

# Dimensionality Reduction for Fast and Accurate Radiative Transfer



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**Abstract:** Line-by-line radiative transfer calculations for the remote sensing of satellite instruments with a high spectral resolution are generally associated with a prohibitive computational cost. Instead, a general approach is to create fast forward models based on look-up tables that relate the atmospheric state to the radiance measured by the satellite. Recently, principal components analysis (PCA) has showed promising results in reducing the number of necessary frequency calculations. Potential for improvement may be sought by generalizing PCA to nonlinear dimensionality reduction.



## The Physical Problem

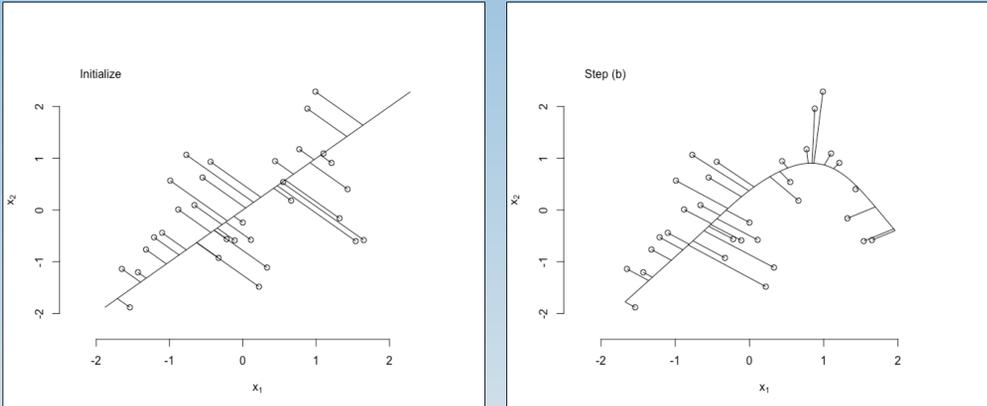
Assimilating satellite radiances in numerical weather prediction requires solving the radiative transfer equation (1) for all relevant trace gases, such as water vapor, carbon dioxide, ozone, and oxygen.

$$I_\nu(z) = B_\nu(T_s) \cdot t_\nu(0, z) + \int_0^z B_\nu[T(z')] \cdot W_\nu(z', z) dz' \quad (1)$$

However, particularly in the important infrared part of the electromagnetic spectrum absorption line spectra of atmospheric trace gases can become very complex and require a very high spectral resolution for an exact calculation of equation (1). For satellite data assimilation and operational remote sensing this requirement for very high spectral resolution is computationally prohibitive. Different approaches have been developed to circumvent this problem, including band models, and correlated-k methods. In the flagship data assimilation codes CRTM [1] and RTTOV [2] a linear regression approach is used successfully. However, the number of necessary atmospheric state variables serving as predictors in the regression is quite high, including temperature profiles, pressure distribution, and all trace gas concentrations and mostly integral functions thereof. Consequently there is room for improvement and any gains in the radiative transfer will allow more data to be assimilated quicker, resulting in cheaper and more accurate weather forecasts and satellite products.

## The Idea

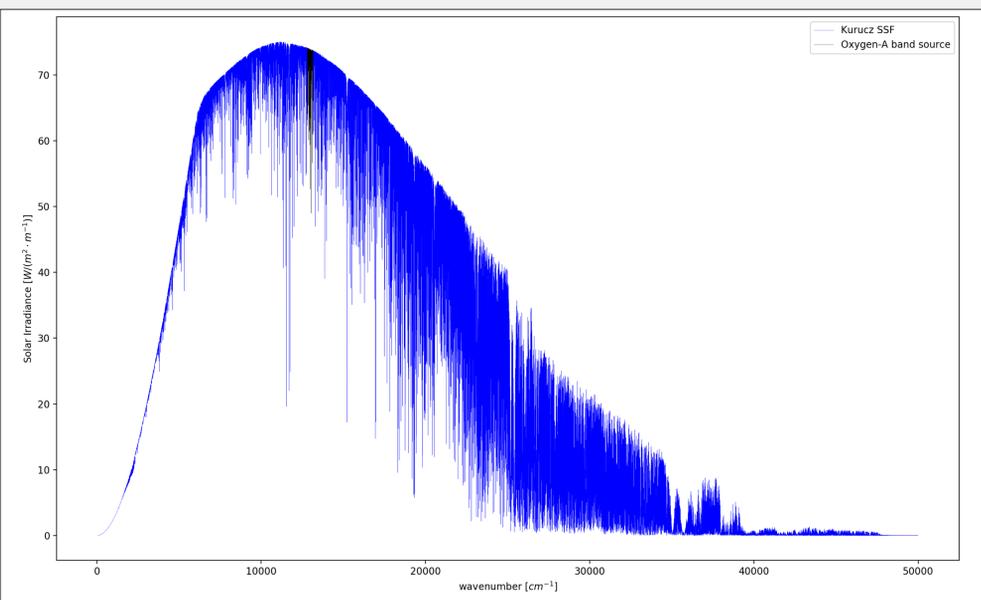
In order to enhance the computational efficiency of the regression approach, it is reasonable to search for a coordinate system that allows for a simpler representation of the data. One approach here is Principal Components Analysis. This method has been successfully applied in Ref. [3] to speed up the radiative transfer forward calculations. Since PCA is a linear approach, a straightforward generalization of this method is to look for a manifold description that simplifies the representation of the data. One example of such a method is Principal Curves [4] (see Fig. 1). Here, a data smoother such as a smoothing spline provides a curve that minimizes the orthogonal projected distance of the data points onto the curve.



**Fig. 1:** Example for a Principal Components axis for a bivariate data distribution (left) and the generalization in terms of a Principal Curve (right) for the same data set.

## Synthetic Data from Line-by-line Calculations

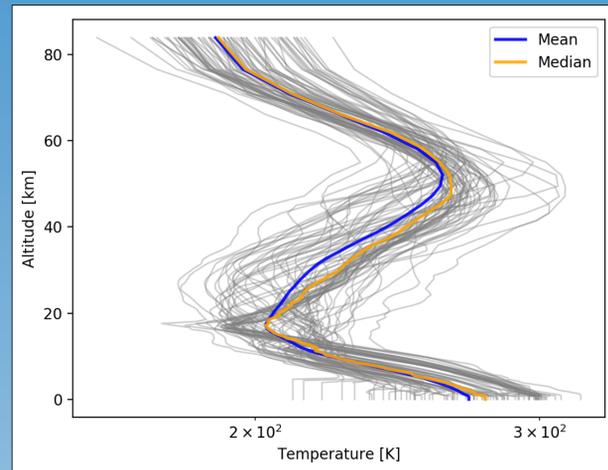
As a simple test case to provide input data for the PCA and nonlinear manifold approaches, the so-called oxygen-A band [5] is selected. This is an absorption band of the oxygen O<sub>2</sub> molecule in the optical part of the solar spectrum that is useful for applications such as cloud top height and aerosol retrievals. The band ranges roughly from 759nm to 780nm. For the high-resolution line-by-line calculations the LBLRTM code [6] from AER was used.



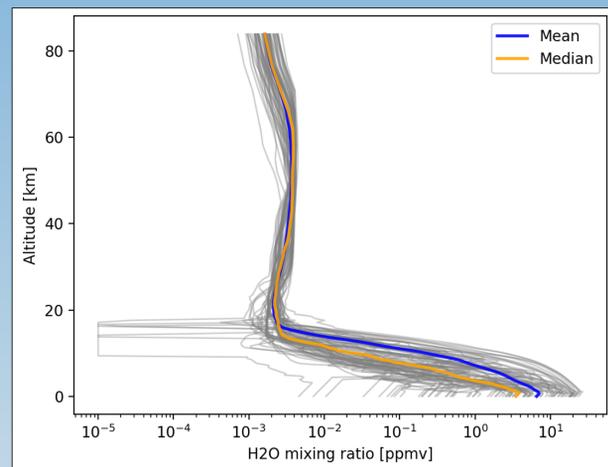
**Fig. 2:** Low-resolution Kurucz spectrum [7] as the solar source function (blue) with oxygen-A band contribution indicated in black.

## Atmospheric State Variables as Predictors

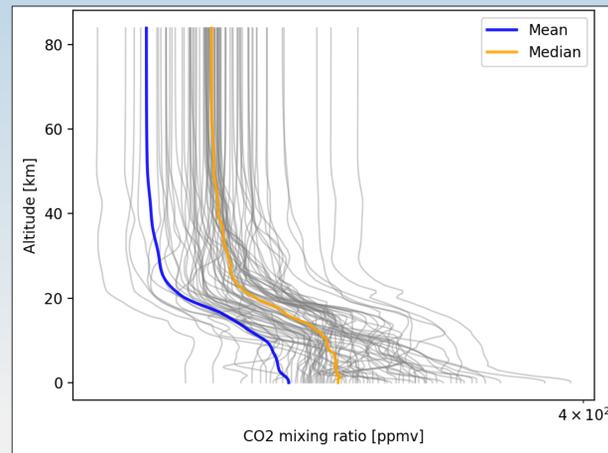
The basis for the line-by-line calculations is provided by the ECMWF83 profile set, which is a selection of 83 atmospheric profiles provided by the ECMWF and specifically selected for radiative transfer calculations. A selection of the profile data is shown in Figs. 3-5.



**Fig. 3:** ECMWF83 temperature profile spaghetti plot with mean and median. The temperature increase in the stratosphere caused by shortwave heating through ozone absorption is clearly visible.



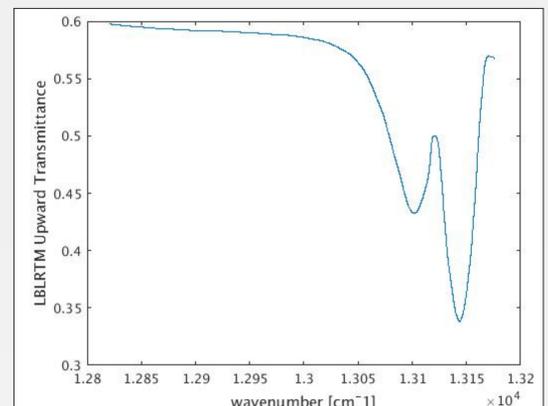
**Fig. 4:** ECMWF83 water vapor mixing ratio profile spaghetti plot with mean and median. Water vapor has a high concentration but also strong variability in the troposphere.



**Fig. 5:** ECMWF83 carbon dioxide mixing ratio profile spaghetti plot with mean and median. Similar to water vapor, the concentration of carbon dioxide is higher in the troposphere and reaches its maximum at ground level.

## LBL Output

Using the ECMWF83 profiles as an input, TOA transmittance and radiances as observed by a weather satellite are computed using LBLRTM to provide dependent variables as PCA and nonlinear dimensionality reduction input. An example is shown in Fig. 6, where the Upward transmittance over the oxygen-A band is shown based on the ECMWF83 profile number 1. Oxygen concentration was assumed to be constant over the entire profile at 209,460ppmv [8].



**Fig. 6:** LBLRTM Upward transmittance sample result for the oxygen-A band.

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