PHY478: Annotated Bibliography

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By Victoria Spada

K. Bognar, X. Zhao, K. Strong, C. Boone, A. Bourassa, D. Degenstein, J. Drummond, A. Duff, F. Goutail, D. Griffin, P. Jeffery, E. Lutsch, G. Manney, C. McElroy, C. Mclinden, L. Millán, A. Pazmino, C. Sioris, K. Walker, and J. Zou, "Updated validation of ACE and OSIRIS ozone and NO2 measurements in the Arctic using ground-based instruments at Eureka, Canada," ***Journal of Quantitative Spectroscopy and Radiative Transfer*****, vol. 238, p. 106571, 2019.**

Summary

This paper shows the validation of OSIRIS and ACE satellite instrument measurements of NO2 and ozone through long-term comparisons with measurements from ground-based instruments at the Polar Environment Atmospheric Research Laboratory (PEARL), near Eureka, Nunavut, Canada. Comparisons of ozone partial columns between OSIRIS v5.10, ACE-FTS v3.5/3.6 data, ACE-MAESTRO v3.13, and ground-based instruments were performed.

Profiles from satellite instruments were extended to the surface using ozonesonde data, Mean absolute differences and correlation plots of ozone and NO2 partial columns were used to compare measurements for each instrument pair. Dynamical coincidence criteria, such as including considerations of sPV and temperature at certain altitudes and imposing a $\pm 1^\circ$ latitude criterion for spring and fall NO2 comparisons, were also tested.

A time series analysis was also conducted for each instrument pair. A linear fit (in time) of the daily mean relative differences was used to estimate the drift between each instrument pair. A bi-square weighted robust fitting method was used for the linear regression. This was more appropriate than an ordinary least squares regression (OLS) method because OLS methods are more sensitive to data gaps and outliers. Bootstrap resampling was used to verify the uncertainties found by the robust, and there were no significant drifts between any of the instrument pairs.

Reflect & Assess

This paper is highly relevant to my research project. The comparison/validation method described in this paper is similar to the method used in (Dupuy, 2009), and the time series analysis method used in this paper is very similar to the method used in (Hubert, 2016). The outlines of these methods, and possibly the articles referred to in this article, will serve as references/guides for when I am doing comparison and drift calculations for my project.

T. V. Clarmann, G. Stiller, U. Grabowski, E. Eckert, and J. Orphal, "Technical Note: Trend estimation from irregularly sampled, correlated data," ***Atmospheric Chemistry and Physics*****, vol. 10, no. 14, pp. 6737–6747, 2010.**

Summary

This paper focuses on the analysis of data that are irregularly sampled in space and time. Irregular spacing of measurements can affect the estimated trend, so the author recommends accounting for the full error covariance matrix. A method for modelling periodic trends by using superimposed periodic functions is outlined. A method for estimating covariance for different sites in global data sets (specifically satellite data) is introduced.

First, models for linearly related data sets are discussed, and a case study using MIPAS temperature measurements is given. Then, data sets with annual cycles are introduced. For datasets that can be modelled as periodic oscillations with a linear term, the process for estimating the periodic correction is explained, and another case study is given, modelling average temperatures at 25 km measured by MIPAS. Finally, models with corrections by discrete empirical functions, continuous empirical functions, and state-dependent amplitudes are discussed, with a case study for each.

Assess & Reflect

This paper provides a clear, detailed background for modelling frameworks that may be incorporated into my project. The frameworks discussed in this paper can incorporate the covariance matrix of the data, but this is likely too complicated to include in my project. The section that discusses modelling data with annual cycles may be particularly useful for my project, as the method is outlined very clearly, and the provided case studies provide useful references.

D. G. Dufour, J. R. Drummond, C. T. Mcelroy, C. Midwinter, P. F. Bernath, K. A. Walker, W. F. J. Evans, E. Puckrin, and C. Nowlan, "Intercomparison of Simultaneously Obtained Infrared (4.8 μm) and Visible (515−715 nm) Ozone Spectra Using ACE-FTS and MAESTRO," ***The Journal of Physical Chemistry A*****, vol. 109, no. 39, pp. 8760–8764, 2005.**

Summary

The ACE-MAESTRO and ACE-FTS spectrometer instruments on the SCISAT-1 were compared before their launch. A comparison of the absorption by ozone in the infrared and visible regions is made in this paper. Since it is challenging to create a stable light source that spans the wide spectral range required for simultaneous visible and infrared absorption band measurements, this type of measurement is rarely done. Ozone measurements obtained from the instruments were compared.

Assess & Reflect

I might revisit this article to compare the results with the results from my work, if I chose to perform comparisons between ACE-FTS and ACE-MAESTRO. The spectral fitting/measurement preparation method used in this paper is not associated with a version number, so the results of the comparison in this article will not be useful for my comparisons of different data versions.

E. Dupuy, K. A. Walker, J. Kar, C. D. Boone, C. T. McElroy, P. F. Bernath, J. R. Drummond, R. Skelton, S. D. McLeod, R. C. Hughes, C. R. Nowlan, D. G. Dufour, J. Zou, F. Nichitiu, K. Strong, P. Baron, R. M. Bevilacqua, T. Blumenstock, G. E. Bodeker, T. Borsdorff, A. E. Bourassa, H. Bovensmann, I. S. Boyd, A. Bracher, C. Brogniez, J. P. Burrows, V. Catoire, S. Ceccherini, S. Chabrillat, T. Christensen, M. T. Coffey, U. Cortesi, J. Davies, C. De Clercq, D. A. Degenstein, M. De Mazière, P. Demoulin, J. Dodion, B. Firanski, H. Fischer, G. Forbes, L. Froidevaux, D. Fussen, P. Gerard, S. Godin-Beekmann, F. Goutail, J. Granville, D. Griffith, C. S. Haley, J. W. Hannigan, M. Höpfner, J. J. Jin, A. Jones, N. B. Jones, K. Jucks, A. Kagawa, Y. Kasai, T. E. Kerzenmacher, A. Kleinböhl, A. R. Klekociuk, I. Kramer, H. Küllmann, J. Kuttippurath, E. Kyrölä, J. C. Lambert, N. J. Livesey, E. J. Llewellyn, N. D. Lloyd, E. Mahieu, G. L. Manney, B. T. Marshall, J. C. McConnell, M. P. McCormick, I. S. McDermid, M. McHugh, C. A. McLinden, J. Mellqvist, K. Mizutani, Y. Murayama, D. P. Murtagh, H. Oelhaf, A. Parrish, S. V. Petelina, C. Piccolo, J. P. Pommereau, C. E. Randall, C. Robert, C. Roth, M. Schneider, C. Senten, T. Steck, A. Strandberg, K. B. Strawbridge, R. Sussmann, D. P. J. Swart, D. W. Tarasick, J. R. Taylor, C. Tétard, L. W. Thomason, A. M. Thompson, M. B. Tully, J. Urban, F. Vanhellemont, C. Vigouroux,, T. von Clarmann, P. von der Gathen, C. von Savigny, J. W. Waters, J. C. Witte, M. Wolff, and J.M. Zawodny, "Validation of ozone measurements from the Atmospheric Chemistry Experiment (ACE)", Atmos. Chem. Phys., vol. 9, pp. 287-343, https://doi.org/10.5194/acp-9-287-2009, 2009.

Summary

This paper presents the validation of ozone measurements from the ACE satellite instruments. The validation includes ACE-FTS (v.2.2 Ozone Update) and ACE-MAESTRO (v.1.2) measurements spanning from February 2004 to August 2006.

The same coincidence criteria were used to search for coincident measurements to compare with ACE-FTS and ACE-MAESTRO, and it was also required that there were profiles available for both ACE instruments for each coincidence to provide a consistent distribution of comparisons for ACE-FTS and ACE-MAESTRO. The data products from ACE-FTS and ACE-MAESTRO were compared with coincident observations from satellite-borne, airborne, balloon-borne, and ground-based instruments (ie, DIAL, FTIR spectrometers), by comparing volume mixing ratio profiles (linearly interpolated or smoothed onto the ACE grid) and partial column densities.

Ozone volume mixing ratio differences were calculated for each pair of profiles. The resulting average differences for a complete set of coincident pairs of profiles were then calculated. For each instrument pair, relative differences as a function of altitude are discussed. For some instrument pairs, comparisons including SS and SR measurements were conducted separately.

While ozone amounts derived from the ACE-MAESTRO sunrise occultation data are often smaller than the coincident observations, the sunset occultation profiles for ACE-MAESTRO show results that are qualitatively similar to ACE-FTS and indicate a large positive bias in this altitude range. The ACE-FTS sunrise and sunset measurements showed no significant bias.

Assess & Reflect

This paper goes into great detail describing comparisons of ozone measurements from ACE-FTS and ACE-MAESTRO with measurements from other instruments. Comparisons of partial columns and volume mixing ratios are thoroughly discussed for each instrument pair. Explanation of choices for coincidence criteria and visuals for the comparisons will serve as a useful reference for comparisons that I will perform between ACE-MAESTRO UV and VIS measurements.

E. Eckert, T. V. Clarmann, M. Kiefer, G. P. Stiller, S. Lossow, N. Glatthor, D. A. Degenstein, L. Froidevaux, S. Godin-Beekmann, T. Leblanc, S. Mcdermid, M. Pastel, W. Steinbrecht, D. P. J. Swart, K. A. Walker, and P. F. Bernath, "Drift-corrected trends and periodic variations in MIPAS IMK/IAA ozone measurements," ***Atmospheric Chemistry and Physics*****, vol. 14, no. 5, pp. 2571–2589, 2014.**

Summarize

Ozone profiles from the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) were studied in this paper. Monthly zonally averaged ozone profiles were used to calculate drifts, trends, and periodic variations.

A multilinear parametric trend model was used, with a constant and a linear term, annual and semi-annual oscillation terms, in addition to several harmonic overtones (*von Clarmann (2010)* is referenced for the in-depth discussion of trend estimation from irregularly sampled, correlated data). The quasi-biennial oscillation was implemented by using the Singapore winds at 30 and 50 hPa as a proxy.

Before analysing derived trends, a potential drift in MIPAS ozone data was identified and accounted for. To estimate the instrument drifts, comparisons were made with other instruments. The difference of MIPAS with the reference instrument was calculated for each data point and the related time series were fitted by the same multilinear parametric trend model. The linear term of the variation of these differences is the drift. The drift was found to oscillate in time, so the full multilinear parametric regression was used for the drift as well. For final analyses in the paper, the drift was subtracted from the calculated trends to examine ozone variation not as seen by MIPAS, but as it truly varied. Note that the coincidence criteria were that measurements closer than 250 km radial spatial distance and 6 h temporal difference to the MIPAS measurements were taken into account.

In most cases, the vertical resolution of the reference instrument was better than that of MIPAS in certain altitude regions. Their vertical resolution is worse than that of MIPAS above 40 km. For all instruments except ACE-FTS, the MIPAS averaging kernel was applied. By applying the averaging kernel, the initially finer profiles (from the reference instruments) are transferred to the MIPAS grid.

Assess & Reflect

This paper provides an excellent framework for my project by thoroughly describing methods that can be employed to analyse trends in ozone (or any other trace gas) profiles over time as seen by a satellite, and also 'as it was', by modelling the drift of the satellite instrument. References in this paper provide a more in-depth mathematical discussion of the analytical tools used.

Tools such as the regression method used to calculate trends will be very useful for my project, and I can further look at other considerations such as the calculation of drift and the use of averaging kernels after my initial analysis.

B. Efron and R. Tibshirani, "Bootstrap Methods for Standard Errors, Confidence Intervals, and Other Measures of Statistical Accuracy," ***Statistical Science*****, vol. 1, no. 1, pp. 54–75, 1986.**

Summary

This article provides an introduction to bootstrap methods, which are used to estimate model parameters using Monte Carlo methods. The paper focuses on outlining methods and their applications as opposed to theoretical considerations.

It begins by describing the bootstrap estimate of standard error for one-sample situations and identically and independently distributed observations, including situations where the data samples and/or their errors are not from a single distribution. Bootstrapping methods are especially useful when there is not an analytical means to estimate parameters/statistics.

The bootstrap methods are further developed to estimate other statistical parameters, such as bias and prediction error. Methods are also developed for censored data, regression models, and time series (two methods are presented for regression models). Several examples are used to demonstrate how these methods are used.

Assess & Reflect

This paper introduces the meaning of "bootstrapping" and shows how to use this method to estimate errors and perform regression analysis, with a choice of confidence interval for the estimated values. These methods could be implemented in my project, but the biggest downside would be the computational power required to employ them. Since I plan on using large datasets for my project, these methods might require copious amounts of time to run on my laptop and thus be inappropriate for me to use. I plan on revisiting these methods for my error estimates and regression models to see if this is the case.

D. Hubert, J.-C. Lambert, T. Verhoelst, J. Granville, A. Keppens, J.-L. Baray, A. E. Bourassa, U. Cortesi, D. A. Degenstein, L. Froidevaux, S. Godin-Beekmann, K. W. Hoppel, B. J. Johnson, E. Kyrölä, T. Leblanc, G. Lichtenberg, M. Marchand, C. T. Mcelroy, D. Murtagh, H. Nakane, T. Portafaix, R. Querel, J. M. R. Iii, J. Salvador, H. G. J. Smit, K. Stebel, W. Steinbrecht, K. B. Strawbridge, R. Stübi, D. P. J. Swart, G. Taha, D. W. Tarasick, A. M. Thompson, J. Urban, J. A. E. V. Gijsel, R. V. Malderen, P. V. D. Gathen, K. A. Walker, E. Wolfram, and J. M. Zawodny, "Ground-based assessment of the bias and long-term stability of 14 limb and occultation ozone profile data records," ***Atmospheric Measurement Techniques*****, vol. 9, no. 6, pp. 2497–2534, 2016.**

Summary

This paper describes the systematic assessment of 14 limb and occultation sounders, with ozone measurements spanning three decades. The paper studies measurements from ACE-FTS (v.3.0), ACE-MAESTRO (v.1.2), MIPAS, and other satellite instruments. The robust analysis of collocated measurement pairs (from satellite and ground-based instruments) included quantifying bias, short-term and long-term variability of the satellite records, and identifying meridional, vertical, and seasonal trends and dependences.

To estimate the drift of satellite instruments, comparisons were made with other instruments. The differences between the satellite instrument measurements and those from the reference instrument were calculated for each altitude point, and the related time series were fitted with a multilinear parametric trend model. The linear term of the variation of these differences is the drift. A bootstrapping technique was used to validate the uncertainty in the drift for each satellite-station pair. The average drift as a function of altitude for each satellite instrument was reported. The MIPAS drift was found to oscillate in time, so the full multilinear parametric regression was used for the drift as well. For final analyses in the paper, the drift was subtracted from the calculated trends to examine ozone variation not as seen by MIPAS, but as it truly varied.

Bias as a function of latitude and altitude was computed for each instrument, and short-term variability and meridional and vertical patterns were discussed.

Assess & Reflect

This paper provides an approach to identifying patterns/trends in trace gas measuring instruments. The method sections describing how to quantify drift and bias, along with cited sources (Street, J.O 1988, and Efron, B. 1986), are of most interest for my project as they can be used to analyse trends in ozone as seen by ACE-MAESTRO. Tools such as the iterative regression model used to calculate drift may be interesting for my project, and I can further look at other considerations such as the calculation of drift and bias after my initial analysis. Discussion of aggregating comparisons for instruments across different ground stations may not be as useful as I may be comparing measurements from ACE-MAESTRO to measurements solely from Eureka, Nunavut.

J. Kar, C. T. McElroy, J. R. Drummond, J. Zou, F. Nichitiu, K. A. Walker, C. E. Randall, C. R. Nowlan, D. G. Dufour, C. D. Boone, P. F. Bernath, C. R. Trepte, L. W. Thomason, and C. McLinden, "Initial comparison of ozone and NO2profiles from ACE-MAESTRO with balloon and satellite data," *Journal of Geophysical Research*, vol. 112, no. D16, 2007.

Summary

This paper is an initial study of v.1.2 measurements from ACE-MAESTRO taken in the UV and visible range. A number of separate algorithms were used to construct vertical profiles of ozone and NO2.

Measurements from ACE-MAESTRO were compared with those from ozonesondes, ACE-FTS, SAGE III, and POAM III. Spatial and temporal coincidence criteria for pairs of measurements were different for each instrument pair. The comparisons were done separately for SR and SS measurements. For comparisons, mean fractional differences were taken for the sets of coincident measurements and averaged ozone profiles were also compared.

For coincidences with POAM III SR or SS, MAESTRO SR retrievals indicate a consistent low bias from 20–50 km, while the MAESTRO SS retrievals show a significant bias above 35 km. The significant SR/SS bias seen in MAESTRO measurements in comparison with the sondes as well as other satellites indicate altitude registration problems.

Assess & Reflect

This paper provides a detailed comparison of data sets for different instruments and visualizes the results of the comparisons in different ways that may serve as a reference/starting point for when I compare ACE-MAESTRO measurements from the UV and VIS ranges. Comparing the mean ozone mixing ratio profiles measured by ACE-MAESTRO UV and VIS and finding their mean fractional differences as a function of altitude are shown to be straightforward, effective tools that I will probably use for my project.

C. T. McElroy, C. R. Nowlan, J. R. Drummond, P. F. Bernath, D. V. Barton, D. G. Dufour, C. Midwinter, R. B. Hall, A. Ogyu, A. Ullberg, D. I. Wardle, J. Kar, J. Zou, F. Nichitiu, C. D. Boone, K. A. Walker, and N. Rowlands, "The ACE-MAESTRO instrument on SCISAT: description, performance, and preliminary results," ***Applied Optics*****, vol. 46, no. 20, p. 4341, 2007.**

Summary

This paper opens with an introduction to the ACE Campaign and a description of ACE-FTS and ACE-MAESTRO. Examining ozone trends and the ozone budget is the highest priority for the ACE mission. The main objectives for ACE-MAESTRO are to collect aerosol extinction data in the 400–1010 nm wavelength range and to measure NO2 and ozone profiles with greater precision and vertical resolution than measurements from ACE-FTS.

ACE-MAESTRO has two independent diode-array spectrometers, one that measures UV and visible spectra and one that measures in the VIS and NIR range. A sunrise or sunset occultation measurement sequence consists of approximately 60 spectra collected at tangent altitudes from 0-100 km, and 20 spectra collected from the thermosphere for calculation of a Sun reference spectrum. Most measurements do not reach below 5–10 km because of clouds.

The paper also outlines the version 1.2 retrieval algorithm from raw data (Level 0) to spectra calibrated in wavelength and corrected for various instrument parameters (Level 1), to slant column densities and vertical profiles (Level 2).

Assess & Reflect

This paper provides an excellent answer to questions regarding the purpose and functions of ACE-MAESTRO. It will serve as a useful reference throughout my project when I have questions about how the instrument is comprised, the spectral range of the two spectrometers, retrieval algorithms, and other technical questions.

J. O. Street, R. J. Carroll, and D. Ruppert, "A Note on Computing Robust Regression Estimates Via Iteratively Reweighted Least Squares," ***The American Statistician*****, vol. 42, no. 2, p. 152, 1988.**

Summary

This paper provides an introduction and discussion of iteratively reweighted least squares regression methods and how to compute standard errors of regression parameters. The introduction explains that ordinary least squares modelling is not "robust against the effects of leverage". A method of creating a linear model for data by using an initial guess and iterating a set of steps until the model converges outlined, and a practical example is given.

Assess & Reflect

This paper is quite brief and provides a concise outline of modelling linearly correlated data through an iterative process. When fitting data, I might refer to this paper to implement an iteratively reweighted least squares method. After doing some further reading on the definition of "leverage" in statistics, my understanding is that leverage describes the points whose independent variable values are very different from the others (outliers). I will be working with satellite measurements that cover a constant altitude range, but some measurements might have large gaps in time, so leverage may be an issue.