects in this comment, which we would like to respond to separately.

First, on the sources of the systematic uncertainty and our (simplified) modeling of it, i.e., on the rationale why we modeled the (systematic and random) uncertainties in the excess phase the way we did it in the particular context of this study:

The main intention of this study was to develop, implement, validate and demonstrate the mathematically correct propagation algorithms for bending angle retrieval, under as few assumptions as necessary for a successful application of the uncertainty algorithm to RO data in the rOPS; so same intention as Schwarz et al. Earth Space Sci. (2017) for refractivity and dry-air retrieval. The quality and realism of the propagation results in absolute terms will of course strongly depend on the uncertainty profiles used as input at excess phase level; as also the test-day *ensemble results indicate. Since for this study realistic full-profile rOPS L1a uncertainty estimates were not yet available at excess phase level, we decided for viable proxy input profiles with realistic order of magnitudes.*

Regarding the altitudes below 30 km, we chose to replace the noise-estimation scheme by a simple linear model below 30 km, because the empirical estimation approach from the noisy time series (as described in section 2.2, esp. Eq. 5 and the related text) becomes increasingly vulnerable to biases and fluctuations below 30 km due to the strong (near-exponential) increase of the excess phase magnitude. The simple linear model chosen was in fact consistent with that ESA/EUMETSAT reference as well as roughly with the overall behavior of COSMIC-profile based estimates below 30 km (which were not stable enough to be used directly). Regarding specifically the simplified Eq.8-modeling of the systematic excess phase uncertainty we also point to the algorithm demonstration focus of this study, rather than very realistic input and output; and also in this specific respect we will of course use the more realistic rOPS L1a-provided estimates once available.

To be more clear with our rationale for the construction of the input profiles used, we updated on p6, L26-28, to: "While in future the excess phase random and systematic uncertainty profiles will be more rigorously estimated by the rOPS L1a processor (Innerkofler et al. 2016) and provided as input to the L1b processor, they had to be estimated for this study from existing excess phase profiles with realistic noise (we chose UCAR/CDACC ones) and simplified modeling. To this end..."
and on p7, L7, to "…roughly following estimates of ESA/EUMETSAT (1998) and the overall behavior of estimates from real excess phase profiles (the latter became too vulnerable to biases and fluctuations to continue using them below 30 km)."
and on p7, L24, to "…linear uncertainty gradient in the troposphere; as noted above this simplified modeling will be replaced in future by realistic uncertainty estimates received as L1b retrieval input from the L1a processor (Innerkofler et al., 2016)."

In general, we will be able to use real uncertainty profiles from the L1a uncertainty propagation when the L1a/L1b interfacing is complete, and we then clearly intend to inter-validate the RO data and uncertainty estimates from the full rOPS chain also against other sources of quality data like from RAOBs and ECMWF.

Second, as response regarding the question of separate estimation of systematic and random uncertainties:

The criteria for separating the evaluation and propagation of estimated random and systematic uncertainties is that the processes giving effect to these uncertainties need to be uncorrelated (if the correlation term is zero, the other terms can be pulled out of the sum). This is independent of the shape of the probability distribution (if a process causes a biased mean of the pdf, it is counted to the (basic) systematic uncertainties, such that the random uncertainty can be assumed unbiased). The basic systematic uncertainty is caused by processes that repeated measurements under (almost) the same conditions could not detect, e.g. insufficiently defined physical constants, most model parameter errors, etc. It can thus not be correlated with effects of processes that give different results under repeated measurements.

The random und apparent systematic uncertainties on the other hand can be seen as uncorrelated for an analogous reasoning: Since we separate them based on *correlation length, the apparent systematic uncertainty appears as a bias within the, e.g., 0.8 seconds of the Blackman window (correlation coefficient of unity over the window range), while the random uncertainties' correlation function typically decays down to zero within this range. So even if random and (apparent) systematic uncertainty were correlated at one side of the Blackman window, they will be clearly uncorrelated at the other. It is crucial, however, that the correlation lengths of the random and the systematic uncertainties remain clearly separable; would the random uncertainty be strongly correlated also over longer time windows (appearing as a bias), it could be also correlated to the systematic uncertainty (a situation that, favorably, does essentially not occur in practice for RO data processing).*

Thus, in practice, while there might be (very) slight correlations between random and systematic uncertainties at times, we consider the additional insight from having random and systematic effects separately available more important than the problem of potentially (very) slightly overestimating the uncertainties of our RO profiles.

In order to further help understand this, we now added on p4, after L20, another sentence/small paragraph as follows: "Since the noise-type effects giving rise to short range-correlated random uncertainties can be considered uncorrelated to the bias-type effects inducing long range-correlated apparent systematic uncertainties, and since both are uncorrelated to basic systematic uncertainties, it is insightful and possible with due care to estimate and propagate each of these uncertainties independently."

2. Although the MC simulations validate the propagation process, whether the propagation results can reflect how real data behave is questionable:

(i) One thing I concern the most is the modeling of **random uncertainty as normal distribution**. While the "residual phase" of the RO signal suffered by thermal noise could be normally distributed (strictly speaking it is not), the excess phase calculated by unwrapping residual phase can contain cycle slips (even bias if the used model is biased) due to signal noise. Obviously the nonlinear unwrapping process is ignored in this article, and I'm wondering if it could impact the uncertainty propagation results? If this has already been considered in the eq. 6, then author should explain how this model is derived rather than simply providing a technical report reference.

In line with our response to the previous comment, we like to refer back first to the argument that our input quantities, including the input uncertainty estimates, will improve in their realism when the L1a part of the propagation chain is available. Second, we of course share the theoretical view that the assumption of a normal distribution is important for the formal validity (and mathematical proof) of the (linear) covariance propagation, but practically – since we remove biases when known, as recommended by the GUM, and therefore have essentially unbiased pdf-means – only skewness could be a (small) issue. Since our uncertainty estimates need not be highly accurate quantitatively, however (several % relative accuracy of an uncertainty estimate is very good already), minor pdf-skewness effects will not be critical.
We also note that the overall combined noise – given that the central limit theorem implies that the superposition of individual non-Gaussian noise sources approaches a Gaussian pdf for the overall noise – can be expected to be fairly close to Gaussian

(which also RO data statistics indicate). We certainly will closely expect the adequacy of the L1a excess phase uncertainty estimates when available, including the effectiveness of cycle slip correction and other potential systematic effects, and their related residual uncertainty.

In order to better reflect in particular the normal-distribution issue also in the text, where we mention the various main noise sources, we have improved on p4, L29ff, to "…the receiving system noise (i.e., thermal noise and residual clock estimation noise) and the ionospheric noise (from scintillations induced by ionospheric irregularities) are essentially normally distributed overall (Kursinski…). These noise sources are the main contribution to…"

(ii) The random uncertainty is highly related to the signal SNR. However, the linear extension used below 30 km removes all the corresponding SNR information. The reason of using **a linear gradient model below 30 km** instead of the calculated ddL_{rm,k} should be given.

We have included the response to this comment in our answer to comment 1 above; please see there.

(iii) A key element this article lack of is the **verification of the propagated uncertainty using the actual data**. The direct comparison in random uncertainty might be difficult, but the system uncertainty, or bias as you defined in P.4, could be observed statistically through the comparison between RO and ECMWF (or other measurement like RAOB). We may have more confidence on the propagated system uncertainty if it matches the comparison results.

[Sokolovskiy, S., C. Rocken, W. Schreiner, and D. Hunt (2010), On the uncertainty of radio occultation inversions in the lower troposphere, J. Geophys. Res., 115, D22111, doi:10.1029/2010JD014058.]

We hope the first part of our response to comment 1 above, and the related text improvements in the manuscript noted there, addressed also this concern. As noted, we will validate the results of the uncertainty propagation also against real data (such as high quality data from RAOBs and ECMWF) when the L1a uncertainty estimates are available and interfaced to L1b. For context, we did compare the output of the rOPS L2a uncertainty propagation (shown in the Schwarz et al. Earth Space Sci. 2017 paper) to empirical/statistical estimates of uncertainties of dry temperature etc., and we also see that the output uncertainties of the L1b chain reasonably corresponds with the assumed input for the L2a chain, so we can be quite confident that our uncertainty propagation will enable a sequential chain of estimates of appropriate quality.

Specific comments

P7,eq. 6&eq. 8

These two equations should be better explained: why linear and where are these constants (3e6 and 3e7) come from? Why eq. 6 is better than the original ddL_{rm,k} in modeling the random uncertainty below 30 km?

Please see the response to comment 1 above and the related text improvements before and near Eqs. 6 and 8 that we have quoted there and included in the revised manuscript.

*** P7, L23 – L26 ***

Why 0.1 mm and 0.2 mm for simMetOp? Why 0.2 and 0.4 mm for the other two? Why are they constants over 8 km to 80 km? What are the causes of the modeled systematic uncertainty?

As explained as part of the response to comment 1 above, this is a simplified model; see also the text improvement now on p7, L24ff, that we quote there, which now explicitly states the fact that this is a simplified modeling that will be replaced in future by the realistic input from the L1a processor.
Regarding the different settings in the current simple model for CHAMP and COSMIC, compared to (sim)MetOp, we added now on p7, L26, as follows "For CHAMP and COSMIC we set us_Lr1 = 0.2 mm and us_Lr2 = 0.4 mm, to roughly reflect the fact that these RO receivers are lower-cost instruments with lower gain, and thus somewhat lower tracking performance, than the GPS receiver GRAS on MetOp (e.g., Luntama et al., 2008; Angerer et al., 2017)."

[Note: Angerer et al., 2017, which inter-compares performances from different RO missions, including CHAMP, COSMIC, and MetOp, is included as a new reference: Angerer, B., Ladstädter, F., Scherllin-Pirscher, B., Schwärz, M., Steiner, A. K., Foelsche, U., and Kirchengast, G.: Quality aspects of the Wegener Center multi-satellite GPS radio occultation record OPSv5.6, Atmos. Meas. Tech., in press, doi:10.5194/amt-2017-225, 2017.]

*** P11, L18 ***

F_{c2} is set noise dependent – How to determine the filter bandwidth? Do you have to check the spectrum first?

As described in Sokolovsky et al. (2009), and in some detail also in the current study in the Appendix section "A.3.1 Adpative Lowpass Filtering…", the filter bandwidth is derived by choosing from a set of cutoff frequencies, based on a minimization algorithm (i.e. there is a loop through the following steps for each frequency: 1. the frequency is chosen, 2. the filter is applied, 3. the ionospheric correction is applied, 4. the noise of the resulting bending angle profile calculated, 5. if smaller than for the preceeding frequency, the profile is kept, 6. the next frequency is chosen).

In the rOPS case, the set of cutoff-frequencies are pre-determined, constant (using the cutoff frequency of the pre-doppler BWS filter as upper bound for the highest frequency), and are independent of the spectrum of the individual event. For the more detailed related description see the Appendix section A.3.1 (p26).

*** P14, L8 ***

What is the criteria used for discarding 5% of the processed profiles?

The QC applied to the uncertainty propagation results was based on the magnitude of the maximum of the u^r_Lr estimate, which appeared to let about 5% of the profiles to be discarded.
To better express this we updated the sentence on p14, L8-9, to: "…because they were detected as outliers based on the magnitude of their random uncertainty profiles (these outliers are not included in the number of profiles shown)."
We note that this was just a temporary solution for this L1b algorithm intro study; a more advanced QC is integrated as part of the rOPS L1a/L1b interfacing.

*** P20, L7 ***

Although the conclusion is the same but shouldn't the BWS filter be 41 points as you stated in P. 16?

Note that we talk in this sentence about the "effective filter width" of eleven points, i.e., the width similar in its smoothing to an eleven-point boxcar filtering. For a more detailed description see Appendix section A1.1 (including explanation also of Figure A1): the window width at half-maximum of the filter function of the 2.5 Hz BWS filter (with a Blackman window of 41 points) corresponds to the filter function of a boxcar filter of about 11 points window width.

*** P23, eq. A33 ***

Why the systematic uncertainty of bending angle is not related to the open angle?

Thank you for spotting this and pointing this out; of course the uncertainty is also related to the opening angle, the corresponding equation (A33) was not properly updated, it is now corrected (p23, L20).

*** P41, Fig. 6(b) ***

When comparing Fig.5(b) and Fig.6(b), it surprised me that the Doppler systematic uncertainty increase at the bottom of the profile vanished in the one of bending angle. In figure 6, it's just a constant all the way down. Is there any specific reason for this? The Doppler uncertainty is too small compared to the orbit uncertainties? So most of the systematic uncertainty of the bending angle comes from the orbit instead of the measured Doppler?

Exactly, given our input uncertainties for the excess phase and the orbit position and velocities, the uncertainty component coming from the systematic uncertainty of the receiver velocity is typically about 2 magnitudes larger than the systematic uncertainty from the Doppler shift. The receiver position uncertainty has about the *same magnitude as the receiver velocity uncertainty, and the transmitter uncertainties are about 1-2 magnitudes smaller.*

To point to this already in the relevant text in section 3.2, we added a brief sentence on p10, L16, as follows: "...(Figure 6b). Compared to this magnitude, the systematic uncertainty contributed by the Doppler shift uncertainty is very small."

*** P45, Fig 10(g) ***

Can you provide an explanation why several cases in simMetOp have larger L_f uncertainty between the impact altitude of 40 and 60 km?

These three simMetOp cases seem to have a somewhat different, but not completely uncommon noise characteristic, stemming from the noise superposition done in the simulation of the excess phase profiles. Some of the discarded simMetOp outliers show similar characteristics, and quite a range of the discarded COSMIC and CHAMP profiles do (and also several remaining ones, as visible in Fig. 10 as well).

We have now included on p15, L29ff, a sentence of explanation on this point, as follows: "Three individual profiles exhibit comparatively high uncertainties of larger than 2 mm within about 40 to 55 km, however, reflecting that the simMetOp error simulations are capable to partly generate higher-noise profiles of the type more frequently seen in the real MetOp data (Figure 10g)."
[Note: the revised manuscript now includes also test-day results for real MetOp data; so this sentence is part of further text updates in this part of the manuscript, based upon suggestion by Reviewer #1]