Neural network scheme for the retrieval of total ozone from Global Ozone Monitoring Experiment data

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A novel approach to retrieving total ozone columns from the ERS2 GOME (Global Ozone Monitoring Experiment) spectral data has been developed. With selected GOME wavelength regions, from clear and cloudy pixels alike plus orbital and instrument data as input, a feed-forward neural network was trained to determine total ozone in a one-step inverse retrieval procedure. To achieve this training, ground-based total ozone measurements from the World Ozone and Ultraviolet Data Center (WOUDC) for the years 1996–2000, supplemented with Dobson-corrected Total Ozone Mapping Spectrometer (TOMS) data to provide global coverage, were collocated with GOME ground pixels into a training data set. Validation of the neural-network-retrieved ozone values relative to independent ground stations yielded a rms error of better than 11 Dobson units. Comparisons performed on the basis of operationally available TOMS and GOME level-3 maps exhibit good agreement in general, with a latitude-dependent offset. © 2002 Optical Society of America

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1. Introduction

Measuring atmospheric parameters and constituents on a global scale has been a challenge to atmospheric scientists ever since the establishment of this discipline and has not as yet lost any of its significance. For the measurement of total ozone, which is one of the most important trace gases to influence our climate and health, a ground-based detection network was set up as early as in the 1930s through the pioneering work of Dobson.[1] Although it has been continually growing since then, this network has never achieved true global coverage, as its horizontal resolution is limited by the number of stations and by their inherent inability to provide arealike measurements. This situation improved dramatically with the advent of orbital instruments in the late 1960s, which for the first time were able to sample the atmospheric state of the entire globe within some hours or days. However, these instruments in turn introduced their own problems, the most troubling of which nowadays appear to be that (a) once in orbit, the instruments are difficult to recalibrate, (b) inverting their data to yield atmospheric constituents is a much more complex operation than for ground-based instruments, and (c) their data rate increases faster than the amount of available computer power and infrastructure needed for real-time data processing or reprocessing of historical data.

To ameliorate these problems, the development of new retrieval algorithms is essential. In an ideal case, such algorithms would not rely on detailed knowledge of all physical processes involved and would be independent of all calibration-related issues and fast enough to be implemented directly at the receiving stations with low-cost hardware. Because neural networks generally exhibit these properties, their use in satellite meteorology has grown in recent years. For instance, Chevallier *et al.*[2] developed a complex neural-network scheme for long-wave radiation budget calculations that increased the processing speed by a factor of 10^6 compared with the classical line-by-line model. Aires *et al.*[3] successfully retrieved various atmospheric parameters from the Special Sensor Microwave/Imager (SSM/I) over land, a task that had not been successfully completed previously because of the many unknown phenomena involved.

In this paper we shall focus on total ozone retrieval from the Global Ozone Monitoring Experiment (GOME), a UV–visible nadir viewing spectrometer that has been operational since June 1995. Ozone

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columns are currently retrieved operationally at the Deutsches Zentrum für Luft- und Raumfahrt by differential optical absorption spectroscopy.[4] In a first step, slant column densities are determined; slant columns are then converted to vertical columns by calculation of an air mass factor (AMF) by use of a multiple-scattering pseudospherical radiative transfer model in which a climatological ozone profile is assumed.[5–7] Validation with ground-based data showed global agreement to within ±4%; however, at solar zenith angles above 60° deviations of 10% and more were observed.[8,9]

The presence of these deviations hints at the fact that a considerable part of the observed errors stem from problems in calculation of AMFs, whose effect is largest at high solar zenith angles. An inherent problem of the Differential Optical Absorption Spectroscopy/AMF approach is that to determine AMFs properly one needs to know the vertical distribution of the corresponding absorber in advance, which is therefore inferred from climatology. A comprehensive discussion of this issue and its possible solutions is beyond the scope of this paper but can be found in those of Marquard et al.[10] and Palmer et al.[11]

As AMF calculation is also the most time consuming part of the retrieval, efforts have been made to speed up this part of the retrieval without jeopardizing precision. Loyola[12] trained neural networks on data calculated with a slow but accurate radiative transfer model, achieving relative AMF differences below 2% while reducing the calculation time to negligible amounts. However, this algorithm is so far not part of the standard retrieval. A similar increase in speed was reported by Del Frate et al.,[13] who used neural networks to effectively emulate the GOME ozone profile retrieval system of the Rutherford Appleton Laboratory.[14]

All the applications mentioned so far have in common the use of neural networks solely as an operational shortcut for already existing physical algorithms. However, the capabilities of those networks go beyond that. When they are applied to a training set of real measurements, they effectively constitute an independent retrieval method that deals with instrument calibration and degradation independently. Krasnopolsky,[15] for instance, examined atmospheric parameter retrieval from SSM/I data over sea. A neural network used for this purpose has a number of independent parameters similar to those in the corresponding physical or empirical methods. All these models have to be tuned to a number of collocated measurements to produce the desired retrieval accuracy. Using these measurements directly as training data for a neural network has led to better results in all respects.

For total ozone, the advantage of using a neural-network-based retrieval system clearly lies in the availability of ample ground data from the Dobson network and its successors. For the NOAA TIROS-N Operational Vertical Sounder (TOVS) instrument suite, which is a combination of infrared and microwave radiometers, it was shown that a neural-network approach is able to account properly for extreme slant viewing geometries at wide scan angles of as much as ±49.5° as well as for cloud-contaminated pixels.[16,17] Whereas the operational TOVS total ozone product exhibits rms errors, with respect to ground stations, in the order of 25 DU greater than those of ground stations,[18] the neural-network approach reaches 15 DU. The same methodology has now been adapted and enhanced for GOME ozone column retrieval, establishing an alternative to the standard retrieval procedures.

2. Data and Methods

A. Collocations

We obtained GOME radiance and irradiance spectra from the years 1996–2000 by applying the GOME Data Processor (GDP) extraction program to the current GOME level-1 data program [Version 2.0 (Ref. 19)]. After Doppler correction of the daily solar spectrum, earthshine and solar spectra were interpolated to a common wavelength grid. This and the following Sun normalization of the earthshine spectra induce some high-frequency noise, especially around the Fraunhofer lines in the solar spectrum. However, as an alternative the neural network would have to be provided with the relative wavelength shift of earthshine versus solar spectrum for each single wavelength, such that it could independently perform some kind of correction based on these shifts. Neural networks are generally quite noise resistant, so using a common grid is preferable to feeding the entire wavelength information into the network, which would roughly double the number of input data and slow training considerably.

The construction of a suitable set of neural network training data requires a considerable amount of what is commonly referred to as ground truth, meaning reliable measurements of the quantity to be retrieved. To this end, ground-based total ozone measurements from Dobson, Brewer, and filter spectrometers that are collected and quality-controlled by the World Ozone and Ultraviolet Radiation Data Centre[20] (WOUDC) have been utilized. We designate this data set ground data in what follows.

However, comparing the data of individual ground stations with satellite measurements reveals considerable biases and variations.[21,22] Also, these stations are not scattered evenly around the globe. Therefore, in an effort to compensate for the sparsity of ground stations in the Southern Hemisphere and in the polar regions, the WOUDC database has been supplemented with virtual stations, namely, fixed geographical locations for which one total ozone value per day was taken from the gridded TOMS Version 7 ozone field.[23]

The question of how to homogenize the resultant mixed total ozone data set then arises. For the purpose of training a neural network it is more desirable to deal with known biases than with random scatter, because the latter slows the training process and in-

creases the achievable minimum error. Biases, however, can be corrected before training commences.

To reduce scatter in the training data we set up an *ad hoc* ranking scheme for the ground stations, that assigns a consistency score to each station based on bias, standard deviation, and mean absolute errors of ground data relative to operational TOMS and GOME total ozone column products. This scheme has been tested extensively with neural networks trained to retrieve total ozone from the NOAA TOVS,[17] and it was found that selecting the most consistent 100 of the 250 stations yields a good basis for the training data set.

Not surprisingly, the stations retained by the ranking process cluster around the northern midlatitudes—where station density is highest—and, to a lesser degree, the tropics, where low ozone variability leads to small differences with respect to satellite measurements. A total of 45 virtual stations were created poleward of 60° latitude. Between 60° S and 60° N, the resulting training data set thus contains only ground data, south of 60° S exclusively TOMS data, and north of 60° N a mixture of both data types, with a prevalence of TOMS data.

Whether TOMS or the ground data are closer to the true total ozone columns will not be discussed here, because the answer is not relevant for neural-network training as long as the data sources themselves are consistent. However, to ensure a smooth transition between the latitude regions dominated by ground data and those dominated by TOMS data it is desirable to correct for offsets between these data. In this paper we assume that the ground data are correct; therefore a time- and latitude-dependent offset function derived by Bodeker *et al.*[22] was applied to the virtual station data (Fig. 1) to make them consistent with the ground data. The function was devised for purposes of trend analysis and contains 22 coefficients, which were fitted to the difference between TOMS and ground data by least-squares regression. As can be seen, the differences reach values of 20 DU (Fig. 1).

The maximum horizontal collocation distance between the GOME field-of-view (FOV) center and the station location was 120 km. Only forward-scan pixels from the same day as the ground data were utilized.

The neural-network test data set originated from the collocation of six selected stations with known data quality, suitable location, or both (Table 1). The retrieval results listed in this table are discussed in Section 3 below. The purpose of this data set is mainly to monitor the generalization ability of the neural network; therefore stations from the various training data regimes were selected. In addition to stations at Hohenpeissenberg and Bangkok, and the virtual stations at 85 °N and 85 °S, which together cover the whole latitude range, we used the station at Boulder to check whether there were any longitudinal effects and the virtual station at 80 °N to check
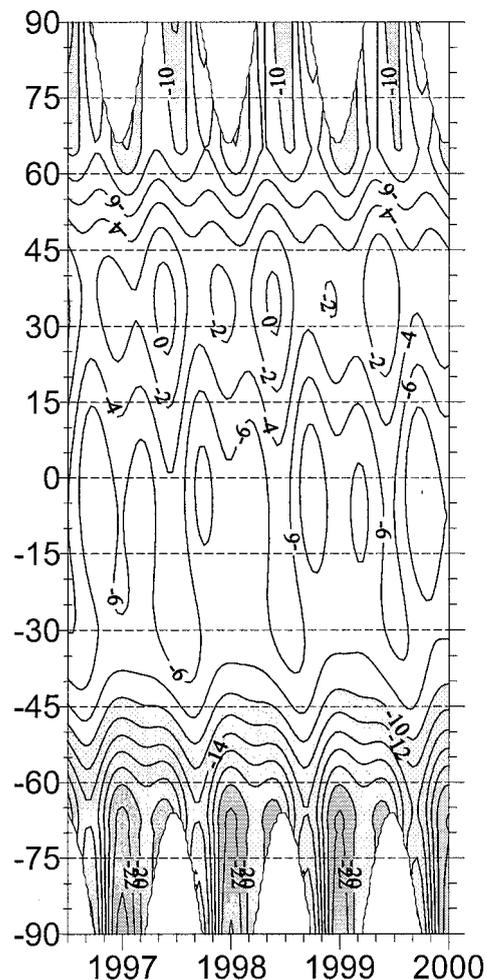

Fig. 1. Fit function for the difference between the ground-based total ozone network minus Earth probe TOMS V.7 ozone columns, in DU (taken from Bodeker *et al.*[22]).

whether the latitudinal transition from ground to TOMS data ran smoothly.

To prevent overrepresentation of certain total ozone values or geographical regions in the training data set, a two-dimensional histogram with bins of 10 DU times 10° latitude was employed. The maximum number of collocations per bin was then limited to 500, whereby excess collocations were randomly selected and discarded. Multiple GOME FOVs collocated with the same total ozone measurement and vice versa have been allowed, because they help the neural network to select relevant features in the input data and allow it to deal with instrument noise as well as with uncertainties of ground and TOMS data. In this manner two data sets that comprised 138,489 training and 16,977 test collocations were created.

B. Neural-Network Technique

The feed-forward type of neural network employed here is called a perceptron and consists of successive one-dimensional layers.[24] The type of training algorithm employed largely determines the time needed for training and the minimum rms error (RMSE)

Table 1. Selected Ozone Stations for the Neural-Network Test Data Set[a]

Station	Latitude	Longitude	Regime[b]	Bias (%)	σ (%)	RMSE (DU)
Hohenpeissenberg	48 °N	11 °E	Ground	2.28	2.60	11.42
Boulder	40 °N	105 °W	Ground	2.48	3.20	12.36
Bangkok	14 °N	101 °E	Ground	−1.21	2.92	8.00
Virtual TOMS station	85 °N	45 °W	TOMS	−0.38	3.15	10.97
Virtual TOMS station	80 °N	90 °E	Both	0.12	3.48	11.96
Virtual TOMS station	85 °S	45 °W	TOMS	0.95	4.63	8.78

[a]Ozone column bias and standard deviation σ were calculated for neural-network retrievals of the collocated GOME pixels as (GOME minus station)/station.

[b]"Regime" refers to the available training collocations in the respective latitude region.

reached after learning. Here the resilient propagation (Rprop) algorithm[25] yielded the best results.

Selection of suitable numbers and sizes of neural-network layers is crucial to the neural network's success. To take advantage of the network's nonlinear approximation capabilities requires, in addition to an input and an output layer, at least one hidden or intermediate layer.[26] The exact size of the hidden layer has to be determined empirically.[27]

The most successful network configuration found in this study uses 20 hidden neurons. The input consists of GOME Sun-normalized earthshine spectra covering the 320–340-nm range and of satellite orientation information, e.g., on line of sight, solar zenith angle, relative azimuth angle between the Sun and the line of sight, and center latitude of the ground pixel. The spectral range used here is greater than the one used to derive the GOME level-2 Version 2.7 total ozone data [325–335 nm (Refs. 6 and 7)]. To speed up the training process we halved the number of spectral samples by averaging pairs of Sun-normalized radiances.

The instrumental lifetime is an additional input parameter that allows for time-dependent corrections, such as instrument degradation functions, to be found by the network.[28] This is not normally a limitation to the applicability of the method beyond the training data time range because the network can extrapolate instrument degradation several months into the future, provided that there are no abrupt changes. In an operational regime the network would be retrained every few months with the new data included in the training set.

No cloud-clearing procedure was employed, which means that cloudy, partially cloudy, and clear scenes were treated in the same way.

3. Results and Discussion

Figure 2 shows the development of the RMSE of neural-network output with respect to the collocated ozone values for the first 10,000 training epochs of the best-trained network. An epoch is defined as one presentation of all training collocations to the neural network. As can be seen, the training data set's RMSE decreases monotonically, which is a characteristic feature of the Rprop algorithm. The test RMSE decreases more irregularly, partially because it is calculated from a much lower number of data, but both

level out after a few thousand epochs, after which training progresses only slowly (note the double-log scaling). The minimum RMSE, 10.7 DU, was reached after ~50,000 epochs. The fact that the test error decreases further than the training error hints at the higher quality of ground data in the test data set.

Table 1 lists the bias and the standard deviation of the retrieved ozone columns with respect to the test stations' total ozone measurements. The RMSE is lowest for Antarctica and the tropics, where day-to-day variations of ozone are also quite low. Stations within the same latitude region do not show significant differences. The bias for virtual station data is less than that for the ground-regime data, as the TOMS measurements are in themselves highly homogenous. The virtual station at 80 °N, which is located close to several training ground stations near the Arctic Sea, does not exhibit much larger errors than do the other test stations, therefore proving that the latitudinal mixing of ground and TOMS data does not have adverse effects. A considerable part of the remaining variance is due to collocation errors: A simple calculation of the day-to-day variations of ozone based on all the WOUDC data reveals that these errors are of the order of 4% within 30° of the equator, ~5% at the poles, and 7–8% in the northern midlatitudes.

Two time series of differences between GOME retrieval and collocated test station data from Hohen-
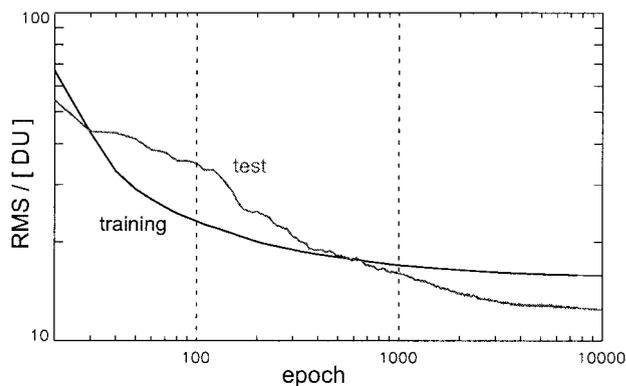

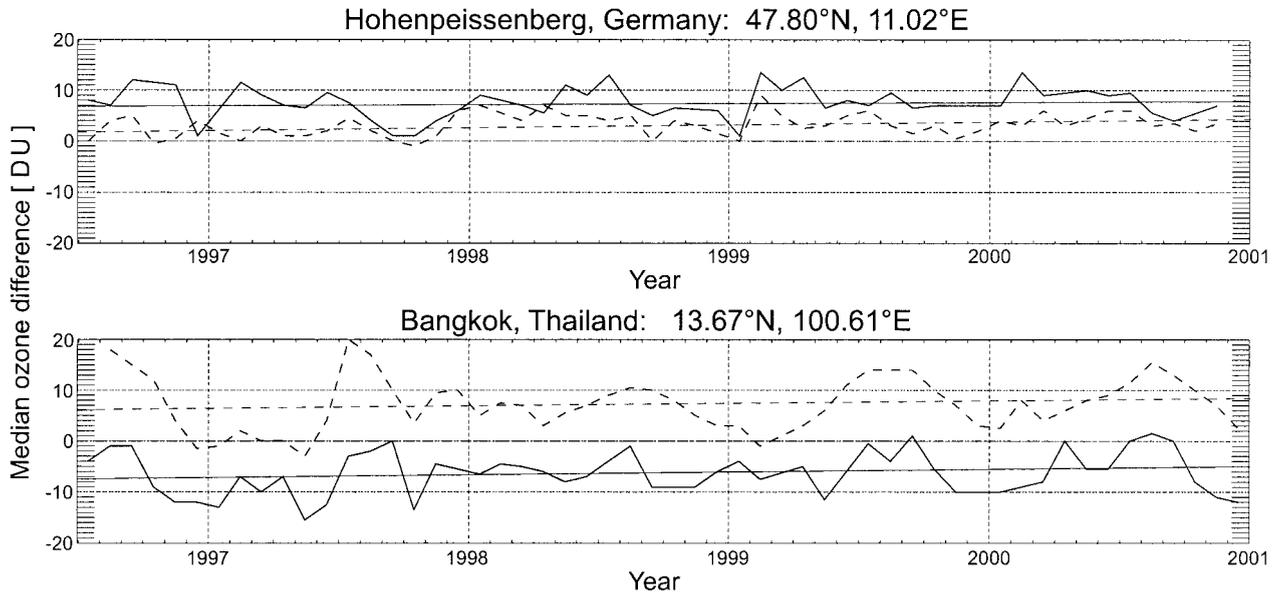Fig. 2. Development of the rms error for training and test data set during neural-network training.

Fig. 3.   Time series of the difference of neural-network-retrieved GOME total ozone (solid curves) and TOMS Version 7 total ozone (dashed curves) with respect to ground measurements.   Neither ground station was used in training the network.   The differences are plotted as monthly median values, whereas the thin straight lines represent linear regression based on all data.

peissenberg (48 °N) and Bangkok (14 °N) are shown in Fig. 3.   The data from Hohenpeissenberg and Bangkok exhibit a more-or-less constant offset with respect to the GOME results, but most data lie within ±10 DU.   Note that these stations are situated in latitude regions where no TOMS data were used for training the network; therefore TOMS level-3 Version 7 ozone data from the same time range have been plotted for comparison.   As can be seen, the monthly variations of the two data sets are of the same magnitude, suggesting that the neural-network-retrieved data are consistent in time.   Also, there seems to be no statistically significant drift in the GOME neural-network total ozone in time with respect to the ground data.   Any effects that may result from the accelerated differential degradation of GOME solar and nadir spectra starting at the end of 1998 (Ref. 28) are obviously compensated for by inclusion of the instrumental lifetime in the neural-network input.

To examine the spatial extent of the time-independent offset seen in Fig. 3 we created monthly means of the global TOMS data (288 × 180 bins) and compared them with neural-network-retrieved GOME ozone data (subsequently denoted NN-GOME) gridded accordingly and averaged over the same time range.   In addition, the operational GDP V2.7 GOME ozone product (GDP-GOME) was obtained and treated similarly.   An example of this comparison is shown in Fig. 4, from which, at first glance, one can see that large-scale structures in the global ozone distribution look much alike on all three maps.   The deviations that are obvious in the equator region and above the oceans near Antarctica hint at a latitude-dependent offset between the NN-GOME and the TOMS.   When NN- and GDP-GOME

data are compared, the largest differences can be observed in the northern midlatitudes, especially near the Pacific Ocean.

Table 2 summarizes the global monthly differences between the satellite data sets for 1999.   Whereas GDP-GOME and NN-GOME agree well from January through April, NN-GOME values are systematically higher later in the year.   When the GDP-GOME retrievals are compared with TOMS data the offset is even higher, averaging to 9.99 DU over the entire year.   This figure can be directly compared with the results of Corlett and Monks,[29] who found a systematic offset of 10.06 DU for the time period 1996–1999.   Because TOMS yields systematically higher values than GOME in almost all cases (cf. Fig. 4), there is not much cancellation of positive and negative errors here.   If all the TOMS data are treated with the fit function introduced above (Fig. 1), the difference from both GOME retrieval methods shrinks considerably.

Zonal means and standard deviations of the GOME–TOMS difference are depicted in Fig. 5.   A plot for April 1999 has been added give an impression of the seasonal variation of the differences.   The distinctive latitude-dependent offset between NN-GOME and TOMS seems to follow the correction function of Bodeker et al.,[22] which is also shown in the figure.   Virtual stations that use this correction were employed only poleward of 60° latitude, whereas below 60° latitude the neural network derived the correction function independently, thereby confirming the statistical analysis presented in Ref. 22.   The deviation from the curve from 30° to 60° can be partially attributed to geography, of which the neural network knows nothing as yet.   Inasmuch as only a few WOUDC stations are situated at a higher eleva-
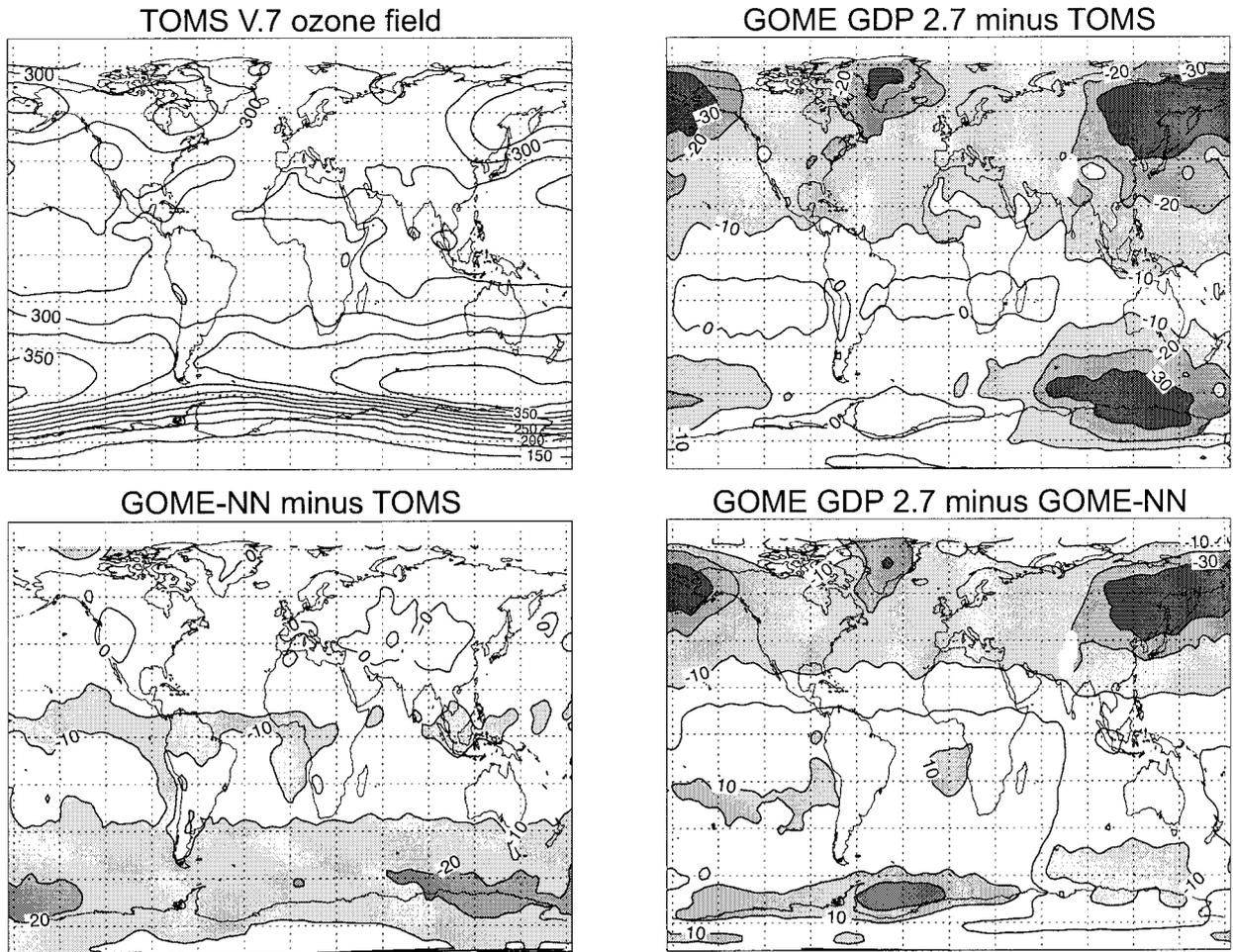
Fig. 4. TOMS monthly mean total ozone field for October 1999 and difference maps for all sensors and processing algorithms considered (DU). Both operational products had been provided as level-3 daily maps; therefore neural-network ozone values were averaged into daily maps as well, before the monthly mean was calculated.

tion, the neural network tends to overestimate total ozone above mountainous regions.

The GDP-GOME data in general agree better with NN-GOME than with TOMS data, but there are major deviations poleward of ±45°. These findings are in line with what Corlett and Monks[29] describe in a much more thorough study that also incorporates TOVS ozone data.

The standard deviation generally lies near 5 DU but in some cases increases quickly at the very edge of the polar night, suggesting high solar zenith angle problems, which are common with all UV-backscatter

Table 2. Monthly Global Mean Deviations for 1999 (DU)[a]

Ozone Fields Compared	Mean Deviation (DU)												
	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Average
GDP–NN	0.85	−0.28	−0.22	2.59	3.40	5.98	5.14	4.14	5.22	3.91	2.63	3.23	**3.05**
Generic TOMS data													
TOMS–GDP	8.52	7.71	7.28	9.12	8.90	11.08	10.03	9.76	11.65	11.79	11.68	12.40	**9.99**
TOMS–NN	7.88	8.27	7.57	6.93	5.66	5.25	5.61	6.35	6.68	7.94	8.97	9.38	**7.21**
TOMS data fitted to ground network[b]													
TOMS–GDP	0.46	−0.48	−0.64	2.02	2.79	5.64	3.89	2.55	3.85	3.76	3.67	4.39	**2.66**
TOMS–NN	−0.27	−0.02	−0.45	−0.25	−0.33	−0.36	−0.70	−1.03	−1.32	−0.26	0.75	−1.09	**−0.44**

[a]NN, neural-network-retrieved total ozone values; GDP, operational GDP V2.7 ozone product; TOMS, Version 7 TOMS ozone values. The means were calculated on monthly averaged level 3 data weighted by surface area.
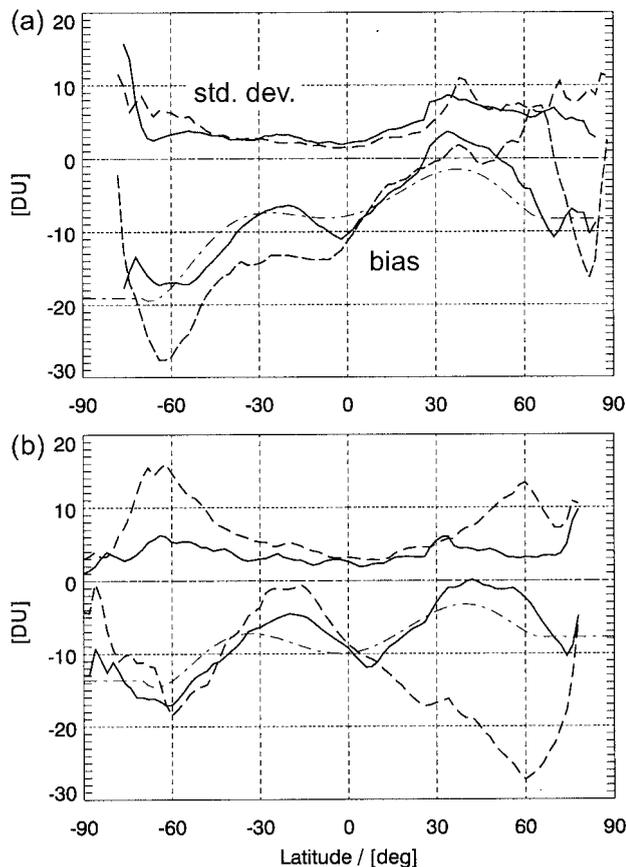[b]Ref. 22.

Fig. 5. Latitudinal mean and standard deviation of GOME ozone minus TOMS ozone for (a) April and (b) October 1999. Neural network and GDP 2.7 ozone are represented as solid and dashed curves, respectively. The correction function applied for creating virtual TOMS stations is plotted as a dashed–dotted curve for comparison.

instruments as the result of physical limitations induced by the slant path geometry.

4. Conclusions and Outlook

It has been shown that neural networks can retrieve high-quality total ozone columns from GOME data if an appropriate collocation database is provided. The retrieved ozone values are consistent in space and time, making them suitable, e.g., for long-term ozone monitoring. In essence, the neural-network technique can be viewed as a method of effectively globalizing ground-based measurements by establishing a nonlinear relationship to spectral satellite data and using supplementary statistical information to correct for instrumental effects such as calibration uncertainties and degradation. Cloud contamination is obviously also accounted for by replacing missing physical information in the spectra with statistical estimates, such that no cloud structures can be discerned in the total ozone maps.

In most cases the retrieved ozone values more closely resemble to the ground data than do those of the TOMS and the GDP-GOME, even in latitude regions where no TOMS data were used for training.

However, this proves that a combined dataset of ground data and corrected TOMS data is consistent enough for a neural network to establish a global relationship between the top-of-atmosphere radiances and total ozone. Should it later turn out that for some reason TOMS is actually more accurate than the ground network, one could in turn correct the ground data by using the same function and train a network to accurately reproduce the TOMS data from GOME measurements. In any case, the neural-network method always takes advantage of the most accurate data source available by directly transforming it into an inverse retrieval model on a global scale.

Current studies focus on some of the remaining problems, such as high elevation and spatially uneven training data distribution; after their completion the neural-network total column ozone from GOME will be made available operationally, as has already been done with a neural-network ozone product from TOVS data.[17] A similar technique for retrieving ozone profiles from GOME data is also currently under development.[30]

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