Empirical RO Uncertainty Estimates Based on Signal Spectra

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Introduction

The calculation of dynamical uncertainty estimates of bending angle data from radio occultation soundings exploiting the spectral characteristics of the measurement was proposed initially by Hocke et al. (1999) and applied in the framework of modern wave optics algorithms like the Canonical Transform by Gorbunov et al. (2006). The idea received renewed attention when Liu et al. (2018) and Zou et al. (2019) introduced their concept of *Local Spectral Width (LSW)* as quality control and dynamical measurement uncertainty estimate in COSMIC RO data assimilation in the tropical lower troposphere.

Spectral energy distribution

The *spectrum* of an RO signal is a spectral energy density distribution of the measured complex signal, mapped into the impact parameter/bending angle space. It can be obtained in two ways:

- By calculating a energy density distribution in the time domain, and then mapping time/doppler points to impact parameter/bending angle space (via the Doppler equation);
- By obtaining a representation of the signal in the impact parameter domain (via the phase transform, see Gorbunov and Lauritsen, 2004), and then calculating the spectrum in the impact domain.

The most commonly used form of a spectral energy density is the spectrogram of the signal $s(\xi)$:

$$P_{sp}(s;\xi,\varepsilon) = |S_h(s;\xi,\varepsilon)|^2$$

with

$$S_h(s;\xi,\varepsilon) = \frac{1}{\sqrt{2\pi}} \int s(\xi)\, h(\tau-\xi) e^{-i\varepsilon\tau}\, d\tau$$

where h denotes an analysis window, and S_h the Short-term Fourier Transform (STFT). Depending on where the spectrum is calculated, $(\xi,\varepsilon) = (t,\omega)$ in the time/doppler domain, or $(\xi,\varepsilon) = (p,-\alpha)$ in the impact parameter/bending angle domain.

An example for the spectral energy distribution of a setting GRAS occultation based on a spectrogram with a Hamming window of 1.3 seconds (65 data points) is shown in the top of Fig. 4.

Consistent spectral bandwidths

Exploiting the spectrum of the RO signal to characterise its uncertainty means interpreting its energy spectral distribution as a probability density function (PDF) for a retrieval.

A nominal approach is to use the second central moments:

$$\sigma = \left(\int (z-\mu)^2 P(z)\, dz \right)^{\frac{1}{2}}$$

with

$$\mu = \int z\, P(z)\, dz\,.$$

μ and σ coincide with the mean and standard deviation of a normal distribution. Gorbunov et al. (2006) and ROPP use moments to estimate bending angle uncertainty.

An alternative is based on the cumulative distribution function (CDF). The *Inner Quartile Range* (IQR) is the width between the 25% and 75% quantiles; it is equivalent to the standard deviation of a normal distribution if properly scaled:

$$\sigma \approx \frac{1}{1.349} IQR\,.$$

The LSW is the width between the breakpoints of a piecewise linear fit to the empirical CDF (Liu et al., 2018). For a normal distribution, this corresponds to the 6.10% and 93.90% quantiles. It should thus be scaled as

$$\sigma \approx \frac{1}{3.093} LSW$$

to be consistent with the standard deviations of a normal distribution as required by NWP data assimilation.

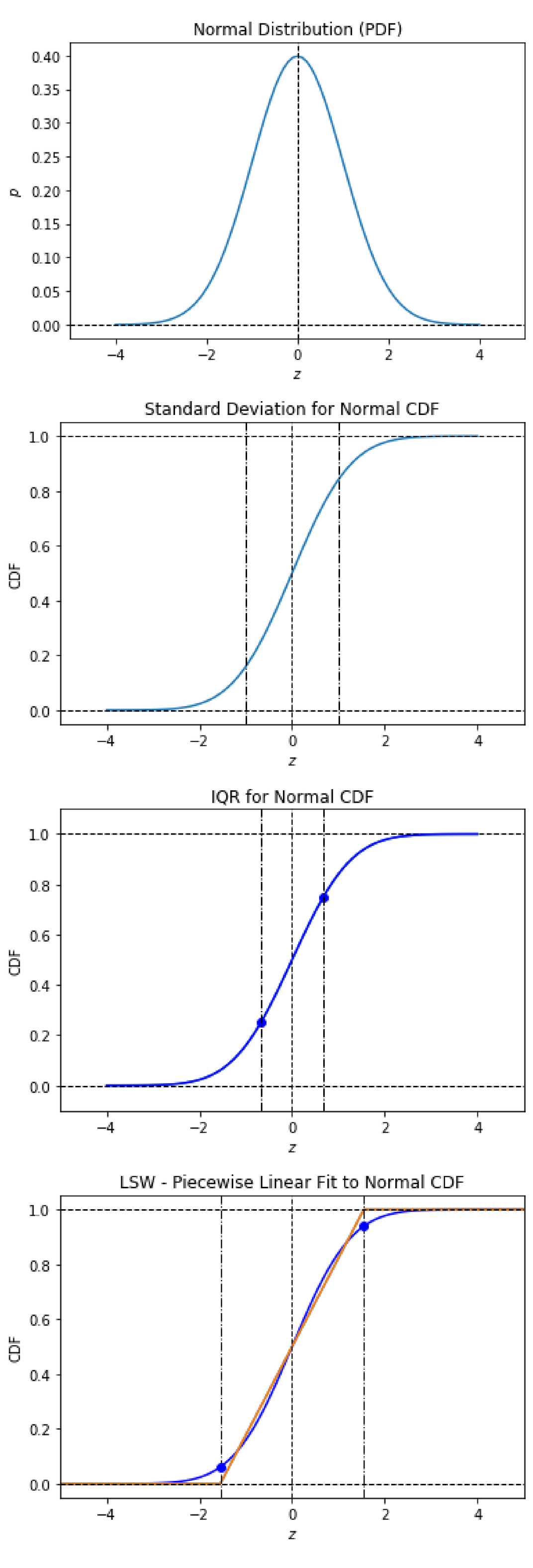

Figure 1. Normal PDF, CDF, IQR and LSW (from top to bottom).

Reassigned spectra

One interpretation of the analysis window (or kernel) h of the STFT is that it smoothes the underlying "true" energy distribution of the signal, thus displacing and smearing out the energy. A sharpened energy distribution can in principle be obtained by "undoing" the dislocation of energy caused by analysis window. The method is known as *reassignment* of the energy distribution. Mathematically:

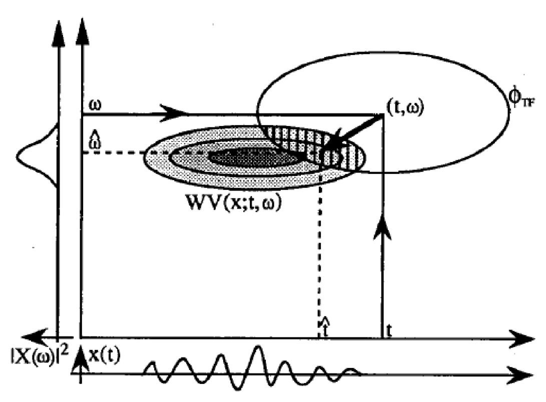

Figure 2. The reassignment method (from Auger and Flandrin, 1995).

$$RS_h(s;\xi',\varepsilon') = \iint S_h(s;\xi,\varepsilon)\, \delta\left(\xi' - \hat{\xi}(s;\xi,\varepsilon)\right) \cdot \delta\left(\varepsilon' - \hat{\varepsilon}(x;\xi,\varepsilon)\right)\, d\xi\, \frac{d\varepsilon}{2\pi}\,.$$

The reassigned coordinates are related to the local group delay

$$\hat{\xi}(s;\xi,\varepsilon) = -\frac{\partial}{\partial\varepsilon}\left[\phi_h(s;\xi,\varepsilon)\right]$$

and instantaneous frequency

$$\hat{\varepsilon}(s;\xi,\varepsilon) = \varepsilon + \frac{\partial}{\partial\xi}\left[\phi_h(s;\xi,\varepsilon)\right]$$

of the phase of the STFTed signal:

$$S_h(s;\xi,\varepsilon) =: M_h(s;\xi,\varepsilon) e^{j\phi_h(s;\xi,\varepsilon)}\,.$$

Fig. 4 (bottom) shows the reassigned energy density distribution. Slices at certain impact heights are shown in Fig. 5, as are moment-based, IQR and LSW estimates of the local spectral bandwidth for normal and reassigned spectra. Profiles of the estimated spectral bandwidth are presented in Fig. 6.

Bandwidth profiles derived from the normal spectrum do not provide physically meaningful results above the region affected by impact multipath. Reassigned estimates are at least somewhat consistent with independent noise estimates above 60 km.

We note that the momentum-based bandwidth estimator is not robust against small noise features far away from the main peaks of the spectrum (see Fig. 5). Therefore, the more robust (scaled) IQR or LSW estimators might be preferable.

Rényi entropy

Entropy is a measure of complexity or information content in a probability or energy distribution function. The generalised Rényi entropy (Baraniuk et al., 2001)

$$H_\alpha(P_s) = \frac{1}{1-\alpha} \log_2 \iint P_s^\alpha(\xi,\varepsilon)\, d\xi\, d\varepsilon$$

(with $\alpha > 0$) counts the "number of components" in a multicomponent signal; a common choice is $\alpha = 3$.

A local (or short-term) form of Rényi entropy was proposed by Sucic et al. (2011). An example for the test case is shown in Fig.3. Note that the Rényi entropy profile was calculated using the normal spectrum, but is nevertheless capable of identifying the layer of apparent impact multipath slightly below 5 km impact height.

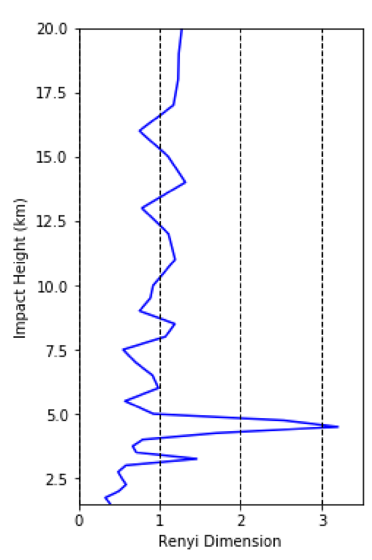

Figure 3. Local Rényi dimension.

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Sample spectra

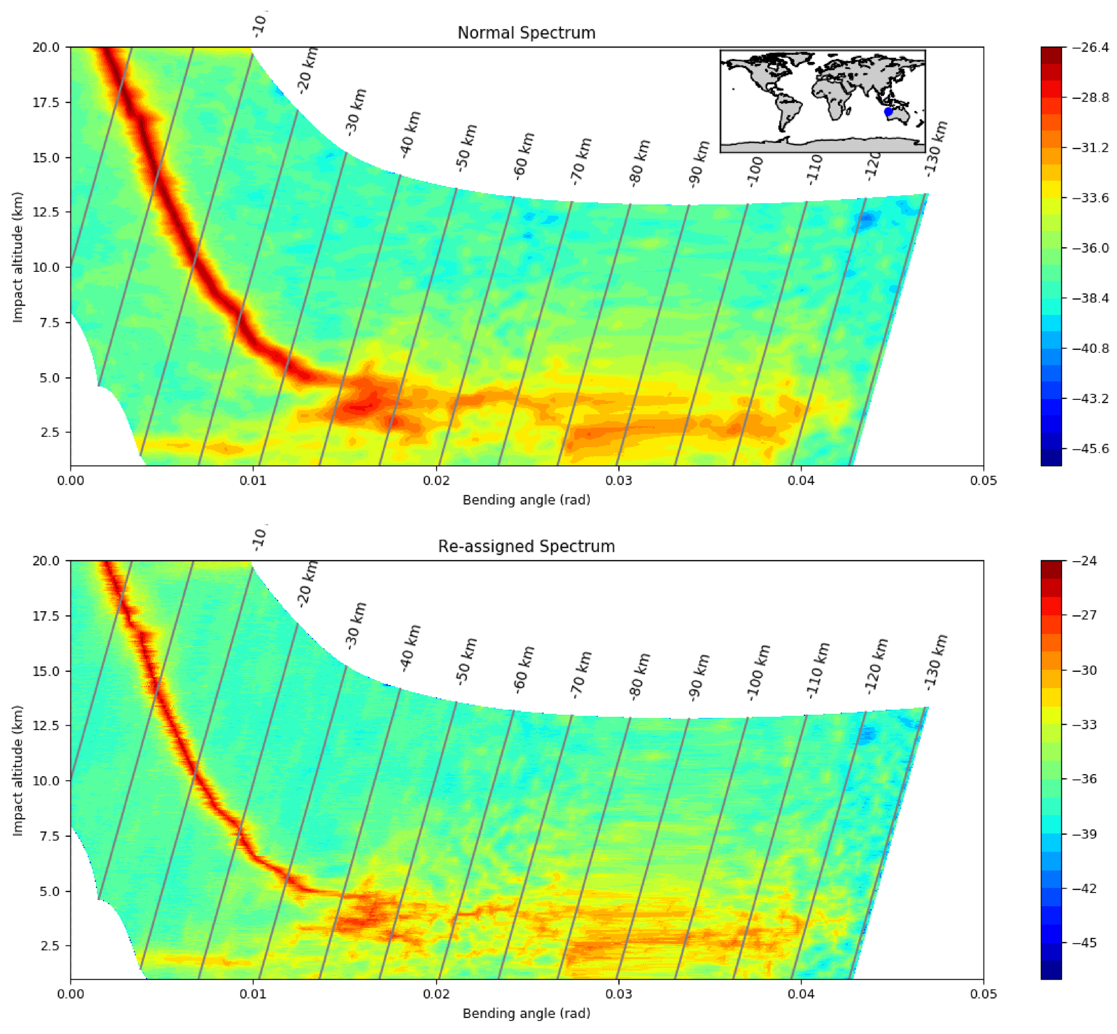

Figure 4. Normal (spectrogram-based, top) and re-assigned spectrum (bottom) of a setting GRAS occultation on 9 Sep 2012 around 00:04 UTC. Grey lines indicate Straight-Line Tangent Altitude (SLTA) during the occultation.

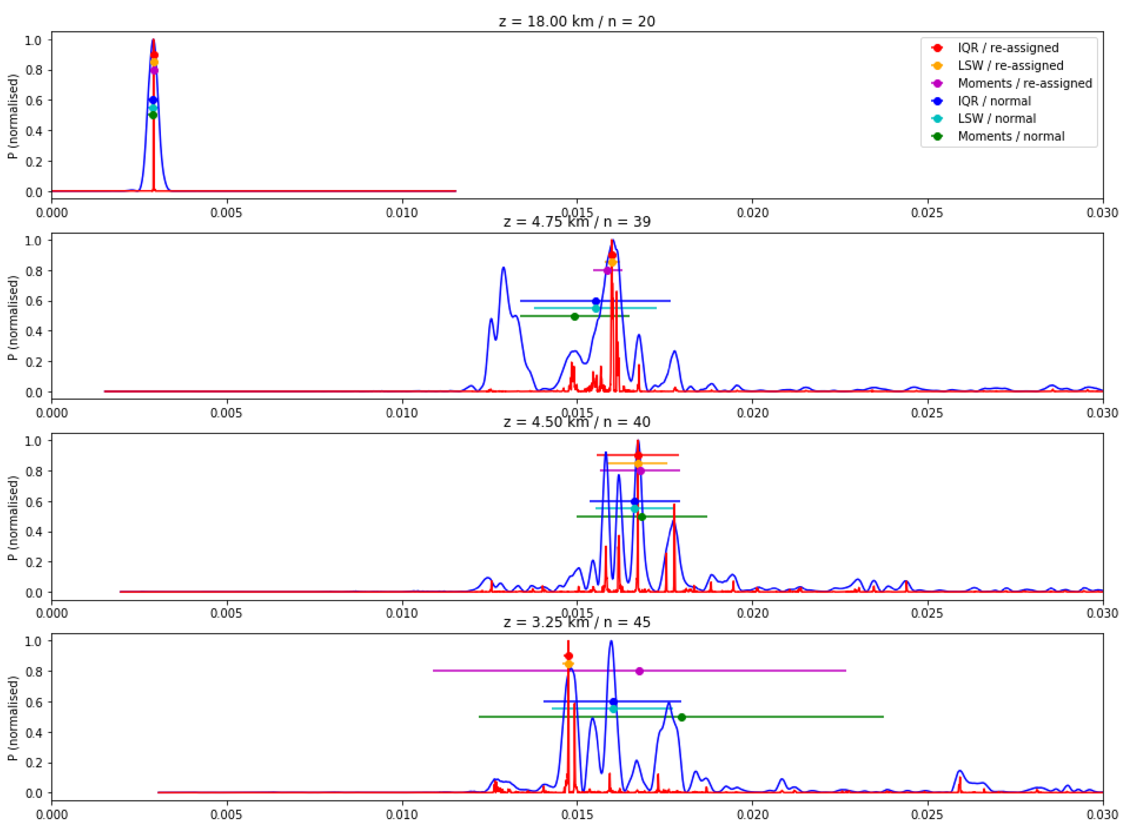

Figure 5. Normalised sample spectra at 18, 4.75, 4.5, and 3.25 km impact height (from top to bottom) for ordinary (blue) and re-assigned (red) spectra. Error bars denote spectral width estimates for various methods.

Error estimates

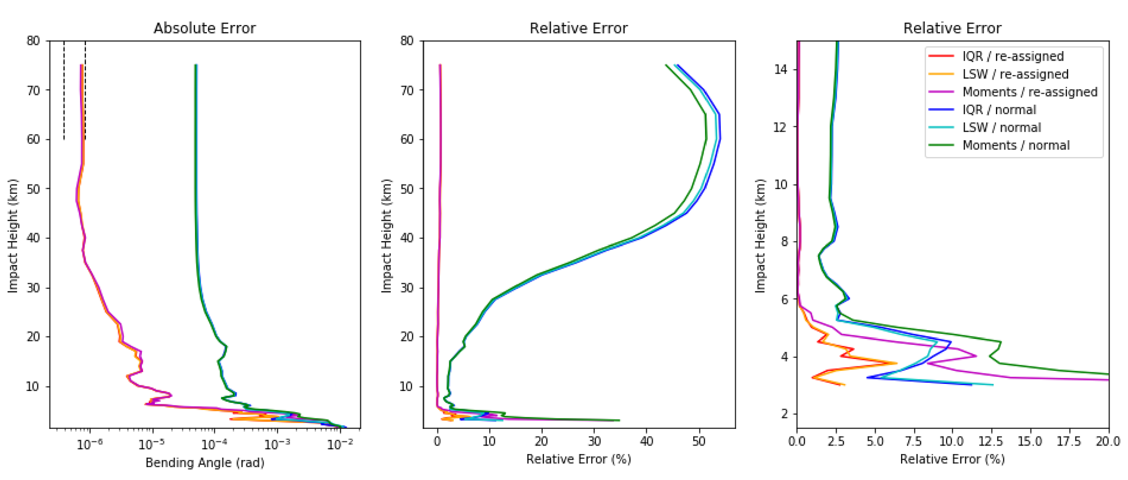

Figure 6. Vertical profiles of absolute (left) and relative (centre and right) spectral L1 C/A bending angle error using various spectral width estimators. Dashed lines in the left plot indicate independent uncertainty estimates of the bending angle above 60 km impact height.

Conclusions

- IQR, LSW and other estimators of spectral width should be scaled to be consistent with normal (Gaussian) standard deviations; see the respective equations on the left.
- In the stratosphere, spectral width estimators based on ordinary spectra do not provide physically meaningful results due to the broadening by the analysis window. The use of high resolution estimators of the spectral energy distribution – such as reassigned spectra – is mandatory.
- In the troposphere, the window continues to affect width estimates, but the robustness of width estimators with respect to small contributions far away from the main beam(s) may become relevant. The moment-based estimator is in particular affected, and may overestimate the spectral bandwidth of the signal.
- Rényi entropy provides an easier-to-interpret metric for the occurrence of impact multipath than spectral width; it might be better suited for quality control applications.

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