Uncertainties in TOC retrieval for Brewer and Dobson data and the role of cross-correlations among influence parameters

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Outline

Just as reminder....

Dobson and Brewer networks.

Total Column Ozone (TOC) measurements performed at a set of wavelengths pairs.

$A \Rightarrow \lambda_1 = 305.5$nm and $\lambda_2 = 325.4$nm.

Beer-Lambert law

$$I_\lambda = I_{0\lambda} \exp\left[-\alpha_\lambda \mu \Omega - \beta m \frac{P}{P_0} - \delta_\lambda \sec(Z)\right] \qquad (1)$$

Double ratio method I

$$I_\lambda = I_{0\lambda} \exp\left[-\alpha_\lambda \mu \Omega - \beta m \frac{P}{P_0} - \delta_\lambda \sec(Z)\right] \quad (2)$$

- I_λ is the direct normal spectra irradiance at λ
- $I_{0\lambda}$ is the extraterrestrial spectral irradiance at λ
- α_λ is the ozone absorption coefficient at λ
- μ is the ratio of actual and vertical paths of solar radiation through the ozone layer.
- Ω is the TOC
- β_λ is the Rayleigh scattering coefficient at λ
- m is the airmass corresponding to solar zenith.
- P is the atmospheric pressure at the measurement station
- P_0 is the mean sea pressure
- δ_λ is the scattering coefficient (optical depth) of aerosol at wavelength λ.
- Z is the solar zenith angle

Double ratio method II

If the spectral irradiance is measured at one pair of wavelengths, then one can, in principle, obtain a value of the O_3 by inverting

$$I_\lambda = I_{0\lambda} \exp\left[-\alpha_\lambda \mu \Omega - \beta m \frac{P}{P_0} - \delta_\lambda \sec(Z)\right] \tag{3}$$

$$\Omega = \frac{N - [(\beta - \beta')mP/P_0] - (\delta - \delta')\sec(Z)}{(\alpha - \alpha')\mu} \tag{4}$$

where $N = \log I/I_0' - \log I/I'$

Double ratio method III

If the measurements at two distinct couples of wavelengths are combined together one gets

$$\Omega = \frac{(N_1 - N_2) - [(\beta - \beta')_1 - (\beta - \beta')_2]\, mP/P_0 - [(\delta - \delta')_1 - (\delta - \delta')_2]\, \sec(Z)}{[(\alpha - \alpha')_1 - (\alpha - \alpha')]\, \mu} \tag{5}$$

It is generally assumed that $(\delta - \delta')_1 - (\delta - \delta')_2 \simeq 0$

Double ratio method IV

The process of determining the total column ozone can be seen as a method where one tries to match the measured quantity

$$y^{(m)} = (\log I/I_0' - \log I/I')_1 - (\log I/I_0' - \log I/I')_2 \tag{6}$$

and the model

$$y = (\Delta\alpha_1 - \Delta\alpha_2)\,\mu\Omega + (\Delta\beta_1 - \Delta\beta_2)\,mP/P_0 + \Delta\delta\,\sec(Z) \tag{7}$$

where
$\Delta\alpha = \alpha - \alpha'$, $\Delta\alpha = \beta - \beta'$ and $\Delta\delta = (\delta - \delta')_1 - (\delta - \delta')_2$.

Jacobian matrix

$\Delta\alpha_1$, $\Delta\alpha_2$, $\Delta\beta_1$,Ω, $\Delta\beta_2$, P, $\Delta\delta$, Z (μ and m are function of Z).
We build the Jacobian matrix

$$\left[J_{jk}\right] = \left[\frac{\partial y}{\partial a_j} \cdot \frac{\partial y}{\partial a_k}\right] \tag{8}$$

$a_j \Rightarrow$ parameter, with $j = 1, \ldots 8$, $a_1 = \Delta\alpha_1$, $a_2 = \Delta\alpha_2$, and so on.
From $\left[J_{jk}\right]$ one can compute the covariance matrix $\left[C_{jk}\right] = \left[J_{jk}\right]^{-1}$.
Degree of cross correlation matrix $[\rho_{jk}]$

$$[\rho_{jk}] = \left[\frac{C_{jk}}{\sqrt{C_{jj}}\sqrt{C_{kk}}}\right] \tag{9}$$

Why are correlations important?

If we have $y = x_1 + x_2$, then, for the uncertainty in y we get

$$u_y^2 = u_{x_1}^2 + u_{x_2}^2 + 2\rho_{1,2} u_{x_1} u_{x_2}$$

- If $\rho_{1,2} = 0$ (no correlation) then $u_y^2 = u_{x_1}^2 + u_{x_2}^2$.
- If, $u_{x_1} = u_{x_2}$ and $\rho_{1,2} = -1 \Rightarrow u_y^2 = 0$ (!!).

Anti-correlations are the main reason of the popularity of some research fields, such as quantum optics

Need for regularization

We need J^{-1}, but the inversion problem is often ill-posed and needs to be regularized.

$$J = U \cdot S \cdot V^T \tag{10}$$

where U and V are orthogonal matrices so that their inverse are equal to their transposes.
S is a diagonal matrix with its diagonal (all positive) elements being the singular values of the original matrix J.
Written in this way, the inverse J^{-1} would take the form

$$J^{-1} = V \cdot \left[diag(1/s_j)\right] \cdot V^T \tag{11}$$

If any of s_i is close to zero, the inverse is very sensitive to noise.

Situation for Brewer Model

For Brewer dataset, one can re-write the measurement equation as in the following

$$\Omega = \frac{N - B}{A\mu} \tag{12}$$

where,

$$N = \sum_{i}^{n} w_i \log \frac{I_i}{I_0} \tag{13}$$

$$A = \sum_{i}^{n} w_i \alpha_i \tag{14}$$

$$B = m \frac{P}{P_0} \sum_{i}^{n} w_i \beta_i \tag{15}$$

Brewer Model

A typical Brewer data set will look like (with meaning of coefficients as in Brewer manual)

Figure : Brewer 070, El Arenosilo 2015. (courtesy A. Redondas)

A1	Ozone	Rayleigh	Pressure	AOD	SZA	airmass	date	ETC	MS9
0.3385	370.0294557	1	1007.7		63.85116641	2.239717799	736108.3059	2950	5755.357874
0.3385	372.1812848	1	1007.7		60.95543503	2.038812779	736108.3165	2950	5518.564943
0.3385	373.0615912	1	1008.3		51.08351434	1.584120693	736108.3526	2950	4950.448975
0.3385	373.1912714	1	1008.3		49.1946256	1.523704952	736108.3596	2950	4874.824019
0.3385	374.0884515	1	1008.4		39.32730405	1.289980267	736108.3965	2950	4583.488348
0.3385	376.1539616	1	1008.5		38.72588121	1.279166188	736108.3988	2950	4578.738207
0.3385	376.000551	1	1008.8		35.49784253	1.226288118	736108.4114	2950	4510.772752
0.3385	374.8214293	1	1008.831		34.29958985	1.20869474	736108.4162	2950	4483.556275
0.3385	375.5418098	1	1008.874		33.19977888	1.193432359	736108.4207	2950	4467.101987
0.3385	375.1339048	1	1008.9		32.6389146	1.18596119	736108.423	2950	4455.967044
0.3385	376.9879481	1	1008.9		29.66998831	1.149690717	736108.4356	2950	4417.125158
0.3385	377.129491	1	1009		27.62181693	1.127638523	736108.4448	2950	4389.524537
0.3385	375.5391251	1	1009		23.31008837	1.088225195	736108.4674	2950	4333.351801
0.3385	376.6040015	1	1009.063		22.93873325	1.0852401	736108.4697	2950	4333.469013
0.3385	378.4930126	1	1008.8		20.19711531	1.065051071	736108.4934	2950	4314.542205

Cross-correlation in Brewer algorithm

For uncertainty purposes, TOC retrieval from Brewer model can be considered as a minimization of the functional

$$\|N^{(measured)} - (A\mu\Omega + B)\| \tag{16}$$

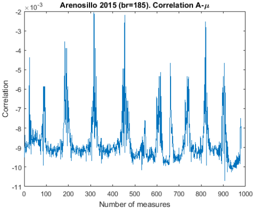
Local optimization ⇒starting values from direct model: $A_{nominal}$,$\Omega_{nominal}$,$\mu_{nominal}$,$B_{nominal}$.
Example at $sza \simeq 41^\circ$

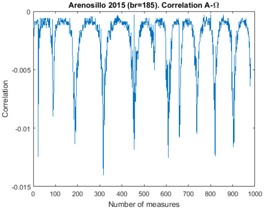
$$[J_{jk}] = \begin{bmatrix} 2.137034729^{13} & 2.087114641^{11} & 5.471782962^{13} & 4.624860617^{10} \\ 2.0871146410^{11} & 2.0383606614^{9} & 5.3439647822^{11} & 4.5168261299^{8} \\ 5.4717829624^{13} & 5.3439647822^{11} & 1.4010258407^{14} & 1.184175117^{11} \\ 4.624860617^{10} & 4.51682612^{8} & 1.18417511^{11} & 1.00088854^{8} \end{bmatrix} \tag{17}$$

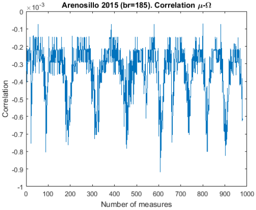
Cond number 1.06980^{22} ⇒ Not possible to invert

Cross-correlation in Brewer algorithm, Brewer 185

After regularizing J (Tickhonov regularization), we obtain







Cross-correlation in Brewer algorithm, Brewer 230

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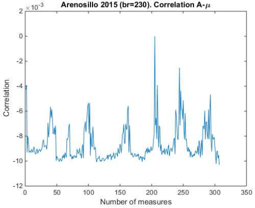

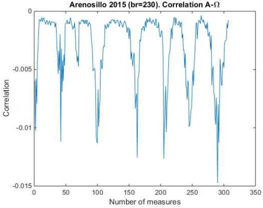

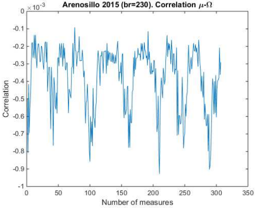

Cross-correlation in Brewer algorithm, Brewer 185

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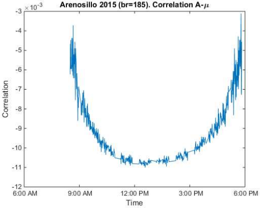

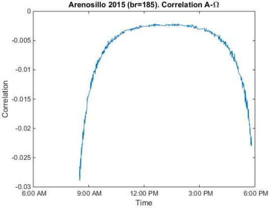

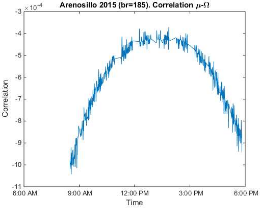

TOC uncertainty

$$u_{\Omega}^2 = u_{a_3}^2 = \frac{u_y^2 + \sum_{\substack{i,j \\ i,j \neq 3}} \frac{\partial f}{\partial a_i} \frac{\partial f}{\partial a_j} \rho_{i,j} u_{a_i} u_{a_j}}{(\frac{\partial f}{\partial a_3})^2} \quad (18)$$

The $\rho_{i,j}$ from the model are available.
The measurements uncertainties u_{a_i} must be determined for each measuring instruments.

Outlook

- We have derived the uncertainties and correlations from the model.
- The total TOC uncertainties combines the measurements/instruments uncertainties and the model uncertainties.
- Now working on the values and entity of atmospheric ad instrumental uncertainties to compile the comprehensive TOC uncertainty budget.