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Aerosol-type retrieval and uncertainty quantification from OMI data

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1 Supplement

Computational implementation of the method

This supplementary material presents a pseudo-code for implementation of the used method introduced earlier in paper Määttä et al. (2014) step-by-step for one Ozone Monitoring Instrument (OMI) pixel. The method is based on Bayesian inference approach.

OMI Data:

- The observed top-of-atmosphere (TOA) spectral reflectance $\vec{R}_{\text{obs}}(\lambda)$ at selected wavelength bands $\lambda = (\lambda_1, \ldots, \lambda_n)$ calculated from the OMI Level 1B VIS and UV radiances and Level 1B Solar irradiance data
- The measurement error variances $\sigma^2_{\text{obs}}(\lambda)$, $\lambda = (\lambda_1, \ldots, \lambda_n)$
- The set of Look-up-tables (LUTs) containing pre-calculated aerosol microphysical models (e.g. hdf5 files)

Outcome:

- Posterior distribution $p(\tau|\vec{R}_{\text{obs}}, m)$ of τ (i.e. AOD) given as a discrete set of values for τ in the range of $[0,\tau_{\max}]$. The posterior distribution is evaluated for each selected best fitting model (maximum of 10) and stored in a table.
- Averaged posterior distribution $p_{\text{avg}}(\tau|\vec{R}_{\text{obs}})$ given as a discrete set of values for τ in the range of $[0,\tau_{\max}]$ and stored in a table
- Point estimate for AOD at 500 nm determined as maximum a posteriori (MAP) estimate, i.e. mode of the averaged posterior distribution

We use a symbol τ for AOD in the formulas. The modeled reflectance $\vec{R}_{\text{mod}}(\tau, \lambda)$ depends on τ and is calculated by interpolation between nodal values of LUT while fitted to the measured reflectance $\vec{R}_{\text{obs}}$ in order to find τ that minimizes

$$\chi^2_{\text{mod}}(\tau) = \vec{R}_{\text{res}}(\lambda)^T \left(\mathbf{C} + \text{diag}(\sigma^2_{\text{obs}}(\lambda))\right)^{-1} \vec{R}_{\text{res}}(\lambda). \tag{1}$$

Here $\vec{R}_{\text{res}}(\lambda) = \vec{R}_{\text{obs}}(\lambda) - \vec{R}_{\text{mod}}(\tau, \lambda)$ is the residual of model fit. This is done for each aerosol microphysical model in turn. In the formula $\sigma^2_{\text{obs}}(\lambda)$ are the measurement error variances and $\mathbf{C}$ is non-diagonal covariance matrix for model discrepancy (i.e. forward modelling uncertainty). In our experiment we calculated the elements of the covariance matrix $\mathbf{C}$ for wavelength pair λ_i and λ_j as

$$\mathbf{C}_{i,j} = \sigma_1^2 \exp\left(-\frac{1}{2}\left(\lambda_i - \lambda_j\right)^2 / l^2\right) + \sigma_0^2 \tag{2}$$

where parameter l is a correlation length, parameter σ_0^2 is non-spectral (i.e. non-spatial) diagonal variance and σ_1^2 is spectral (i.e. spatial) variance. We like to note that our used parameter values are specific for this study with OMI data and have been empirically evaluated. These parameter values were estimated from an ensemble of the residuals, i.e. the differences between the observed and modeled reflectances, as described in the paper Määttä et al. (2014). Here we used $l = 90$ nm and for σ_0^2 and σ_1^2 we used values of 1% and 2% of the observed reflectance, respectively.

By Bayes' formula the posterior distribution for τ within the model m and given the observed reflectance $\vec{R}_{\text{obs}}$ is

$$p(\tau|\vec{R}_{\text{obs}}, m) = \frac{p(\vec{R}_{\text{obs}}|\tau,\, m)\, p(\tau|m)}{p(\vec{R}_{\text{obs}}|m)}. \tag{3}$$

In this case we have one unknown τ (i.e. AOD at 500 nm) and the full posterior distribution is calculated as described below.

The posterior is evaluated at a dense grid, e.g. at 200 points, of τ values, basically in the range of $[0,\, \tau_{\max}]$. The maximum allowed $\tau_{\max}$ is determined by the model LUT.

We calculate the likelihood as

$$p(\vec{R}_{\text{obs}}|\tau,\, m) = c\, \exp(-\frac{1}{2} * \chi^2_{\text{mod}}(\tau)), \tag{4}$$

where $\chi^2_{\text{mod}}(\tau)$ is calculated from Eq. 1 for the set of τ values in the range of $[0,\, \tau_{\max}]$. The constant c ensures that the probability distribution is properly defined and it is the same for all the models m.

We assume that a prior distribution $p(\tau|m)$ for τ within aerosol microphysical model m follows a log-normal distribution

$$p(\tau|m) \propto \log N(\tau_0, \sigma_\tau^2). \tag{5}$$

This confirms that $p(\tau|m)$ can take only positive real values and ensures that AOD is positive. We set mean value $\tau_0 = 2$ for the log-normal distribution.

We calculate the normalizing constant (or scaled factor) of the posterior numerically as

$$p(\vec{R}_{\text{obs}}|m) = c \int p(\tau|m) * \exp(-\frac{1}{2} * \chi^2_{\text{mod}}(\tau))d\tau. \tag{6}$$

Consequently, we have now calculated all the elements of the posterior distribution for τ (Eq. 3).

In our study we call $p(\vec{R}_{\mathrm{obs}}|m)$ as the model evidence that is used to make the model selection. We select models with the highest evidence value until the cumulative sum of the selected models' evidences pass the value of 0.8 or the number of chosen models is 10.

Next we calculate relative evidence for model m_i with respect to the other models selected above (max 10) by

$$p(m_i|\vec{R}_{\mathrm{obs}}) = \frac{p(\vec{R}_{\mathrm{obs}}|m_i)}{\sum_j (\vec{R}_{\mathrm{obs}}|m_j)}. \tag{7}$$

These relative evidence values are used to compare models among the set of selected best fitting models.

The averaged posterior distribution over the selected best models m_i is calculated as

$$p_{\mathrm{avg}}(\tau|\vec{R}_{\mathrm{obs}}) = \sum_{i=1}^{n} p(\tau|\vec{R}_{\mathrm{obs}},\, m_i)\, p(m_i|\vec{R}_{\mathrm{obs}}), \tag{8}$$

where n is the number of models.

We accept the solution for the pixel if the threshold value $\chi^2 \leq 2$ calculated by following modified chi-squared formula

$$\chi^2 = \frac{1}{n-1} \vec{R}_{\mathrm{res}}(\lambda)^{\mathrm{T}} \left(\mathbf{C} + \mathrm{diag}(\sigma^2(\lambda))\right)^{-1} \vec{R}_{\mathrm{res}}(\lambda). \tag{9}$$

We do this test only for the best model.

As a summary, we do the following for model selection, calculation of posterior distributions and getting MAP estimate of AOD:

1. fit each model from LUT (i.e. $\vec{R}_{\mathrm{mod}}(\tau,\, \lambda)$) in turn to the measured reflectance $\vec{R}_{\mathrm{obs}}(\lambda)$
2. for each model, find τ that minimizes $\chi^2_{\mathrm{mod}}(\tau)$ (Eq. 1)
3. for each model, calculate posterior distribution $p(\tau|\vec{R}_{\mathrm{obs}}, m)$ (Eq. 3)
4. use model evidence (Eq. 6) to select max 10 best models
5. calculate the relative evidence (Eq. 7) for each model among the selected best models. Actually, we first carry out steps 2.-3. once more for the selected best models and then calculate the relative evidences.

6. calculate the averaged posterior distribution (Eq. 8) and get point estimate for AOD, i.e. MAP estimate

7. finally, do the goodness-of-fit test (Eq. 9)

References

Määttä, A., Laine, M., Tamminen, J., and Veefkind, J. P.: Quantification of uncertainty in aerosol optical thickness retrieval arising from aerosol microphysical model and other sources, applied to Ozone Monitoring Instrument (OMI) measurements, Atmos. Meas. Tech., 7, doi:10.5194/amt-7-1185-2014, 2014.