A New Unconstrained Approach to GNSS Atmospheric Water Vapor Tomography

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Abstract A new atmospheric tomographic model totally based on Global Navigation Satellite System (GNSS) observations is proposed and tested against field observations. The method does not require a first guess, does not contain specific constraints on the variability of water vapor density inside the tomographic domain, and is able to produce reasonable results at 6 km horizontal and 500 m vertical resolutions, from short (30 min) GNSS data samples. The inversion method uses the Moore-Penrose pseudoinverse, which is made possible by increasing the rank of the design matrix through angular interpolation and extrapolation of the observations. Comparisons against 30 consecutive 4-h radiosonde observations and model simulations suggest the ability of the method to detect inversions and local maxima aloft, and behave sensibly in the far-field. Further improvements from this method may be expected from higher density and multi-constellation networks.

Plain Language Summary Knowing the three-dimensional distribution of water vapor is a key goal of atmospheric observation that has been very difficult to attain, given its space and time variability. A new method of water vapor tomography is proposed, exclusively based on Global Navigation Satellite System observations, such as GPS, which is found to lead to sensible results. These results suggest a feasible tomographic system, using data from all satellite constellations (GPS, Glonass, Beidou, and Galileo) with a dense network of ground stations.

1. Introduction

Since the establishment of Global Navigation Satellite System (GNSS) meteorology (Bevis et al., 1992, 1994) indicating the possibility of using GNSS ground stations delay anomalies to infer column integrated water vapor (IWV or precipitable water vapor, PWV), the value of such information for meteorology has been explored in different ways, as a new weather nowcasting variable (e.g., Baker et al., 2001; Benevides et al., 2015; Champollion, Masson, Van Baelen, et al., 2004; Foster et al., 2003; Liu et al., 2019; Van Baelen et al., 2011) or as a variable to assimilate in numerical weather prediction (NWP). The impact of such data on NWP operations has, however, been limited because available GNSS ground stations data were not yet able to produce PWV observations at sufficient horizontal resolution, and its assimilation tends to produce rather smooth fields with little (but positive) impact on forecasts (Mateus et al., 2018).

GNSS PWV represents the observation of an inverted atmospheric cone, encompassing a diameter of around 35 km at 850 hPa (about 1.5 km) when GNSS data is accepted from an elevation of 5° (Hanssen, 2001). GNSS PWV can be estimated every few minutes. The quality of that data has been assessed against radiosonde observations in different studies and found to have an accuracy of the order of 1 mm or less (cf. details in Adams et al., 2011 and Alshawaf et al., 2015), as long as it is processed by high-precision scientific software such as GAMIT/GLOBK (Herring et al., 2018). The assimilation of these 2D fields into NWP models has been found to be challenging, with positive impact on rainfall prediction in spite of a relatively small influence on the 3D structure of the water vapor field (Guo et al., 2000). Some studies also indicate the potential of the direct assimilation of slant delays in nowcasting (Bauer et al., 2011; Risanto et al., 2021).

The possibility of using GNSS data one step further to compute tomographic 3D images of the troposphere has also been considered, starting with a case study of severe rain in Hawaii by Flores et al. (2000), and has led to the development of different tomographic inversion methods applied to field experiments (Champollion, Masson, Bouin, et al., 2004; Champollion et al., 2009; Nilsson et al., 2007; Van Baelen et al., 2011), in some cases to countrywide networks (Bender et al., 2011). However, these developments could not be made...
without the inclusion of extraneous data from different sources, namely from NWP analysis or forecasts, from radiosonde observations or other remote sensing platforms, imposing direct constraints on the water vapor field. The feasibility of doing these inversions in real time was recently assessed (Sá et al., 2021).

GNSS tomography is computed from the distribution of GNSS delays between the different available satellites and a network of closely located ground stations, computed along each slant line connecting stations and satellites. In the case of the GPS constellation, it means at most 10 delays per ground station on each observation instant. By accumulating observations during a period like 1 h (an epoch), and assuming a stationary atmosphere, it is possible to gather a large number of observations. Each of these observations can be converted into an estimation of the IWV along the “slant” line, a well-established result (Bevis et al., 1992; Hopfield, 1971). The computation of the 3D distribution of water vapor from those observations is thus equivalent to solving the linear problem:

$$\tilde{S}_{\text{IWV}} = D\hat{\rho},$$  

(1)

where $\tilde{S}_{\text{IWV}}$ is a vector containing $N$ available slant integrated water vapor (SIWV) observations (in all ground stations), $\hat{\rho}$, is a vectorized version of the 3D water vapor distribution in the tomographic domain with $n_v = n_x \times n_y \times n_t$ voxels and $D$ is an $N \times n_v$ design matrix, where each term contains the size, in meters, of the GNSS microwave ray path from the corresponding observation (the matrix line) crossing the corresponding voxel (the matrix column). In general, $N \gg n_v$ but the matrix rank is smaller than $n_v$, implying that the problem is largely underdetermined, because of redundancy between observations at sequential instants and of observational noise. GNSS tomographic algorithms have dealt with this problem by adding constraints to the distribution of water vapor inside the tomographic domain, which are equivalent to imposing extra observations affecting non-observed voxels. Examples of such constraints are described in Yao et al. (2020).

The inclusion of independent remote sensing observations from multiple GNSS constellations (Li et al., 2015), from InSAR (Benevides et al., 2016), and from optical bands, including the AIRS multispectral sensor (Benevides et al., 2018) and MODIS (Zhang, Zhang, Ding, et al., 2021; Zhang, Zhang, Zheng, et al., 2021), have proved to be beneficial, but not at the point of making the inversion feasible without extra non-GNSS data. The comparison of Benevides et al. (2018) between solutions initialized by a radiosonde and by the corresponding AIRS profile clearly indicates a strong dependence of current tomographic methods on their initial guess.

Rohm (2013) tried to address this issue, with synthetic data, by extending the observation period, concluding that a successful “unconstrained” solution could be obtained with 10 h of observations, a period which is in general far too long even for a very stationary atmosphere. However, with four GNSS constellations, such period may be reduced.

In the present study, we try a somewhat different approach. First, we follow Rohm (2013) by performing a tomographic study with real data from the rather stationary atmosphere observed in the SMOG (Structure of Moist convection in high-resolution GNSS observations and models) field experiment in July 2013, and previously analyzed with standard tomographic methods (Benevides et al., 2018). Next, we propose a new approach to increase the rank of the design matrix, but without direct constraints on the voxel variability or first guesses from non-GNSS data. In both cases, we proceed to the solution by applying the Moore-Penrose pseudoinverse algorithm (Moore, 1920; Penrose, 1955) and evaluate the results against real observations.

### 2. Data and Methods

The SMOG field experiment took place in the Lisbon area (Portugal) in July 2013 and included the deployment of a network of 17 GPS receivers (including those from the permanent network) with a station spacing down to about 6 km (Figure 1) and the launching of 4-h radiosondes during six consecutive days near the center of the field domain. The procedure taken to compute SIWV was described in Benevides et al. (2018). The choice of the location and timing of the experiment was justified by the expected stationarity of the lower troposphere in summer, with little synoptic forcing, and by the frequent occurrence of strong water vapor gradients just above the boundary layer (Salgado et al., 2015), a challenge for tomography. The 4-h radiosonde cycle offers a unique data set to evaluate the tomographic results.
Because the radiosondes only provide detailed information along specific ascent paths, the Weather Research and Forecast (WRF) model (Skamarock et al., 2008), version 4.1, at 3 km horizontal resolution and 70 layers, forced by ERA5 (Hersbach et al., 2020) reanalysis, was used to simulate the flow in the region. The simulations were initialized every 24 h (at 18 UTC), with the first 6 h taken out to account for model spin-up. Parameterization options are the same as in Mateus et al. (2021).

A sensitivity analysis was performed with two unconstrained tomographic solutions at different horizontal and vertical resolutions (Table 1). Both solutions use a tomographic grid regularly spaced in the horizontal, with a vertical terrain-following coordinate (Gal-Chen & Somerville, 1975; Figure 1):

\[
\hat{z} = \frac{H_0(z - z_s)}{H_0 - z_s},
\]

which can contain layers of different vertical resolutions. In Equation 2, \(H_0 = 10\) km is the altitude of the top boundary of the tomographic domain, \(z_s\) in the terrain altitude, and \(\hat{z}\) is the altitude. The use of a terrain-following coordinate follows standard practice in atmospheric modeling, and has the advantage of avoiding unobserved (or poorly observed) voxels at low levels in the case of complex terrain, which can lead to spurious solutions. In the case of flat terrain at sea level (\(z_t = 0\)) \(\hat{z} = z\).

In the first solution, the design matrix \((D_\lambda)\) is computed in the standard way from the ray-path of the observations within a chosen time window, the observation vector \((\hat{S}_{\text{obs}})\) contains the observed SIWV, and the solution is obtained by applying the pseudoinverse algorithm to Equation 1. In the second solution, the design matrix \((D_\lambda)\) is computed for sets of rays, at each ground station, regularly spaced in the angular

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**Figure 1.** Tomographic domain for the SMOG field experiment. Black triangles locate the Global Navigation Satellite System ground stations. The lower wireframe shows the height of the topography at the 6 km tomographic resolution. One of the tomographic layers (2–2.5 km), in terrain-following coordinates, is shown aloft, with three of the voxels being observed by one or two stations. The green line represents the path of one of the radiosondes (RS). All data in a UTM projection (zone 29°N).
domain (in both azimuth and elevation), and the corresponding observation vector \((\mathbf{S}_\alpha, \mathbf{S}_\eta)\) at the prescribed azimuths and elevations) is computed by a least-squares fitting of the slant observations to a continuous function of azimuth and elevation:

\[
S_{\text{IWV},k} = a_i \cos(\alpha_{i,k}) + b_i \sin(\alpha_{i,k}) + \frac{c_i}{\sin(\eta_{i,k})} + d_i + \varepsilon_{i,k} \quad (i = 1, \ldots, n; \quad k = 1, \ldots, N),
\]

where \(S_{\text{IWV},k}\) is the \(k\)th slant observation at station \(i\) within a 30 min time window, \(\alpha_{i,k}\) and \(\eta_{i,k}\) are the corresponding co-azimuth and elevation, and \(\varepsilon_{i,k}\) is the fitting error. From the coefficients \((a_i, b_i, c_i, d_i, i = 1, \ldots, n)\), we then compute:

\[
\mathbf{S}_\alpha = \mathbf{S}_{\text{IWV},i} = a_i \cos(\alpha_i) + b_i \sin(\alpha_i) + \frac{c_i}{\sin(\eta_i)} + d_i \quad (i = 1, \ldots, n),
\]

\[
\mathbf{S}_\eta = \mathbf{S}_{\text{IWV},j} = a_j \cos(\eta_j) + b_j \sin(\eta_j) + \frac{c_j}{\sin(\eta_j)} + d_j \quad (j = 1, \ldots, J),
\]

where \(\alpha_i, \eta_j\) are the prescribed regularly spaced co-azimuths and elevations. Finally, the solution is obtained by solving (for \(\mathbf{\bar{\rho}}\)) the underdetermined system of equations:

\[
\mathbf{S}_\alpha = \mathbf{D}_\alpha \mathbf{\bar{\rho}},
\]

again by the pseudoinverse technique.

One further detail was included in the tomographic model for both methods. When a given ray \((m)\) to station \((j)\) enters the tomographic domain through its lateral boundaries, the SIWV observation is corrected by:

\[
S'_{\text{IWV},m} = S_{\text{IWV},m} \frac{1 - \exp\left(-\frac{z_m}{H_w}\right)}{1 - \exp\left(-\frac{z_m}{H_s}\right)},
\]

where \(z_m\) is the altitude of the ray when it crosses the wall, \(H_w\) is the altitude of the top boundary of the tomographic domain (10 km), and \(H_s = 2\) km is the scale height of the atmospheric water vapor (Tomasi, 1984). Equation 6 assumes that the water vapor density decays exponentially with height in the atmosphere outside the tomographic domain. It is important to stress that Equation 4 applies to an unbounded plane atmosphere, the first two terms representing the zonal and meridional structures of the IWV field (at constant elevation) and the third term the effect of elevation, so correction Equation 6 needs to be applied after the computation of the \((a_i, b_i, c_i, d_i)\) coefficients.

### 3. Results

Table 1 shows parameters and mean error statistics for five tomographic experiments applied to time windows around 30 consecutive radiosonde ascents in experiment SMOG. The first three experiments use the first inversion method from directly observed SIWV at different resolutions (horizontal and vertical) and for two different time windows (3 h and 30 min). The shortest time window (S3) is of course unusable, but the corresponding design matrix will be needed later. Experiment S2 (at 10 km horizontal, 500 m vertical...
resolution) not only results in poorer mean statistics than S1, but also does a very poor job in the lowest layers, largely overestimating (by a factor of 2) the low-level water vapor density. In the two inversions with the method here proposed, the first (A1) matches the resolution of S1, leading to the best overall statistics from just 30 min of assimilated data. The second (A2), at higher horizontal and vertical resolutions, requiring finer angular interpolation, shows slightly worst statistics but is able to capture some fine details of the water vapor field.

Figure 2 shows results from Experiment A2, compared with the radiosonde observations and with the WRF simulations, with both model results taken along the grid point nearest to the radiosonde launch (Figure 1). The low-level structure of the water vapor field is mostly very well captured by the tomography, often better than by WRF. The tomography is in some cases able to detect secondary maxima aloft (especially in day 201 and 202), and the far-field appears very well-conditioned, with the profiles converging smoothly to zero at
the top of the domain. Averaging over all experiments leads to the values shown in Table 1. An analysis of the vertical distribution of the errors (not shown) indicates that the mean low-level RMSE in Experiment A2 is near 2.4 g m\(^{-3}\) (with 1.2 g m\(^{-3}\) in WRF), with values around 1.4 g m\(^{-3}\) for the voxel above 3 km (with 0.8 g m\(^{-3}\) in WRF) and 0.15 g m\(^{-3}\) for the voxel above 8 km (with 0.08 g m\(^{-3}\) in WRF).

Figure 3 shows a comparison between S1, A2, and WRF, in the zonal cross-section closer to the radiosonde ascent taken at 12 UTC on each of the 5 days simulated. In doy 198 and 199, both tomographic models are excellent in the lowest layer (better than WRF) but overestimate the water vapor density above the boundary layer (between 2 and 4 km); in doy 201 and 202, A2 (and WRF) are able to simulate a dry intrusion at the boundary layer top, with a secondary maximum aloft; in doy 200 and 203, A2 detects a secondary maximum aloft, as observed, but wider and slightly higher than observed, possibly a consequence of the 500 m vertical resolution. A comparison between S1 and A2 in Figure 3 indicates that the latter is much better conditioned.
at the boundaries and its spatial structure appears rather natural, suggesting that the approach could lead to valuable results in operation.

To clarify the validity of the hypotheses taken in the tomography design, we will now look at two post-processing checks. Figure 4 presents results from Equation 3 computed from 30 min of observations around 12 UTC. Note that each graphic includes all stations, each at a different color, each with a different set of computed fitting coefficients, which also vary in time. Each station has limited coverage in SIWV, which means a limited range in elevation, and the full combination of stations and GPS satellites, at a given time, leaves significant regions of the parameter space (co-azimuth and elevation) unobserved. However, the fitting is remarkably good with RMSE under 0.5 mm (about 1% of the mean SIWV of 40 mm). The final check is shown in Figure 5, where the design matrix from Experiment S2 is used to compute slant synthetic observations from the water vapor density computed by the A2 tomography (at the same resolution and time window), and these “observations” are compared with GNSS observations for the same epoch. RMSE is between 1.2 and 1.8 mm (3%–4.5% of mean SIWV), comes mostly from the less observed low elevation (high SIWV) region of the parameter space, and appears evenly distributed around the 45° perfect fitting line.

With respect to Figure 5, it is interesting to add that the high SIWV values are often associated with rays entering the domain through its lateral boundaries, for which Equation 6 was applied to correct for the missing IWV outside the domain. That correction is included in the observed data of Figure 5 (but not in Figure 4 as previously explained). The synthetic data does not require correction as it only works within the domain. Figure 5 gives some extra assurance to the consistency of the method.

Extra experiments, not shown, suggest that with the SMOG data it is not possible to further increase the spatial resolution, even with higher resolution in the angular interpolation, suggesting the need for a denser network and/or the use of multiple GNSS constellations. Another experiment, in the line of Rohm (2013), extending the assimilation of slant observations to 6 h was also unsuccessful for all available observational windows, certainly due to the non-stationarity of the real atmosphere at those extended time scales.

Figure 4. Verification of the goodness of fit provided by Equation 3. Each graphic includes all stations (in different colors), each with different fitting coefficients, for the 12 UTC simulations. Root mean square error is shown in each subtitle. All data in mm.
4. Conclusions

A new tomographic method is proposed to compute the 3D distribution of atmospheric water vapor from GNSS observations, without the need for extraneous constraints coming from in-situ observations or model data. The method proceeds by parameterizing SIWV observations as a function of their co-azimuth and elevation, and then using those parameterized curves to produce SIWV observations at specified elevations and co-azimuths, which are consistent with observations. This increases the rank of the design matrix to a level where the pseudoinverse algorithm is able to produce sensible results. The underdetermined linear problem is then solved without the need for other data or assumptions on the variability of the water vapor density.

Results obtained from the 2013 SMOG experiment, with GPS only data, were found to produce good results against 4-hourly radiosondes, some with challenging vertical structure, from just 30 min of GNSS data (and it could be done with shorter periods). Those results were obtained at 6 km horizontal and 500 m vertical resolution, the former close to the closest spacing in the GNSS network. A more straightforward method, doing the pseudoinverse directly from 3 h of slant observations, was also found to work, although only at a coarser resolution, confirming the theoretical study of Rohm (2013). While the present approach recovers IWV values, including PWV, with great accuracy (cf. Figure 5), the errors on the vertical distribution of water vapor density were found to be, on average, larger those obtained by WRF (forced by ERA-5, corresponding to a “perfect model approach”). However, an analysis with a larger data set covering different weather conditions is required to characterize the vertical structure of such errors and their dependence on the geometry of observations and tomographic options.

The proposed method is in many ways simpler than the standard approach, as it does not require multiple constraints on the tomography field. It may constitute the basis of remote sensing of the vertical structure of tropospheric water vapor, with application to boundary layer studies, whenever sufficiently dense GNSS networks are in operation.
The main weakness of the proposed approach comes from the need to extrapolate GNSS observations into very low elevations, where those observations are considered unreliable. In the SMOG experiment, that weakness appeared manageable. At those low elevations, the inclusion of multiple constellations or products such as InSAR and MODIS will not improve the tomography. However, GNSS-RO (Radio Occultation) could be easily merged, although with challenges coming from its very extended atmospheric paths outside the tomographic domain. Further work to develop a fully unconstrained tomographic model is still ahead.

A final note concerns the computational cost of the proposed method. For one inversion in a new tomographic grid around a network of ground stations, its computational cost can be much higher than the conventional approach, and its cost (in time and memory) will increase substantially with the size of the design matrix. However, if the geometry of both observations (location of the stations and angular resolution) and voxels are fixed, most computations (including the evaluation of the pseudoinverse) can be done only once and used for all subsequent observations, making this approach much less expensive than conventional methods.

If GNSS tomographic results can be made operationally for large domains one may expect a significant impact on weather forecasting, maybe complementing InSAR observations that will be available at much higher horizontal resolutions but only offer 2D PWV fields. Recent results indicate that InSAR data assimilation can consistently improve forecasts (Mateus et al., 2021; Miranda et al., 2019). The joint use of both data sources is a promising prospect, although there are many challenges concerning the real-time availability of such data.

Data Availability Statement

ERA5 data were downloaded from the European Center for Medium-Range Weather Forecasts (ECMWF), Copernicus Climate Change Service (C3S) available at https://cds.climate.copernicus.eu/; GNSS and radiosonde data sets used in this study are available from the figshare repository (https://dx.doi.org/10.6084/m9.figshare.14778378).

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