New Algorithm for High-Accuracy, Low-Baseline-Shape Frequency Switching

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In this memo I present a summary of those concepts from Winkel, Kraus, & Bach (2012) ("Unbiased flux calibration methods for spectral-line radio observations", A&A, 540, A140) that I believe are most salient to scalar and vector calibration of GBT data. In particular, section 4.7 of the paper describes a model for a potential new technique that the authors claim could significantly improve both the baseline structure and calibration of frequency-switched observations. Since the paper is a theoretical approach to baselines and calibration, the authors never tried the technique on real data. Here I correct some significant algorithmic errors in that section, provide a more in-depth analysis of the theoretical results. Test data taken with the GBT clearly shows how much better the new technique performs over the 'classic' tactics and algorithms for frequency switching.

It is important to note that the new method will substantially increase the scientific output of the GBT. The technique requires approximately half the time to achieve the same noise level for many projects that, up to now, were forced into using the more expensive technique of position switching. It also provides much better calibration accuracy then does the GBTIDL algorithms for position- and frequency-switched observations.

Bandpass Model

Observing toward your astronomical source, while flickering the noise diode, gives two outputs from a spectrometer that will be modeled as:

$$P(\nu) = G_{RF}(\nu)G_{IF}(\nu)[T_L(\nu) + T_{Rcvr}(\nu) + T_S^P] \tag{1}$$

$$P_{On}(\nu) = G_{RF}(\nu)G_{IF}(\nu)[T_L(\nu) + T_{Rcvr}(\nu) + T_{Diode}(\nu) + T_S^P] \tag{2}$$

Items in red either are scalars or have a frequency shape that is so smooth across the bandpass that they can be thought of as being scalars for this level of analysis. In contrast, all items in black have a non-negligible frequency structure and are treated as vectors in this analysis.

- P's = The raw bandpass outputs of a spectrometer when on source
- G_{RF} and G_{IF} = The gains before and after the receiver's mixer.
- T_S = Proxy for any contribution to T_{sys} that has no or only a smooth frequency structure. $T_{Spill} + T_{CMB} + T_{ATM} + T_{Continuum}$
- T_{Rcvr} = Proxy for any contribution to T_{sys} that has a frequency structure.
- T_{Diode} = Frequency spectrum of the noise diode. If using a calibration load, T_{Diode} can be considered a scalar.
- T_L = Desired line

Position Switching

Observing off your astronomical source

$$Q(\nu) = G_{RF}(\nu)G_{IF}(\nu)\left[T_{Rcvr}(\nu) + T_S^Q\right] \tag{3}$$

$$Q_{On}(\nu) = G_{RF}(\nu)G_{IF}(\nu)\left[T_{Rcvr}(\nu) + T_{Diode}(\nu) + T_S^Q\right] \tag{4}$$

Intrinsic assumption with all position switching is to switch faster than the time in which frequency structure changes in T_{Rcvr} and G's.

Solve for T_L

From (1): $T_L = \frac{P}{G_{RF}G_{IF}} - (T_{Rcvr} + T_S^P)$

From (3): $G_{RF}G_{IF} = \frac{Q}{T_{Rcvr}+T_S^Q}$ and substitute into above.

$$T_L = \frac{P}{Q}\left(T_{Rcvr} + T_S^Q\right) - \left(T_{Rcvr} + T_S^P\right) + \left(T_S^Q - T_S^Q\right)$$

$$T_L + \Delta T_S = \left(\frac{P}{Q} - 1\right)\left(T_{Rcvr} + T_S^Q\right)$$

Where the difference in T_{sys} between P and Q is $\Delta T_S = T_S^P - T_S^Q$

From (3) and (4): $T_{Rcvr} + T_S^Q = T_{Diode}\frac{Q}{Q_{On}-Q}$ and substitute into above:

$$T_L + \Delta T_S = \left(\frac{P-Q}{Q}\right)\left[T_{Diode}\frac{Q}{Q_{On}-Q}\right]$$

Notes:

1. In the 'classical' algorithm, the last term in square brackets is converted into a scalar by averaging over the bandpass. Here, I leave these as vectors.
2. We usually expect the noise in a position-switched observation to increase by √2 over that in the P or Q spectra, as one is differencing two vectors. However, with this algorithm the increase in noise is $\sim\sqrt{2\left[1+\left(\frac{\Delta T_S}{T_{Diode}}\right)^2\right]}$. Any difference in T_S will increase noise above √2. One must smooth Q_{on}-Q appropriately. One must use enough smoothing to reduce the noise but not enough to smooth over frequency structures in Q. Using the notation < > to denote a smoothed quantity.

In all that follows, I strongly suggest using SAVITZKY-GOLAY smoothing functions (See "Numerical Recipes", Press et al, section 14.8). SAVGOL retains large-scale structure while significantly reducing noise. It preserves a line's width and height better than boxcar, Hanning. It produces less artifacts than median filtering near strong features. SAVGOL replaces data with a running polynomial, in contrast to the running DC offset of boxcar smoothing.

Thus, position-switched vector calibration uses the algorithm:

$$T_L + \Delta T_S = T_{Diode} \frac{P-Q}{\langle Q_{On}-Q \rangle} \tag{5}$$

You probably have noticed that we haven't used (2) yet. Repeat above with (2), (3), and (4) to derive:

$$T_L + \Delta T_S = T_{Diode} \frac{P_{On} - Q_{On}}{\langle Q_{On} - Q \rangle}$$

Then construct weighted average of this and (5). For simplicity, here I ignore doing the weighted average and the final vector calibration algorithm is:

$$T_L + \Delta T_S = \frac{T_{Diode}}{\langle Q_{On}-Q \rangle} \frac{[(P+P_{On})-(Q+Q_{On})]}{2} \tag{6}$$

Aside: Determining T_{Diode}

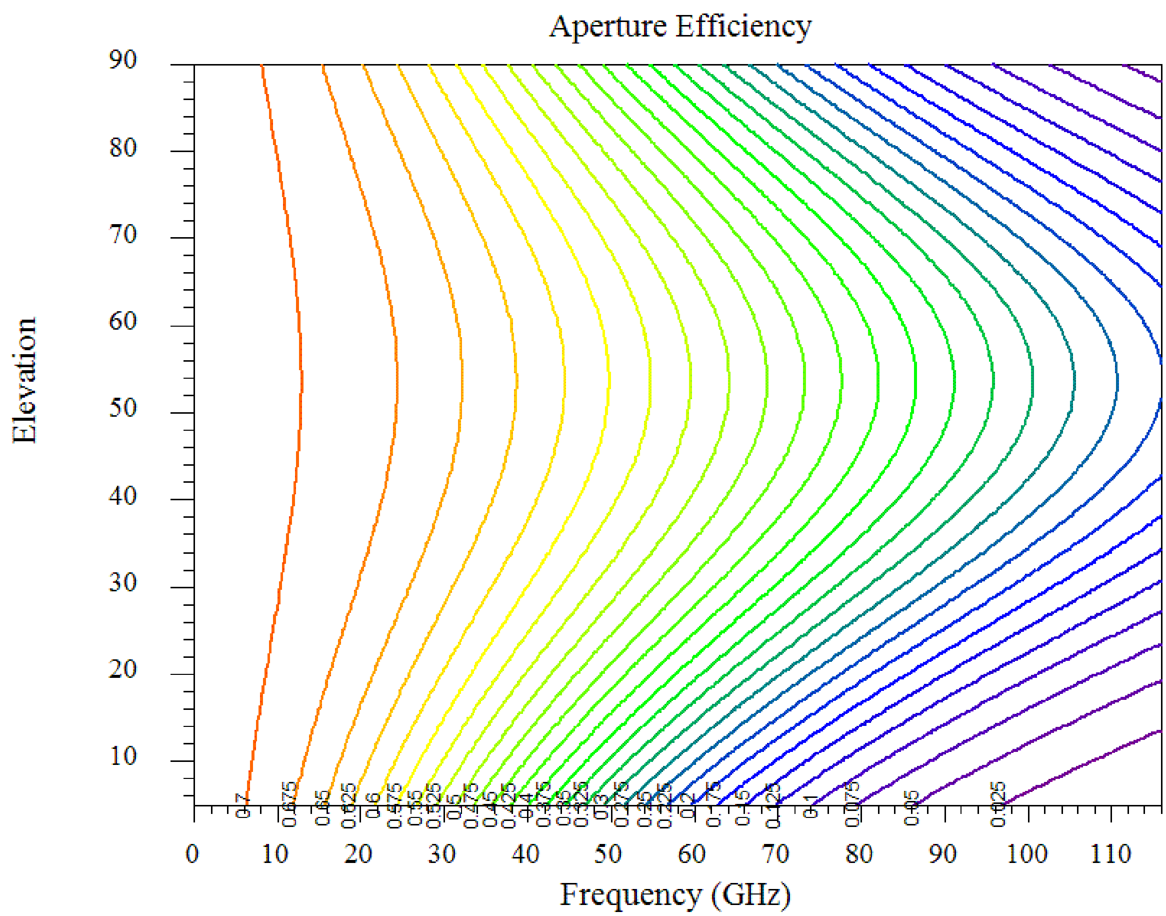
The above requires knowing T_{Diode} with high accuracy and as a function of frequency. You can use a point-source calibrator of known flux S(ν). Solve (6) for T_{Diode}.

$$T_{Diode} = \frac{2\langle Q_{On}-Q \rangle (T_{Calib}(\nu)+\Delta T_S)}{[(P+P_{On})-(Q+Q_{On})]} \tag{7}$$

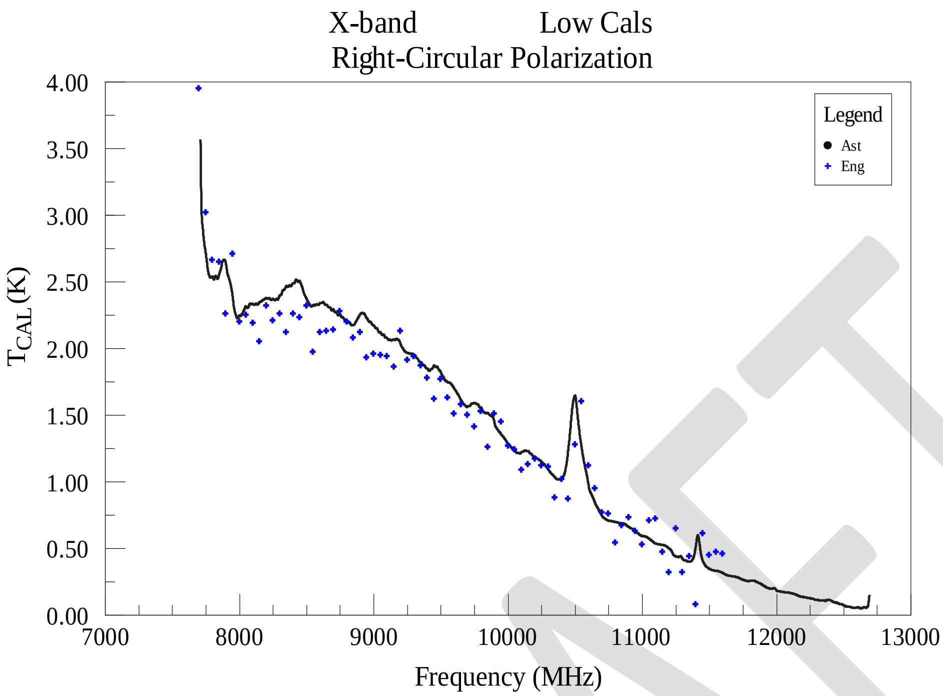
Where the expected antenna temperature from the calibrator is:

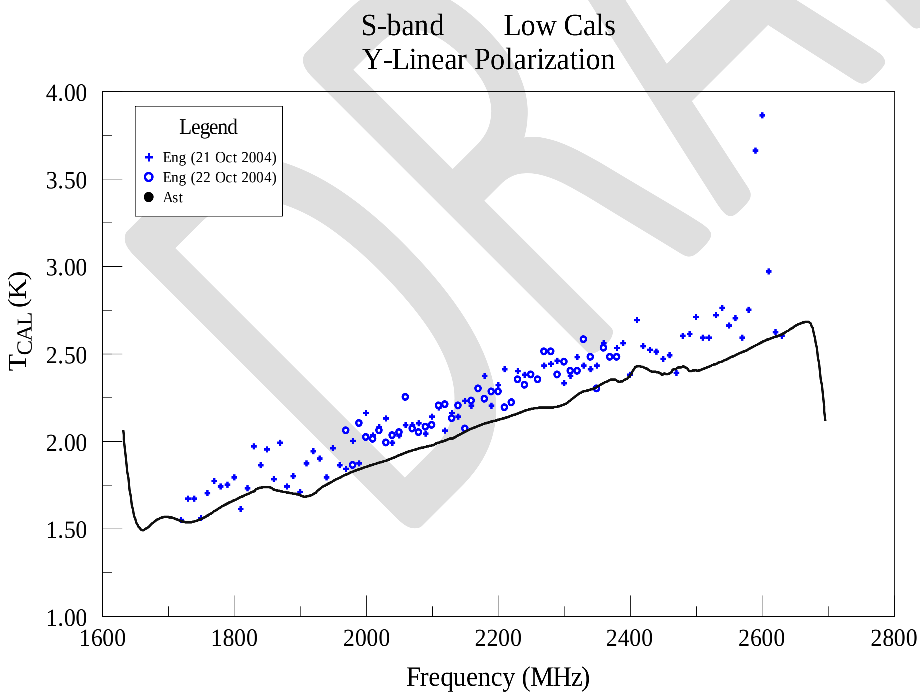
$$T_{Calib}(\nu) = \eta_A(\nu, Elev) \cdot Area \cdot S(\nu) \cdot exp\big(-\tau(\nu) \cdot A(Elev)\big)/2k$$

See ~rmaddale/myPros/scalUtils.pro for IDL routines that use the best models we have for η and air mass, A. File includes a function that will retrieve τ from my weather database. The following is a plot of the best model for η.


Aperture Efficiency
Elevation
90
80
70
60
50
40
30
20
10
0
10
20
30
40
50
60
70
80
90
100
110
Frequency (GHz)

Here are comparisons of engineer's and astronomically-determined values for T_{Diode}. Engineer's values have course resolution, thereby missing structure, and significant noise. If treated as a vector, the 'noise' would introduce unreal structure to the baselines.





What does GBTIDL, CLASS, UniPOPS, … do with Position-Switched Observations?

Answer: Not the above. For GBTIDL:

$$T_a = \frac{[(P+P_{On})-(Q+Q_{On})]}{(Q+Q_{On})} \left\{ \frac{Q+Q_{On}}{Q_{On}-Q} T_{Diode} \right\} - T_{Diode}/2 \qquad (8)$$

T_{sys} is a scalar, averaged over the center 90% of the bandpass.

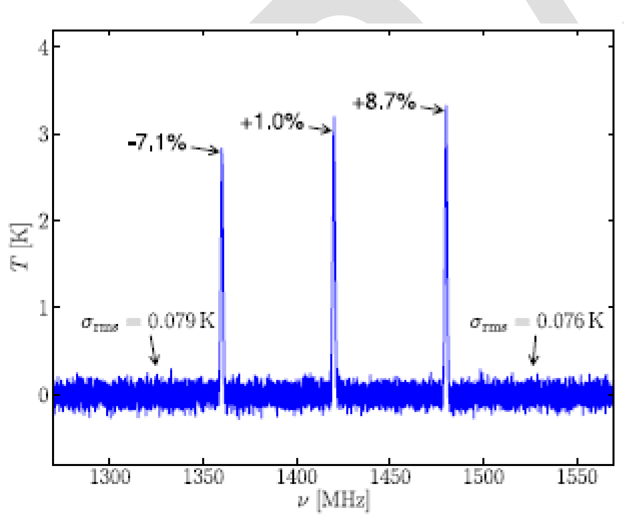
Also note that noise increase is ~√2, an advantage over (6) if ΔT_S is not zero and one can't or hasn't enough smoothing.

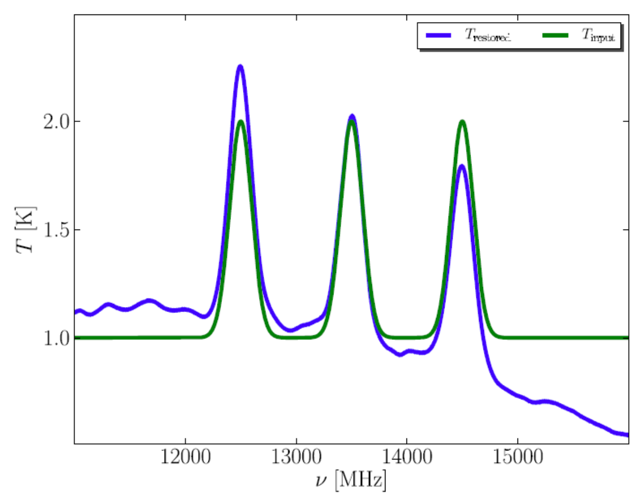
Does $T_a = T_L$? No!! Substitute (1) through (4) into the above:

$$T_a(\nu) = T_L(\nu) \frac{T_{Rcvr} + T_S^Q}{T_{Rcvr}(\nu) + T_S^Q} + \Delta T_S \frac{T_{Rcvr} + T_S^Q}{T_{Rcvr}(\nu) + T_S^Q} \qquad (9)$$

1. Line Intensities will only be properly calibrated at those frequencies where $T_{Rcvr}(\nu) = T_{Rcvr}$, the average value of T_{Rcvr} across the bandpass.
2. Baseline structure will occur whenever $T_{Rcvr}(\nu)$ isn't a constant across the band and $\Delta T_S \neq 0$ (there exists some ΔElev, Δτ, ΔSpill, ΔContinuum)
3. Historically has worked well for narrow bandwidth spectrometers when T_{Rcvr} can be taken to be essentially constant. Fails for our ever increasingly wide bandwidth spectrometers

Here are examples of the errors in calibration and introduced baseline structure from Winkel, Krauss, & Bach (from Figs. 8 and 13)





Classical Frequency Switching

The bandpasses for the Signal and Reference frequencies of the frequency switch:

$$P^{Sig}(\nu) = G_{RF}^{Sig}(\nu)G_{IF}(\nu)\left[T_L^{Sig} + T_{Rcvr}^{Sig} + T_S^P\right]$$

$$P_{On}^{Sig}(\nu) = G_{RF}^{Sig}(\nu)G_{IF}(\nu)\left[T_L^{Sig} + T_{Diode}^{Sig} + T_{Rcvr}^{Sig} + T_S^P\right]$$

$$P^{Ref}(\nu) = G_{RF}^{Ref}(\nu)G_{IF}(\nu)\left[T_L^{Ref} + T_{Rcvr}^{Ref} + T_S^P\right]$$

$$P_{On}^{Ref}(\nu) = G_{RF}^{Ref}(\nu)G_{IF}(\nu)\left[T_L^{Ref} + T_{Diode}^{Ref} + T_{Rcvr}^{Ref} + T_S^P\right]$$

Note that the Ref versions of G_{RF}, T_L and T_{Rcvr} the Sig versions shifted by the amount of the frequency switch, $\Delta\nu$.

$$G_{RF}^{Ref}(\nu) = G_{RF}^{Sig}(\nu + \Delta\nu) \approx \Delta\nu \frac{dG_{RF}^{Sig}}{d\nu}$$

$$T_{Diode}^{Ref}(\nu) = T_{Diode}^{Sig}(\nu + \Delta\nu) \approx \Delta\nu \frac{dT_{Diode}^{Sig}}{d\nu}$$

$$T_L^{Ref}(\nu) = T_L^{Sig}(\nu + \Delta\nu)$$

G_{IF} is identical for the Sig and Ref phases as G_{IF} lies after the receiver's mixer. In-band frequency switching is when $\Delta\nu$ is small enough that both T_L's are covered by the spectrometer's bandwidth. Out-of-band switching is equivalent to using $T_L^{Ref} = 0$.

The classical analysis constructs:

$$T_a = \frac{(P^{Sig} - P^{Ref})}{P^{Ref}}\left[T_{Rcvr}^{Ref} + T_S^P\right] \qquad (11)$$

I will make some simplification to illustrate frequency-switched baselines:

Assume $T_{Rcvr}(\nu)$=constant (flat), and out-of-band frequency switching.

Substitute the P's above gives:

$$T_a = T_L^{Sig}\frac{G_{RF}^{Sig}(\nu)}{G_{RF}^{Ref}(\nu)} + \left[\frac{G_{RF}^{Sig}(\nu)}{G_{RF}^{Ref}(\nu)} - 1\right]\left[T_{Rcvr} + T_S^P\right] \qquad (12)$$

1. T_a should equal T_L^{Sig} but is not. Line strengths are calibrated at only those frequencies where $G_{RF}^{Sig}(\nu) = G_{RF}^{Ref}(\nu)$
2. Second term introduces baseline structures.
3. If $T_{Rcvr}(\nu)$ not constant, baseline problems are even further compounded.
4. Using vector calibration still cannot resolve the calibration error or introduced baseline from not knowing the frequency structure in the ratio of G_{RF}'s.

Advantages over position switching:

- G_{IF}'s shape and time variability always completely cancel out. For some observing G_{IF} is the major source of gain changes.
- Immune to variability in the ***magnitude*** of G_{RF}
- Source continuum level, changing atmosphere, etc. won't introduce baseline shapes
- In-band switching reduces noise by $\sqrt{2}$ (and observations take ½ the time).
- The narrower the spectra-lines, the smaller the frequency switch can be, and the more the G_{RF} ratio becomes 1.

Position-Frequency Switching

Here one frequency switches on and then off your source. The raw bandpasses will be:

$$P^{Sig}(\nu) = G_{RF}^{Sig}(\nu)G_{IF}(\nu)\left[T_L^{Sig} + T_{Rcvr}^{Sig} + T_S^P\right]$$

$$P^{Ref}(\nu) = G_{RF}^{Ref}(\nu)G_{IF}(\nu)\left[T_L^{Ref} + T_{Rcvr}^{Ref} + T_S^P\right]$$

$$Q^{Sig}(\nu) = G_{RF}^{Sig}(\nu)G_{IF}(\nu)\left[T_{Rcvr}^{Sig} + T_S^Q\right]$$

$$Q^{Ref}(\nu) = G_{RF}^{Ref}(\nu)G_{IF}(\nu)\left[T_{Rcvr}^{Ref} + T_S^Q\right]$$

There will be four more like these if one flickers the diode. There are two ways to treat these bandpasses:

Position-Frequency Switching as Two Classical Position-Switched Observations.

Algorithm:

$$T_a = \frac{\left(P^{Sig} - Q^{Sig}\right)}{Q^{Sig}}\left[T_{Rcvr}^{Sig} + T_S^Q\right] - \frac{\left(P^{Ref} - Q^{Ref}\right)}{Q^{Ref}}\left[T_{Rcvr}^{Ref} + T_S^Q\right]$$

Substitute the above P's:

$$T_a(\nu) = T_L^{Sig}\frac{T_{Rcvr}^{Sig} + T_S^Q}{T_{Rcvr}^{Sig} + T_S^Q} - T_L^{Ref}\frac{T_{Rcvr}^{Ref} + T_S^Q}{T_{Rcvr}^{Ref} + T_S^Q} + \Delta T_S\left[\frac{T_{Rcvr}^{Sig} + T_S^Q}{T_{Rcvr}^{Sig} + T_S^Q} - \frac{T_{Rcvr}^{Ref} + T_S^Q}{T_{Rcvr}^{Ref} + T_S^Q}\right]$$

Again, one gets calibration errors and bandpass shapes.

Instead, if one uses vector calibration to remove baseline shapes and improve calibration. Then, $T_a(\nu) = T_L^{Sig}$

However, still making all the same assumptions regarding the time scales over which one must position-switch. One is still concerned with changes in both G_{IF} and G_{RF}. It's hard to see any advantage of using this technique over position switching with vector calibration?

Position-Frequency Switching as Two Classical Frequency-Switched Observations.

Here is the 'classical' algorithm:

$$T_a = \frac{\left(P^{Sig} - P^{Ref}\right)}{P^{Ref}}\left[T_{Rcvr}^{Ref} + T_S\ \right] - \frac{\left(Q^{Sig} - Q^{Ref}\right)}{Q^{Ref}}\left[T_{Rcvr}^{Ref} + T_S\ \right]$$

Really bad idea….. Has almost all the 'bad' characteristics' of frequency and position switching combined. Instructional simplified cases.

Case 1: Calibration Error

- Assume: Out-of-band switching ($T_L^{Ref} = 0$), $\Delta T_S = T_S^P - T_S^Q = 0$

$$T_a = T_L^{Sig}\left(\frac{T_{Rcvr}^{Ref} + T_S}{T_{Rcvr}^{Ref} + T_S}\right)\left(\frac{G_{RF}^{Sig}(\nu)}{G_{RF}^{Ref}(\nu)}\right)$$

Case 2: Baseline Shapes

- Assume $T_L^{Ref} = 0$ and $T_L^{Sig} = 0$, ΔT_S is not zero, $T_{Rcvr}(\nu)$=constant (flat)

$$T_a = \frac{G_{RF}^{Sig}(\nu)}{G_{RF}^{Ref}(\nu)}\left\{\frac{T_{Rcvr}^{Sig} + T_S^P}{T_{Rcvr}^{Ref} + T_S^P}\left(T_{Rcvr}^{Ref} + T_S^P\right) - \frac{T_{Rcvr}^{Sig} + T_S^Q}{T_{Rcvr}^{Ref} + T_S^Q}\left(T_{Rcvr}^{Ref} + T_S^Q\right)\right\} - \Delta T_S$$

Even with vector calibration:

$$T_a = \Delta T_S\left(\frac{G_{RF}^{Sig}(\nu)}{G_{RF}^{Ref}(\nu)} - 1\right)$$

New Algorithm for Frequency Switching

To make the algebra easier to understand, I assume out-of-band switching. One frequency switches on source (P) and then, ever-so-often, does a short frequency switched observation off source (Q):

$$P^{Sig}(\nu) = G_{RF}^{Sig}(\nu)G_{IF}(\nu)\left[T_L^{Sig} + T_{Rcvr}^{Sig} + T_S^P\right]$$

$$P_{On}^{Sig}(\nu) = G_{RF}^{Sig}(\nu)G_{IF}(\nu)\left[T_L^{Sig} + T_{Diode}^{Sig} + T_{Rcvr}^{Sig} + T_S^P\right]$$

$$P^{Ref}(\nu) = G_{RF}^{Ref}(\nu)G_{IF}(\nu)\left[T_{Rcvr}^{Ref} + T_S^P\right]$$

$$P_{On}^{Ref}(\nu) = G_{RF}^{Ref}(\nu)G_{IF}(\nu)\left[T_{Diode}^{Ref} + T_{Rcvr}^{Ref} + T_S^P\right]$$

$$Q^{Sig}(\nu) = G_{RF}^{Sig}(\nu)G_{IF}(\nu)\left[T_{Rcvr}^{Sig} + T_S^Q\right]$$

$$Q^{Ref}(\nu) = G_{RF}^{Ref}(\nu)G_{IF}(\nu)\left[T_{Rcvr}^{Ref} + T_S^Q\right]$$

The full algorithm is embedded in the file ~rmaddale/mypros/vectorTcals/scalFSW.pro. A simplified expression of the new algorithm is

$$T_a = \left(\frac{\langle Q^{Ref}\rangle P^{Sig}}{\langle Q^{Sig}\rangle P^{Ref}} - 1\right)\langle T_{Sys,P}^{Sig}\rangle \tag{13}$$

Where:

$$\langle T_{Sys,P}^{Sig}\rangle = \langle T_{Rcvr}^{Sig} + T_S^P\rangle = T_{Diode}^{Sig}\frac{\langle P^{Sig}\rangle}{\langle P_{On}^{Sig} - P^{Sig}\rangle}$$

As before, the < > indicates quantities that have been smoothed. Must smooth $T_{Sys,P}^{Sig}$ and Q using SAVGOL in order to keep increase in noise close to $\sim\sqrt{2}$. Smoothing must be sufficient to remove noise yet not enough to introduce baseline shapes.

Important to note: If a line is present, one needs to interpolate $\langle T_{Sys,P}^{Sig}\rangle$ over the frequencies of the line. Some intensity errors can arise if T_{sys} is a rapidly-changing function across the frequencies that the line occupies. Such a fast-changing T_{sys} is a very rare possibility for the typical GBT receiver.

Substitute the P's from above:

$$T_a = T_L^{Sig} + \Delta T_S\left(\frac{T_{Rcvr}^{Sig} + T_S^P}{T_{Rcvr}^{Ref} + T_S^P} - 1\right) \tag{14}$$

Line is perfectly calibrated but there will be some baseline shapes if ΔT_S is not zero.

For in-band switching, can obtain a factor of 2 savings in time.

$$T_a = \left(\frac{\langle Q^{Sig}\rangle P^{Ref}}{\langle Q^{Ref}\rangle P^{Sig}} - 1\right)\langle T^{Ref}_{Sys,P}\rangle \tag{15}$$

$$\langle T^{Ref}_{Sys,P}\rangle = \langle T^{Ref}_{Rcvr} + T^P_S\rangle = T^{Ref}_{Diode}\frac{\langle P^{Ref}\rangle}{\langle P^{Ref}_{On} - P^{Ref}\rangle}$$

$$T_a = T^{Ref}_L + \Delta T_S\left(\frac{T^{Ref}_{Rcvr} + T^P_S}{T^{Sig}_{Rcvr} + T^P_S} - 1\right)$$

Shift (15) by the amount of the frequency switch and construct weighted average with (13).

- Must switch faster than time of frequency-structure changes in G_{RF}
- Changes in G_{IF} are of no concern
- Magnitude changes in G_{RF} between Q and P are of no concern, just changes in the shapes of G_{RF} between Q and P.
- Unlike position switching, can balance the IF attenuators between Q and P, thereby allowing for higher dynamic range, more linear observing than position switching.
- Baseline could be a problem if both ΔT_S is large (atmosphere, source continuum, etc.) and if the frequency derivative of T_{Rcvr} is also significant.
    - If both G_{IF} and G_{RF} are really stable, position switching will still be better
- Can invert the above equations to determine T^{Sig}_{Diode} and T^{Ref}_{Diode} from observations of a point-source calibrator.
- New algorithm should increase number of observations that can profitably use frequency switching, thereby saving nearly 50% of the needed observing time.

What of Gain Changes?

For position switching, if $G = G_{RF} G_{IF}$ changes between P and Q, then baseline shapes will be for scalar and vector calibration:

$$T_a \sim T_{SYS} \left[\frac{G_{RF}^{Q} G_{IF}^{Q}}{G_{RF}^{P} G_{IF}^{P}} - 1 \right]$$

$$T_a \sim T_{SYS} \left[\frac{G_{RF}^{Q} G_{IF}^{Q}}{G_{RF}^{P} G_{IF}^{P}} - 1 \right]$$

Thus, both magnitude and shape changes will add baseline shapes. Vector calibration more susceptible since one will see the T_{sys} shape as well.

For new frequency-switching algorithm:

$$T_a \sim T_{SYS} \Delta\nu \left[\frac{1}{G_{RF}^{Q}} \frac{dG_{RF}^{Q}}{d\nu} - \frac{1}{G_{RF}^{P}} \frac{dG_{RF}^{P}}{d\nu} \right]$$

$$T_a \sim T_{SYS} \Delta\nu \frac{d}{d\nu} \left[ln \left(\frac{G_{RF}^{Q}}{G_{RF}^{P}} \right) \right]$$

Immune to magnitude changes in G_{RF}, requires a change in shape. If there is a change in shape, will also see the shape of T_{sys}.