DEVELOPMENT OF A PC-BASED RADIATIVE TRANSFER MODEL

and its application to IASI CH_4 retrievals

C. Robert, S. Vandenbussche, A.C. Vandaele, J. Erwin, M. De Mazière

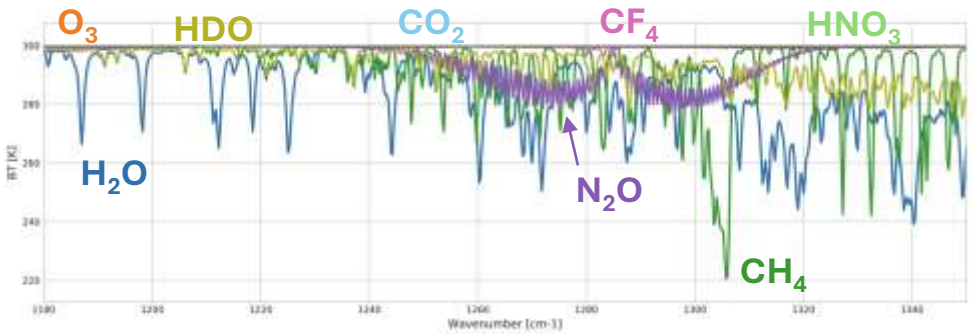
Royal Belgian Institute for Space Aeronomy

IWGGMS-21 Conference • June 2025• Takamatsu, Japan

SPEED

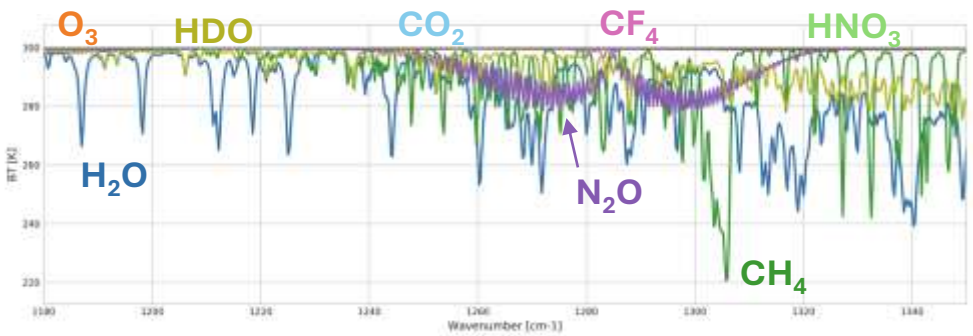
Retrieval of methane in the TIR

Top-of-Atmosphere BT contributions
from different species

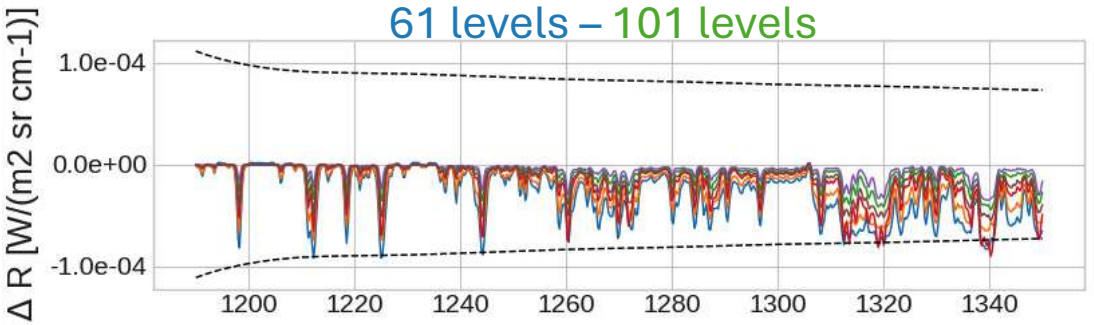


Retrieval of methane in the TIR

Top-of-Atmosphere BT contributions from different species

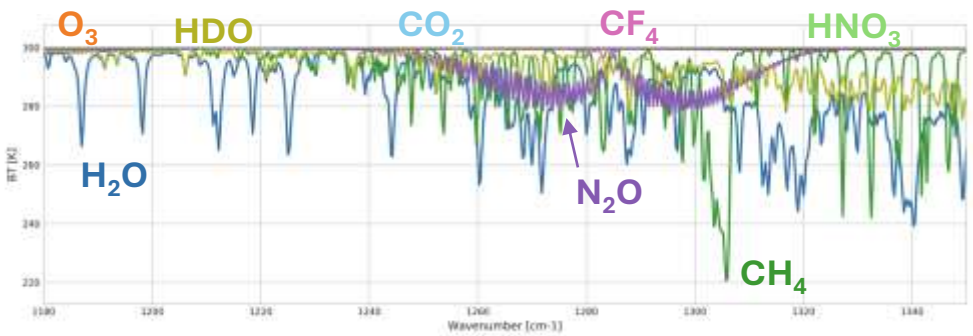


Spectral residuals due to undersampling of model vertical discretization

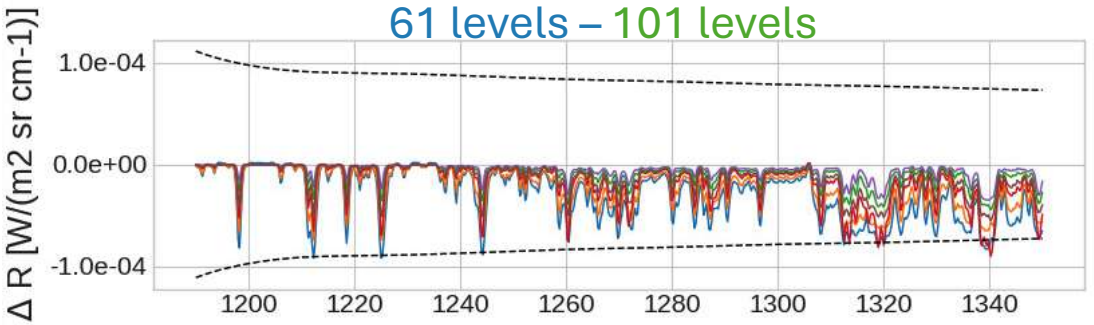


Retrieval of methane in the TIR

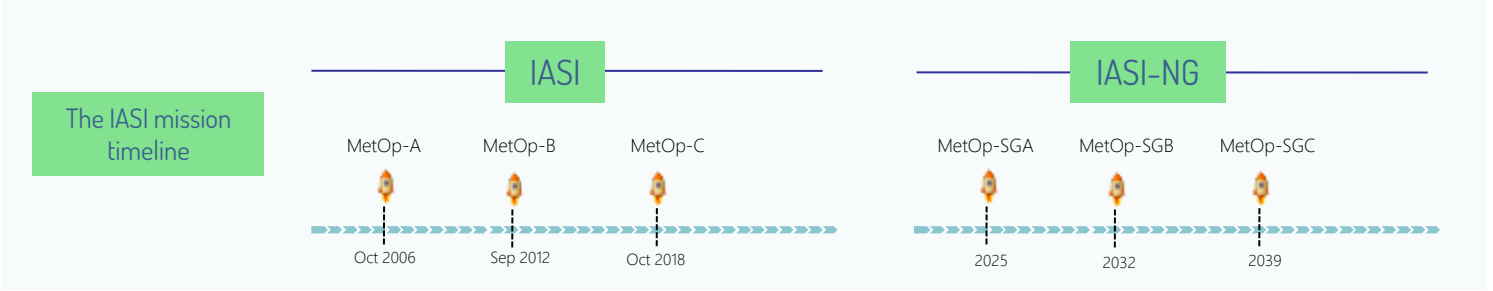
Top-of-Atmosphere BT contributions from different species



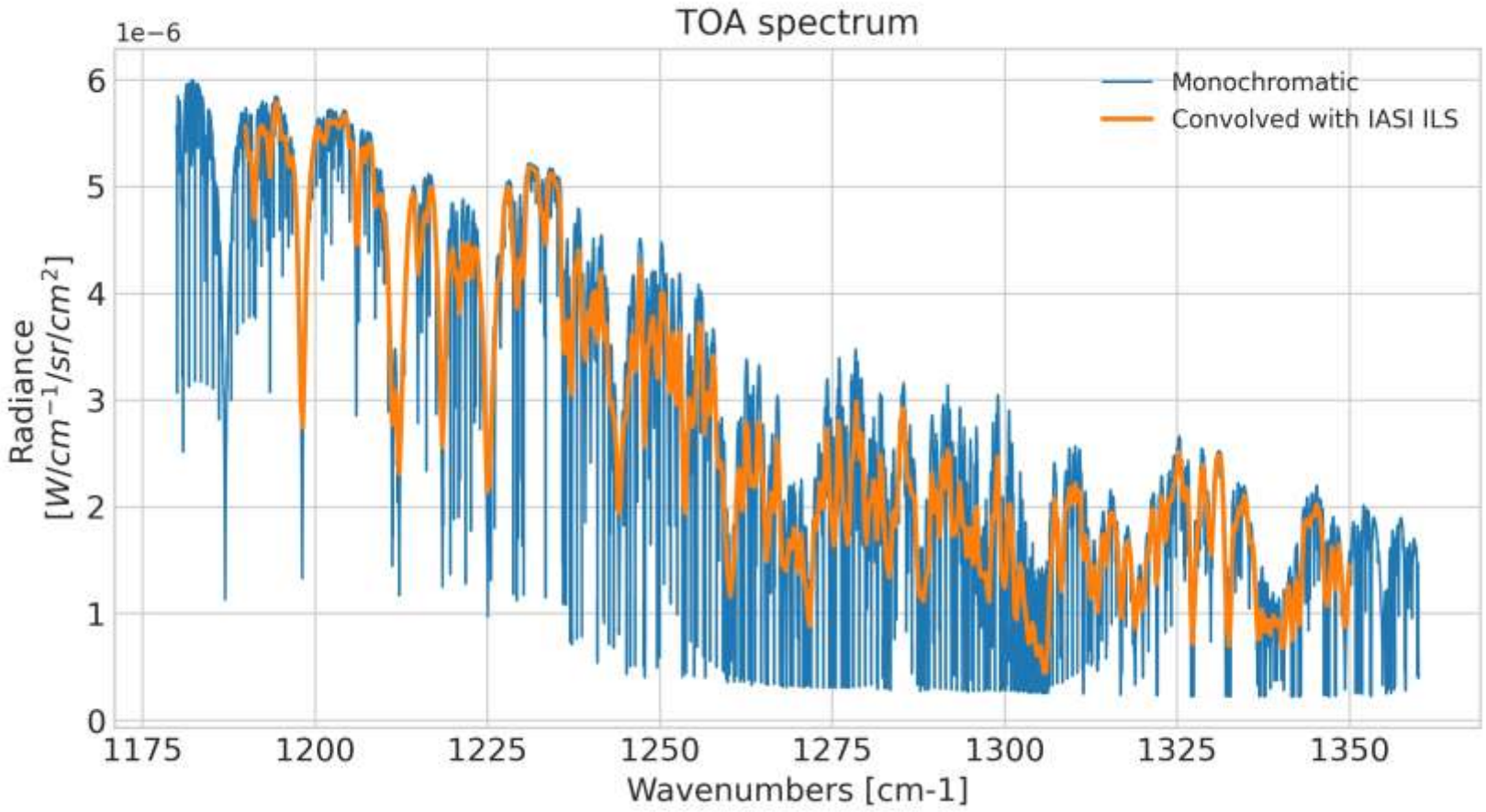
Spectral residuals due to undersampling of model vertical discretization



Large data volume to process / reprocess /upcoming



Conventional RTM



For CH_4 retrievals

1190 – 1350 cm^{-1}

60 000 monochromatic calc.

641 IASI channels

(Also outputs Jacobians)

PCRTM : Compress and Reduce

> “The number of independent pieces of information is much less than the number of monochromatic radiances”

PCRTM : Compress and Reduce

> “The number of independent pieces of information is much less than the number of monochromatic radiances”

1. The convolved spectra can be reconstructed with good accuracy using a few Principal Components ($\mathbf{U}_i$)

$$\mathbf{R}^{ch} = \sum_{i=1}^{N_{PC}} \mathbf{Y}_i \mathbf{U}_i + \boldsymbol{\varepsilon}$$

PCRTM : Compress and Reduce

> “The number of independent pieces of information is much less than the number of monochromatic radiances”

1. The convolved spectra can be reconstructed with good accuracy using a few Principal Components ($\mathbf{U}_i$)

$$\mathbf{R}^{ch} = \sum_{i=1}^{N_{PC}} \mathbf{Y}_i \mathbf{U}_i + \boldsymbol{\varepsilon}$$

2. The PC scores $\mathbf{Y_i}$ can be calculated as a multilinear model based on a set of monochromatic radiances $\boldsymbol{R_{mono}}$

$$\mathbf{Y}_i = \left(\sum_{j=1}^{N_{mono}} a_j R_j^{mono} \right)$$

PCRTM : Compress and Reduce

> “The number of independent pieces of information is much less than the number of monochromatic radiances”

1. The convolved spectra can be reconstructed with good accuracy using a few Principal Components ($\mathbf{U}_i$)

$$\mathbf{R}^{ch} = \sum_{i=1}^{N_{PC}} \mathbf{Y}_i \mathbf{U}_i + \boldsymbol{\varepsilon}$$

2. The PC scores $\mathbf{Y_i}$ can be calculated as a multilinear model based on a set of monochromatic radiances $\boldsymbol{R_{mono}}$

$$\mathbf{Y}_i = \left(\sum_{j=1}^{N_{mono}} a_j R_j^{mono} \right)$$

Typically, N_{mono} << 60 000

PCRTM

Pros

10-100x faster than conventional RTM

Based on direct physical modelling

Can be used with any monochromatic RTM code

PCRTM

Pros

10-100x faster than conventional RTM

Based on direct physical modelling

Can be used with any monochromatic RTM code

Cons

Only applies to observations with a constant ILS

Data intensive when building the model

Need to reconstruct the model for any changes in the underlying model

PCRTM

Pros

10-100x faster than conventional RTM

Based on direct physical modelling

Can be used with any monochromatic RTM code

Cons

Only applies to observations with a constant ILS

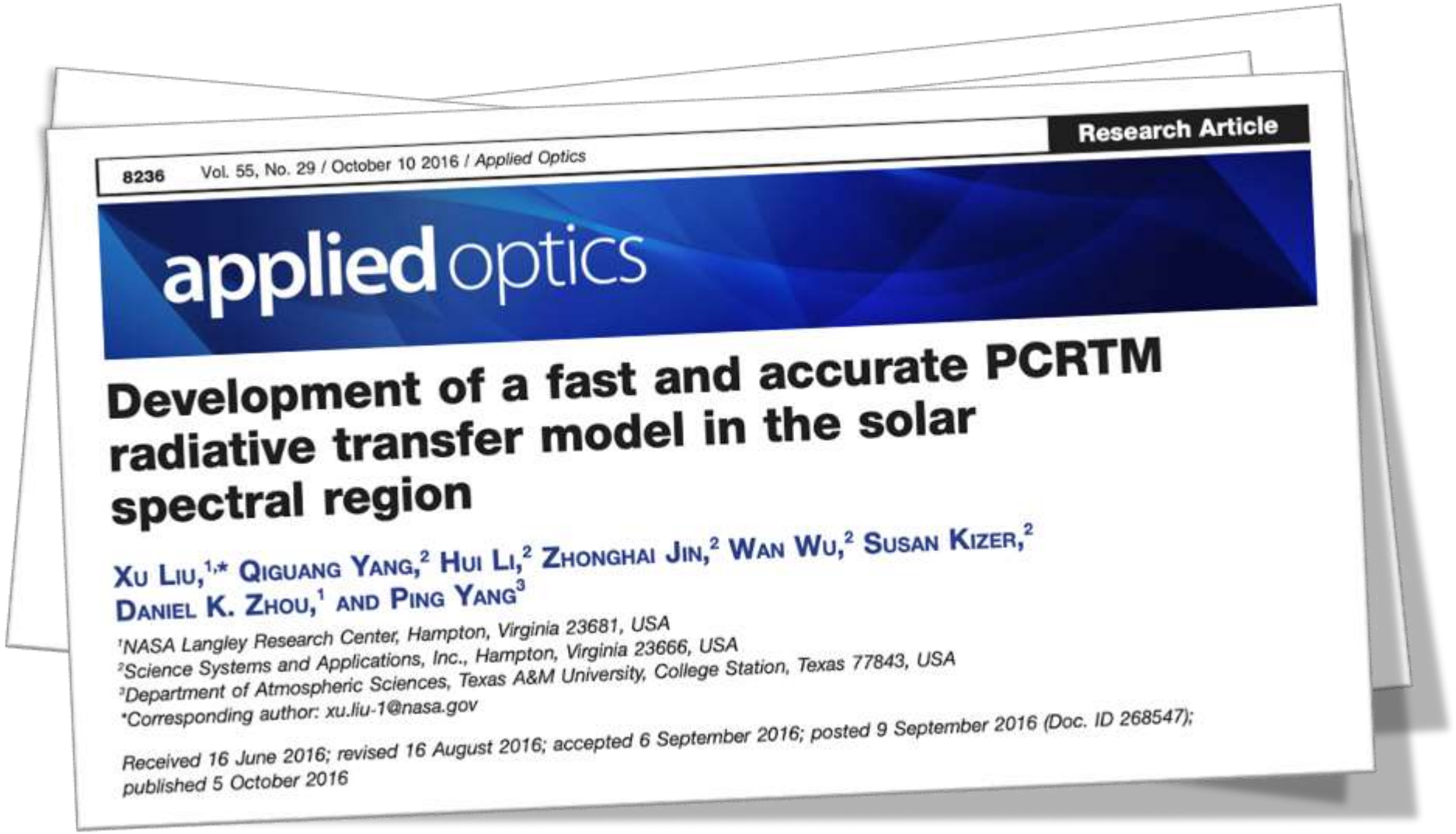
Data intensive when building the model

Need to reconstruct the model for any changes in the underlying model

Goal

Provide a framework for construction of the PCRTM model in a more systematic way

PCRTM



8236 Vol. 55, No. 29 / October 10 2016 / Applied Optics

Research Article

applied optics

Development of a fast and accurate PCRTM radiative transfer model in the solar spectral region

Xu Liu,[1,*] Qiguang Yang,[2] Hui Li,[2] Zhonghai Jin,[2] Wan Wu,[2] Susan Kizer,[2] Daniel K. Zhou,[1] and Ping Yang[3]

[1]NASA Langley Research Center, Hampton, Virginia 23681, USA
[2]Science Systems and Applications, Inc., Hampton, Virginia 23666, USA
[3]Department of Atmospheric Sciences, Texas A&M University, College Station, Texas 77843, USA
*Corresponding author: xu.liu-1@nasa.gov

Received 16 June 2016; revised 16 August 2016; accepted 6 September 2016; posted 9 September 2016 (Doc. ID 268547); published 5 October 2016

HOW TO PCRTM?

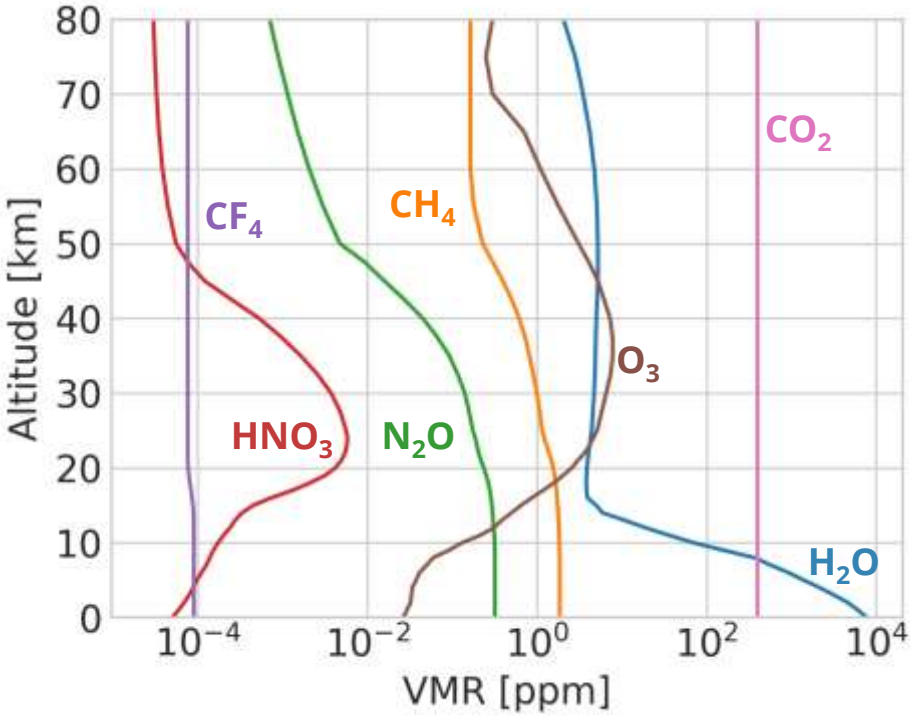
STEP 1

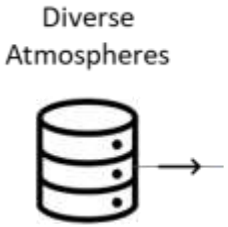
Build a database of high-resolution AND convolved spectra (training / testing)

Sources of diverse atmospheres

- AFGL
- ECMWF 83 diverse profiles*
- MACC60L profiles *
- ACE-FTS
- Models (WACCM)

+ varied observational parameters:
SZA, VZA, emissivity ...

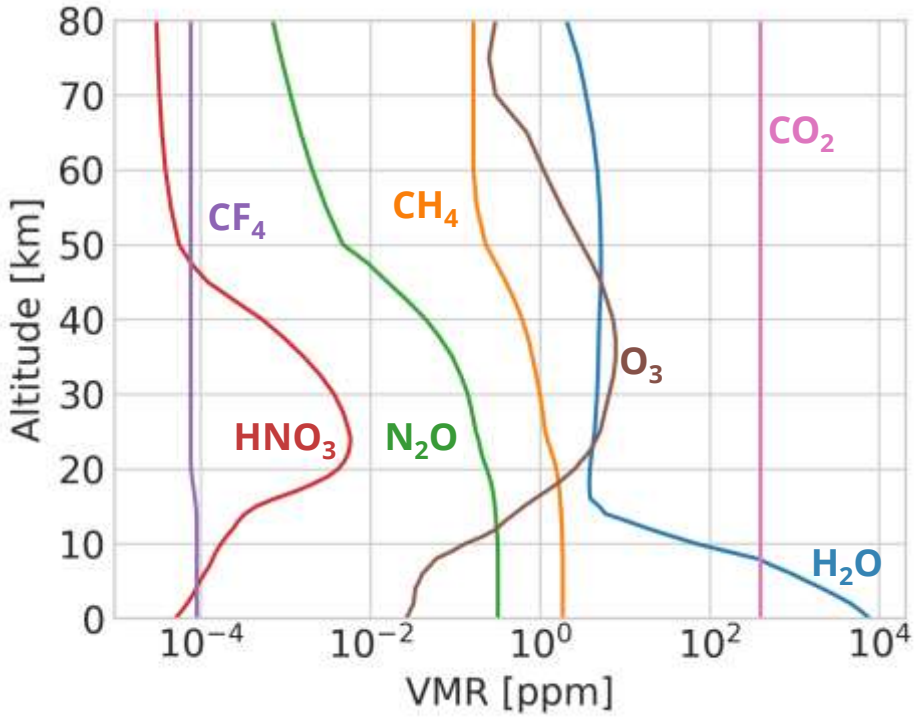


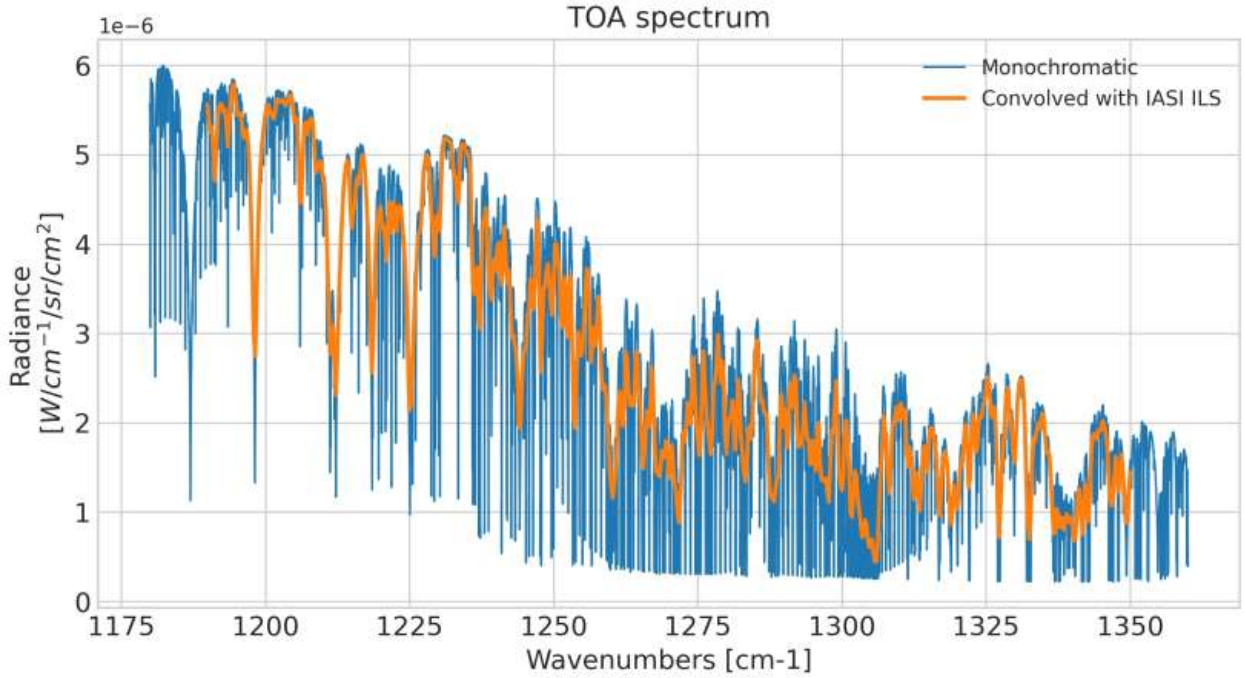


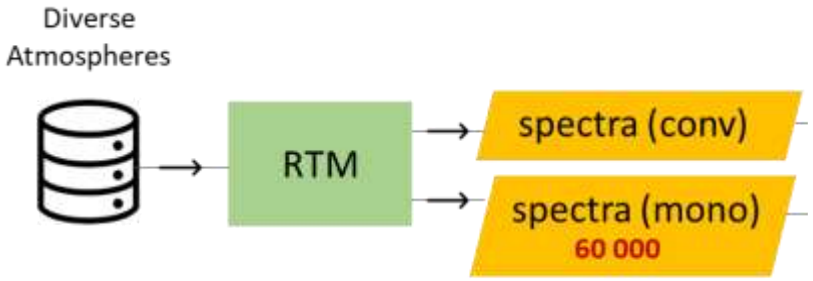
* https://nwp-saf.eumetsat.int/site/software/atmospheric-profile-data/

STEP 1

Build databases of high-resolution AND convolved spectra for training and testing

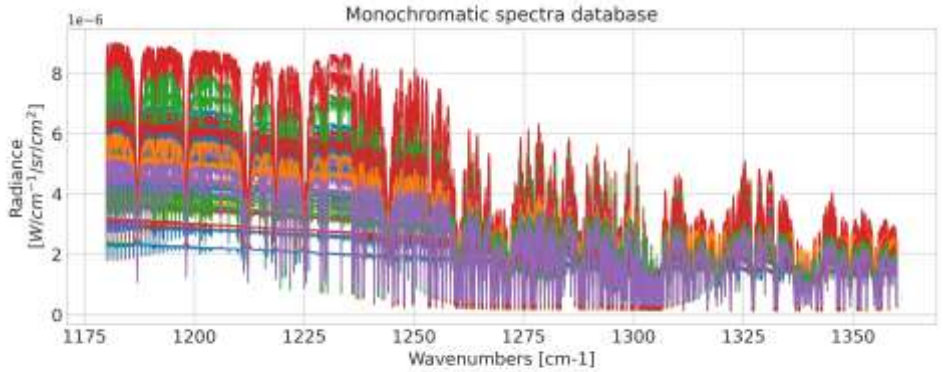






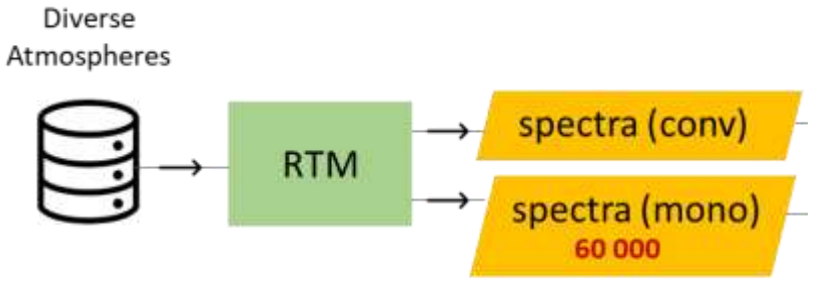
STEP 1

Build databases of high-resolution AND convolved spectra for training and testing



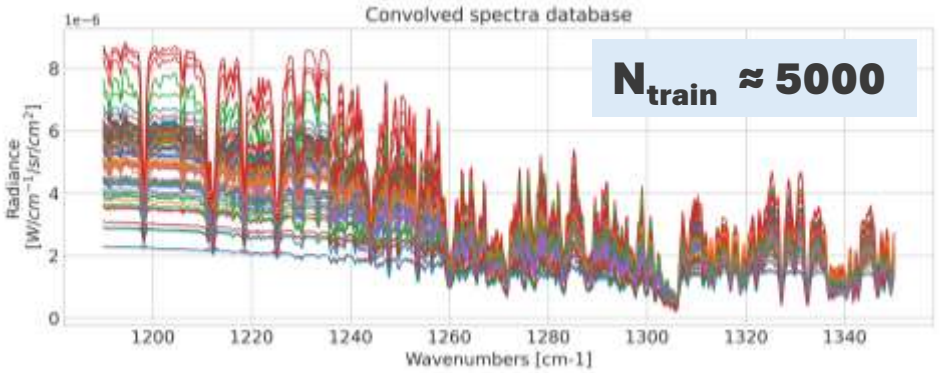
$N_{train} \approx 8000$

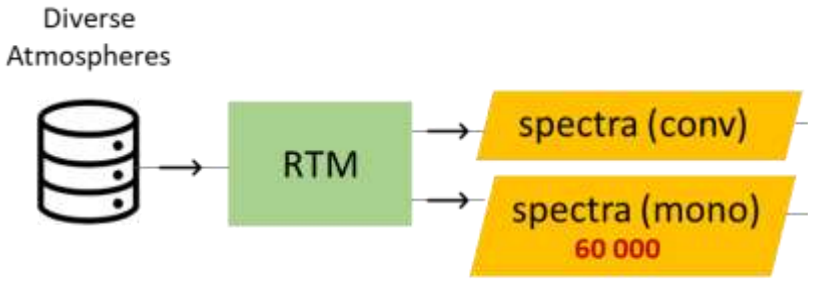
$N_{test} \approx 3000$



STEP 2

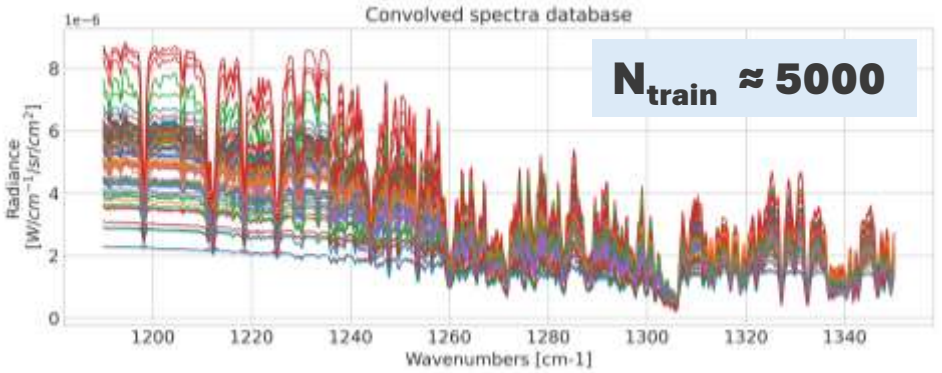
Extract the principal components and associated scores



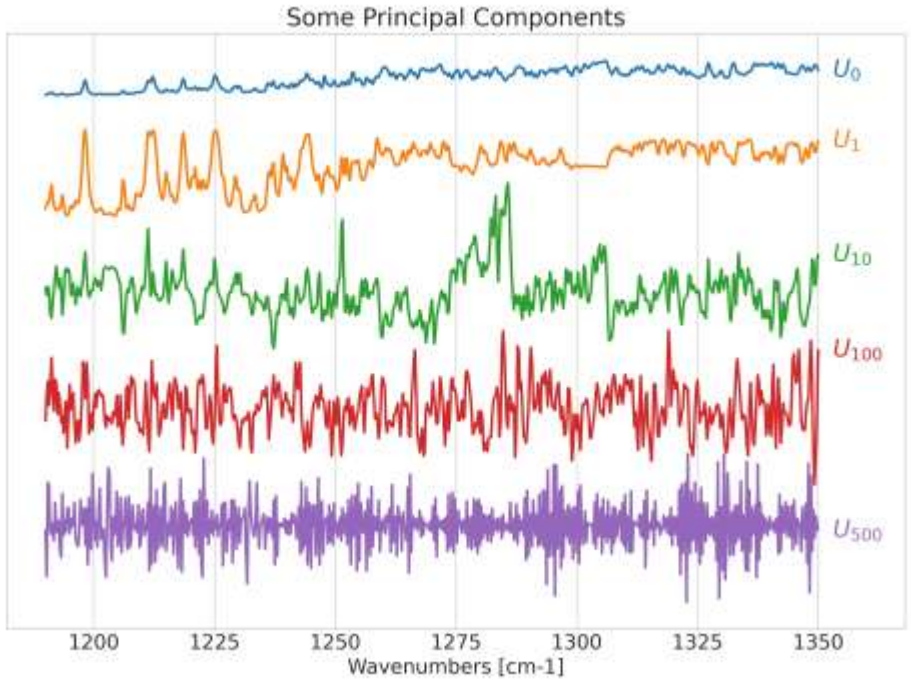


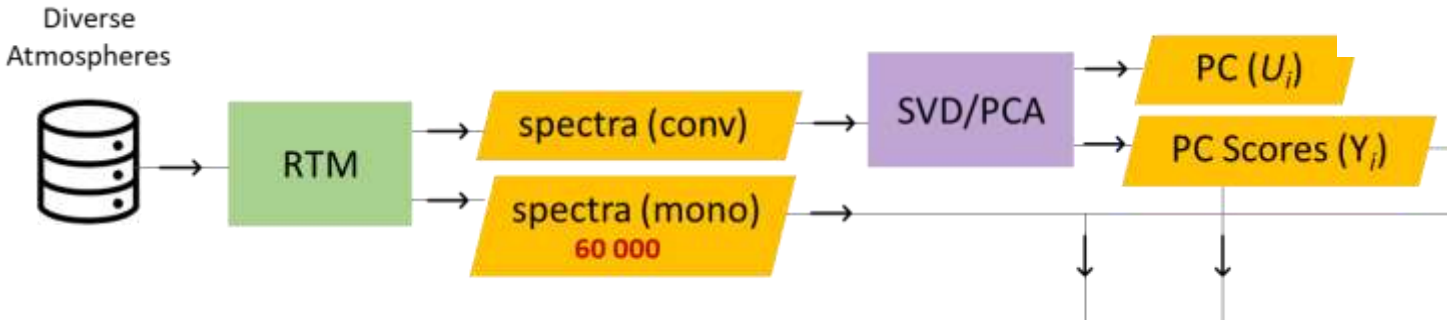
STEP 2

Extract the principal components and associated scores



SVD



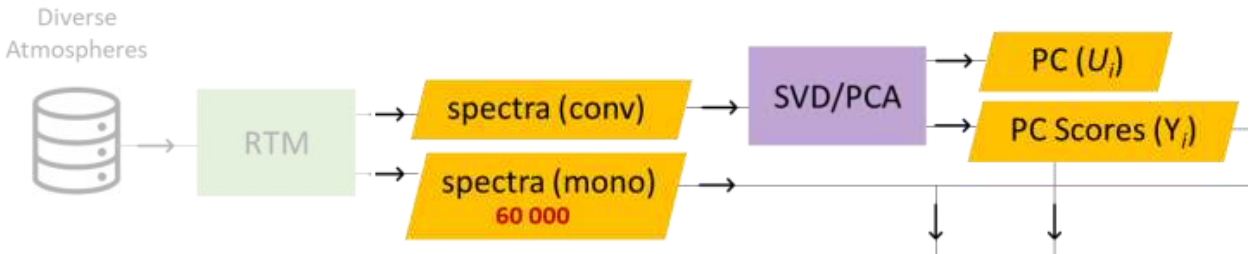


STEP 2

Extract the principal components and associated scores

How many PCs to keep?

→ Inspect residuals of reconstructed Testing spectra

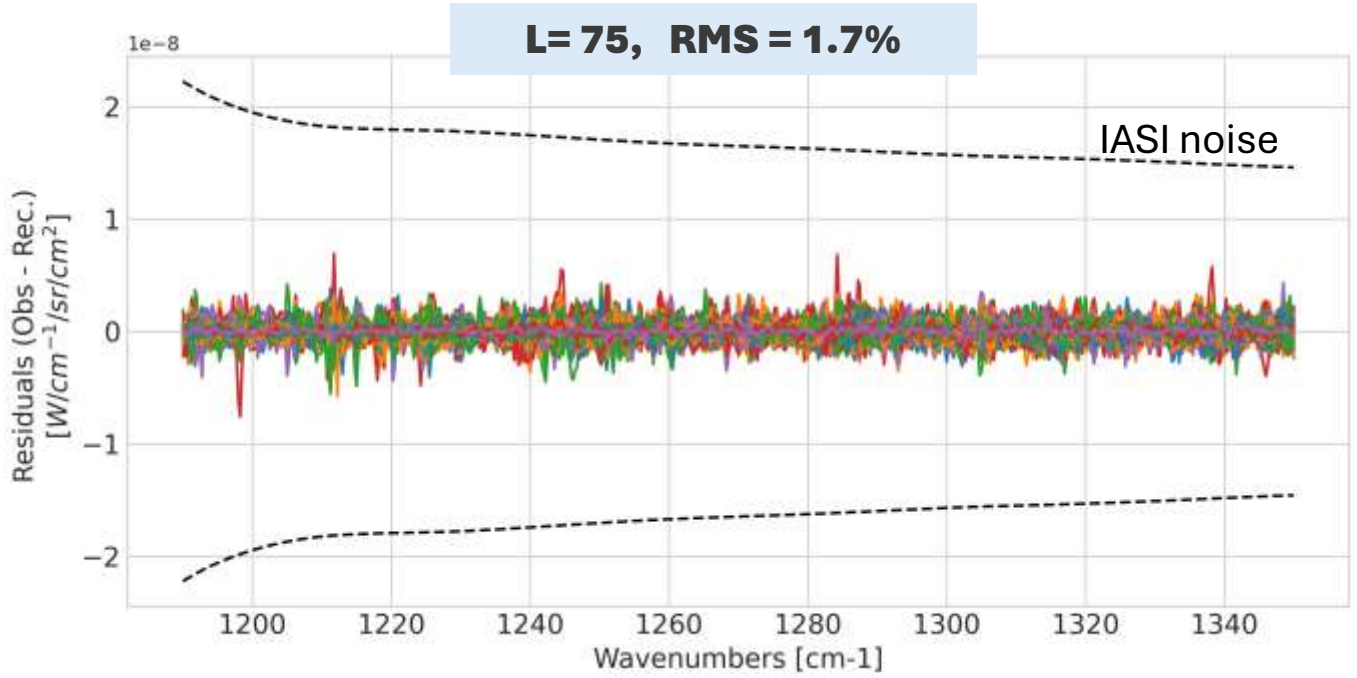


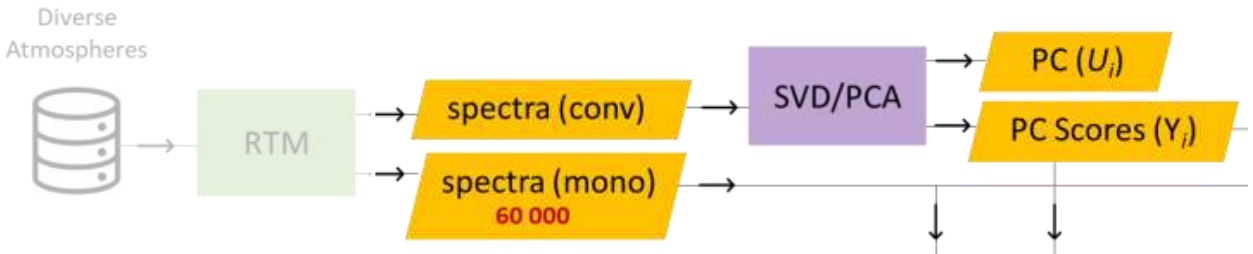
STEP 2

Extract the principal components and associated scores

How many PCs to keep?

→ Inspect residuals of reconstructed Testing spectra



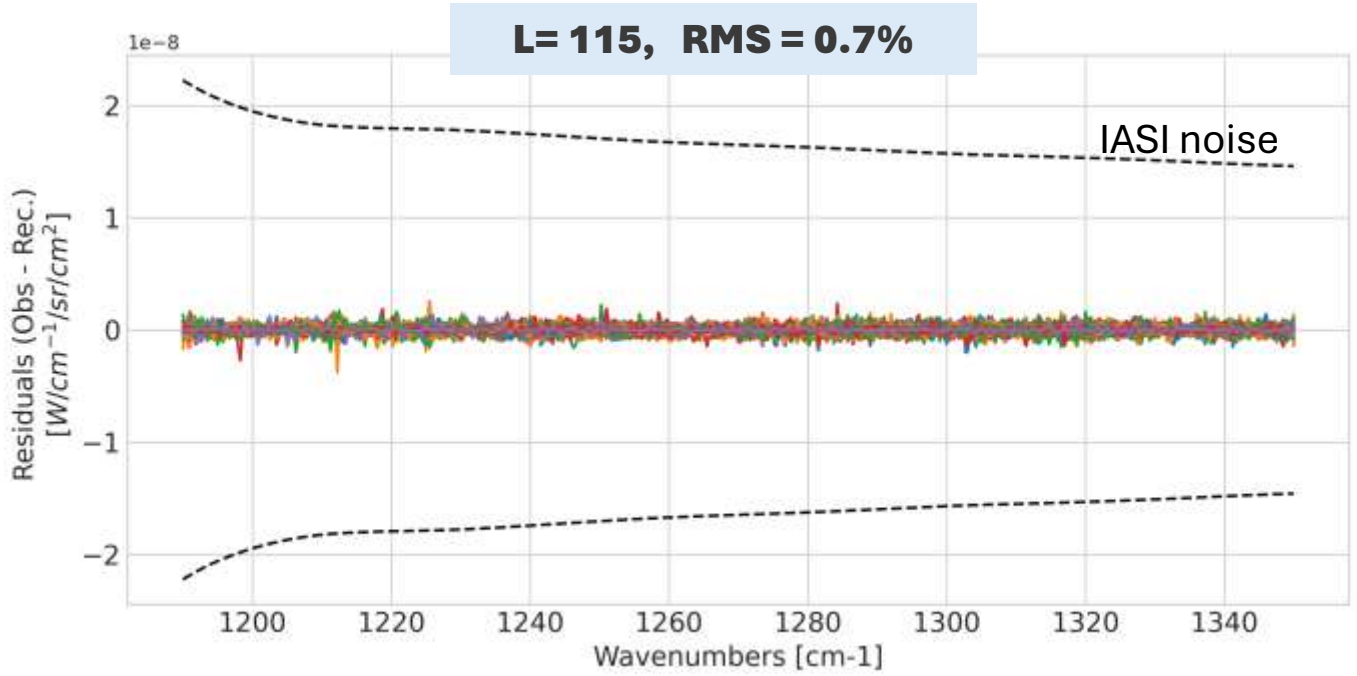


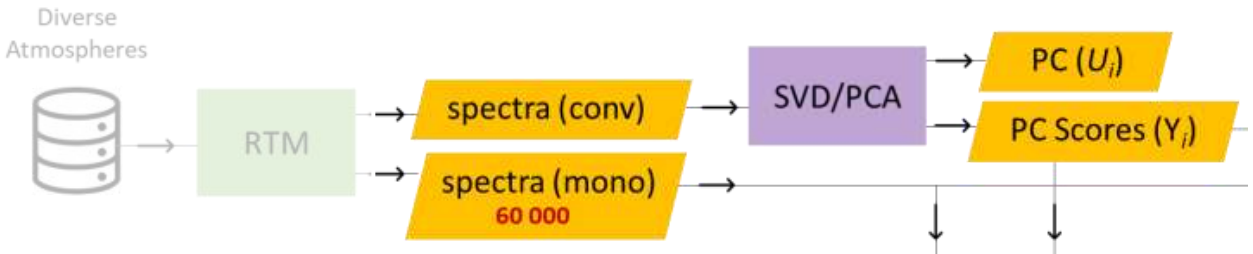
STEP 2

Extract the principal components and associated scores

How many PCs to keep?

→ Inspect residuals of reconstructed Testing spectra



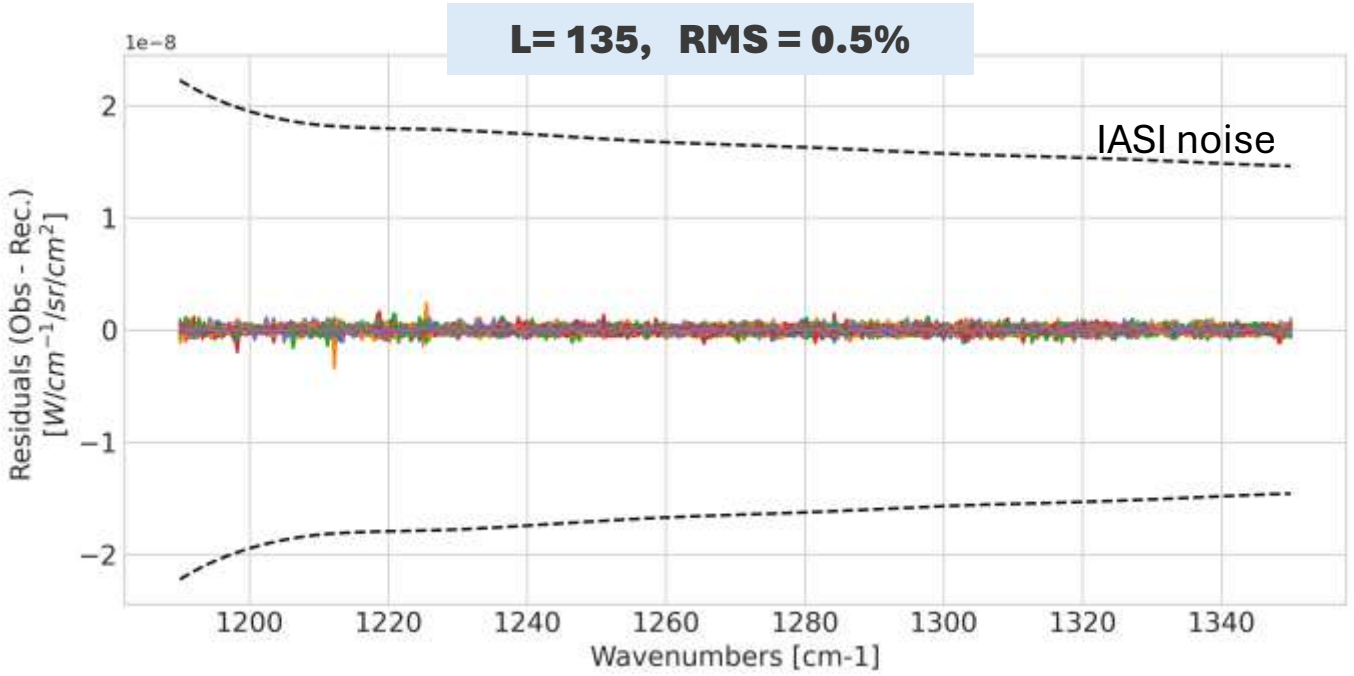


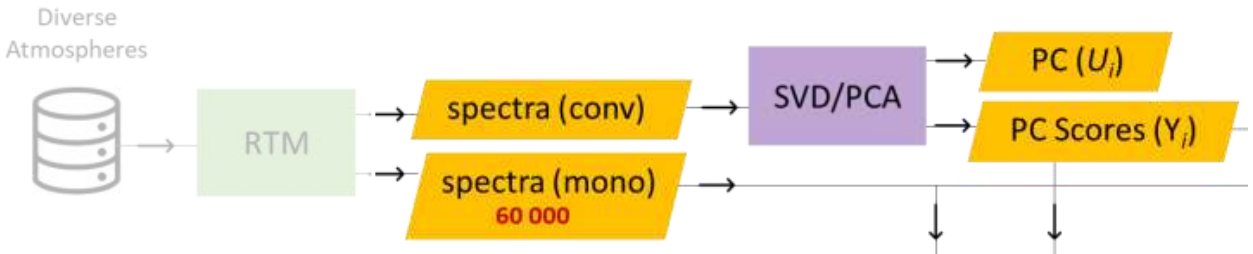
STEP 2

Extract the principal components and associated scores

How many PCs to keep?

→ Inspect residuals of reconstructed Testing spectra





STEP 3

Choose the monochromatic features to best model the PC scores

$$\mathbf{Y}_i = \left(\sum_{j=1}^{N_{mono}} a_j R_j^{mono} \right)$$

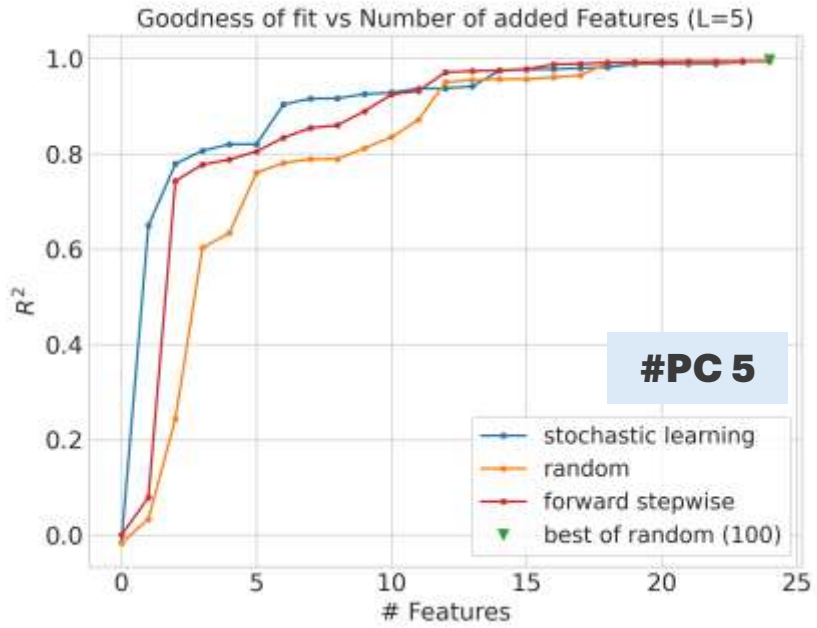
For each Principal Component $\mathbf{U}_i$, we need to find the (optimal) monochromatic radiances $\mathbf{R}_j^{mono}$ to reconstruct the PC scores $\mathbf{Y}_i$

STEP 3

Choose the monochromatic features to best model the PC scores

$$\mathbf{Y}_i = \left(\sum_{j=1}^{N_{mono}} a_j \, R_j^{mono} \right)$$

For each Principal Component $\mathbf{U}_i$, we need to find the (optimal) monochromatic radiances $\mathbf{R}_j^{mono}$ to reconstruct the PC scores $\mathbf{Y}_i$

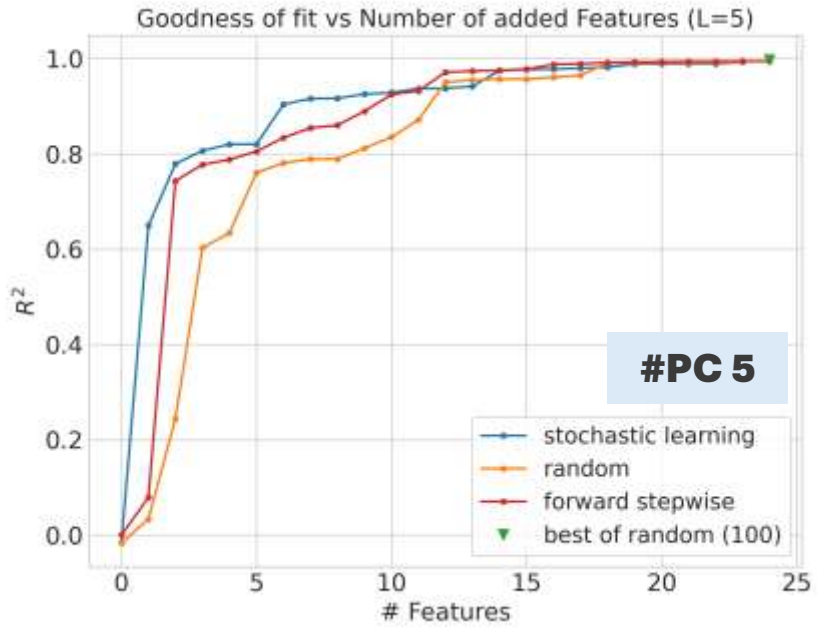


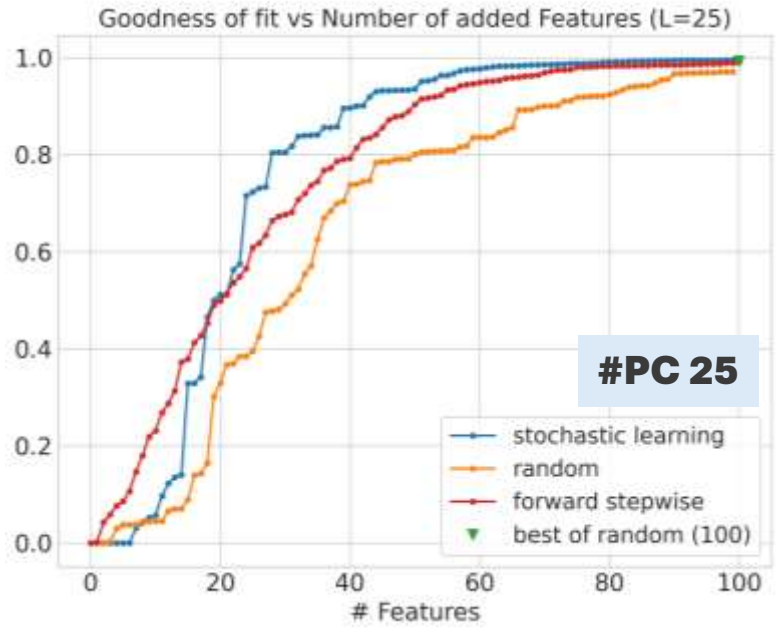
STEP 3

Choose the monochromatic features to best model the PC scores

$$\mathbf{Y}_i = \left(\sum_{j=1}^{N_{mono}} a_j \, R_j^{mono} \right)$$

For each Principal Component $\mathbf{U}_i$, we need to find the (optimal) monochromatic radiances $\mathbf{R}_j^{mono}$ to reconstruct the PC scores $\mathbf{Y}_i$



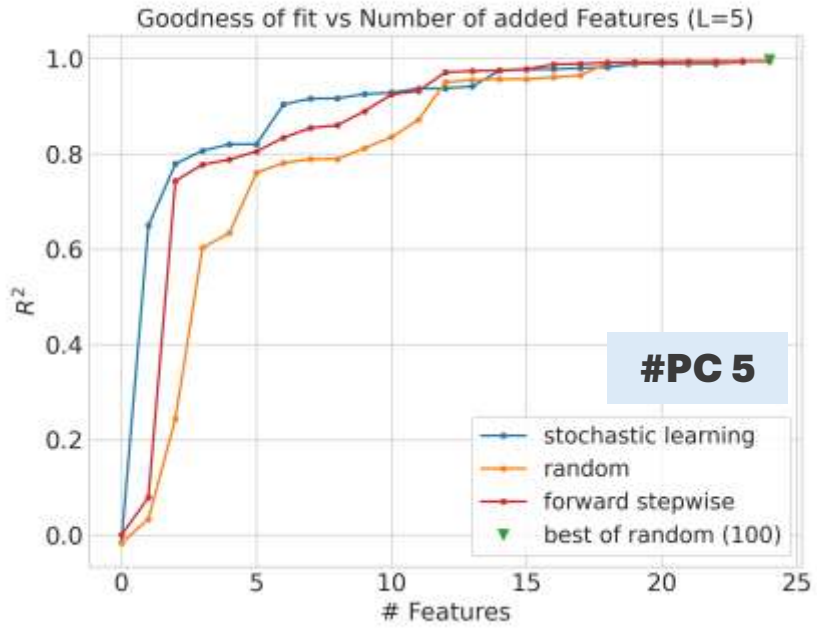


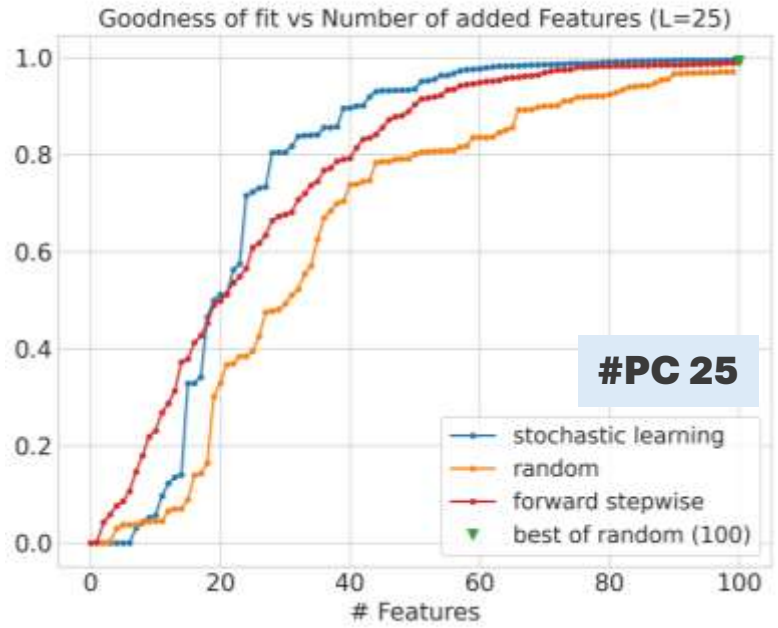
STEP 3

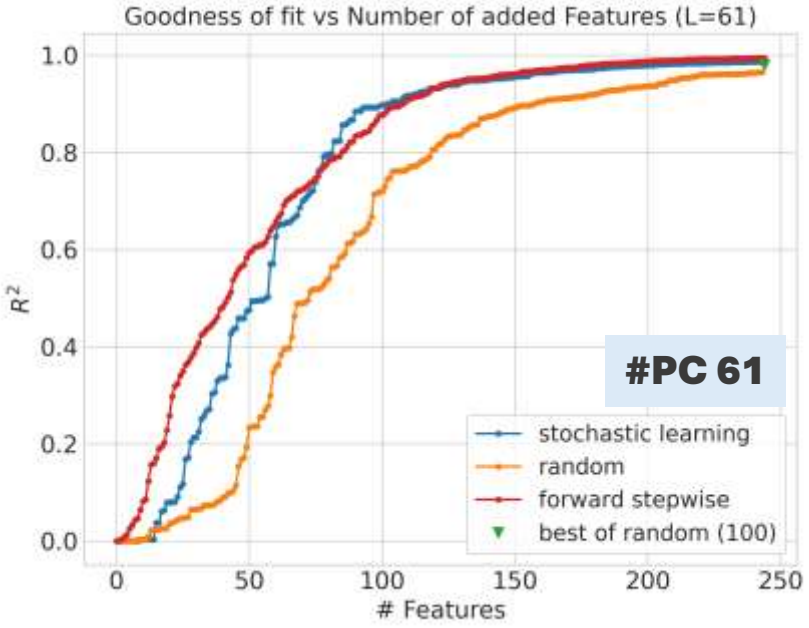
Choose the monochromatic features to best model the PC scores

$$\mathbf{Y}_i = \left(\sum_{j=1}^{N_{mono}} a_j \, R_j^{mono} \right)$$

For each Principal Component $\mathbf{U}_i$, we need to find the (optimal) monochromatic radiances $\mathbf{R}_j^{mono}$ to reconstruct the PC scores $\mathbf{Y}_i$







STEP 3

Choose the monochromatic features to best model the PC scores

When are we satisfied with our model fit?

→ What R^2 value should we set as threshold?

For a given PC #i:

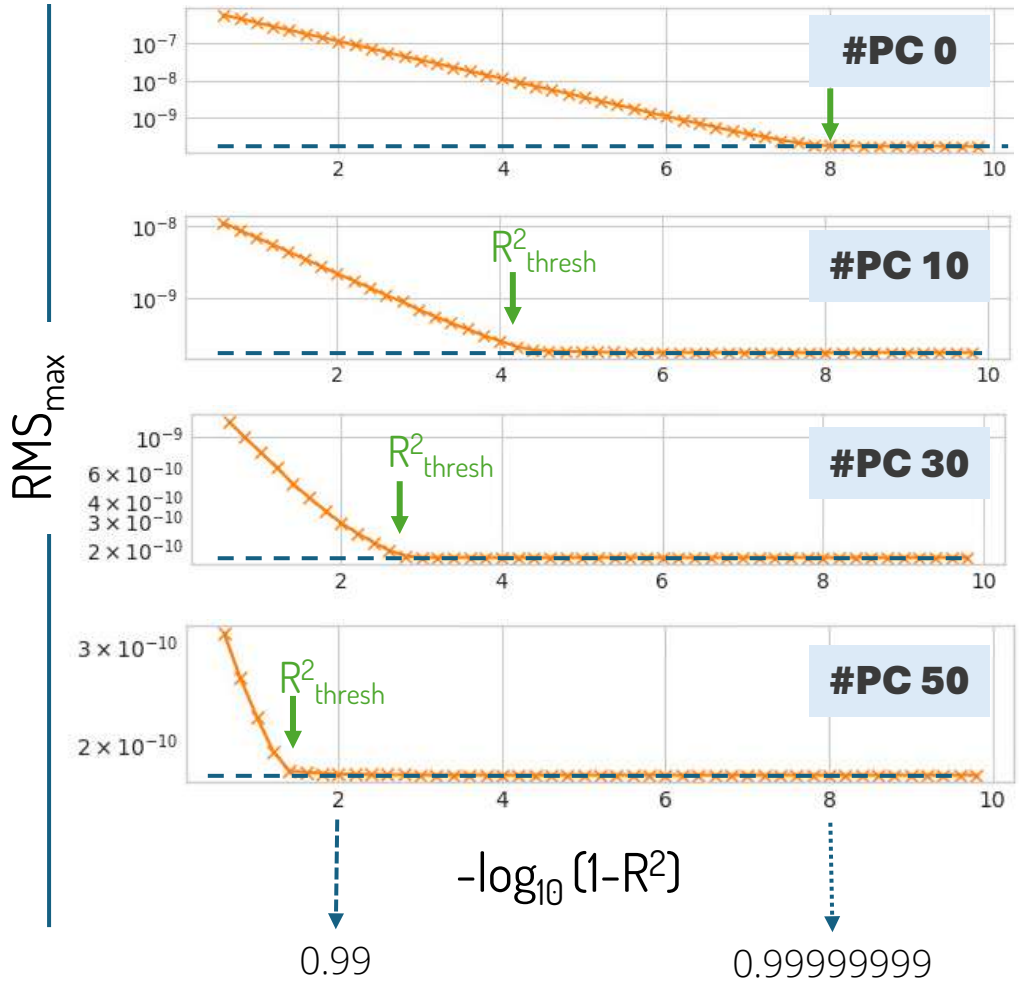
- **Add noise to** PC scores Y_i to model different values of R^2

$$\mathbf{Y_i^{noisy} = Y_i} + \sigma \;; \qquad \sigma = \sqrt{\left(\frac{TSS \cdot (1 - R^2)}{N_Y}\right)}$$

- Keep original scores fixed for all other PCs $\{Y_k, k \neq i\}$
- Reconstruct the radiances
- Calculate RMS_{max} of the spectral residuals

We can define: $R^2_{thresh}(PC\#)$

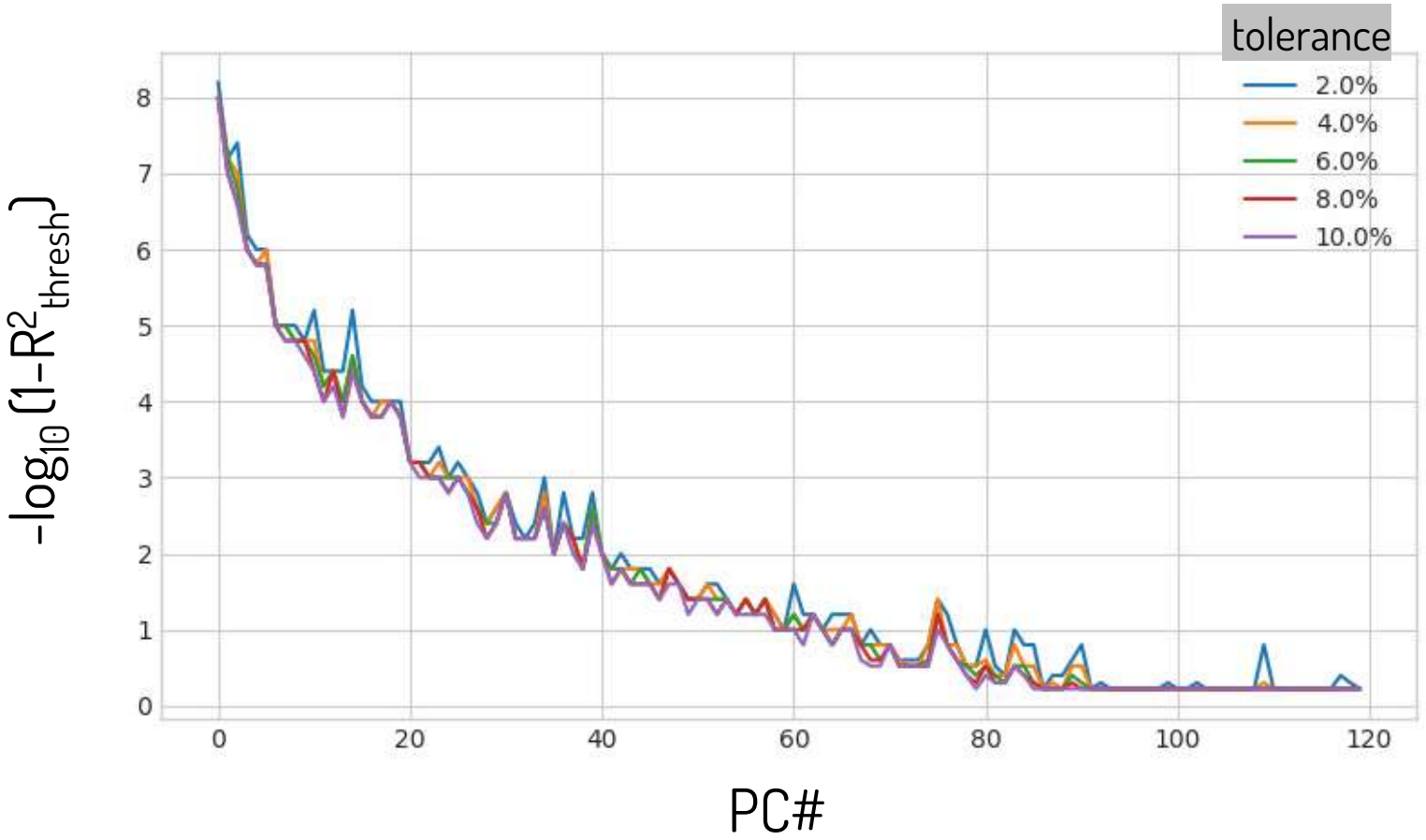
RMS_{max} vs R^2 for different #PC



STEP 3

Choose the monochromatic features to best model the PC scores

We can define: $R^2_{thresh}(PC\#)$

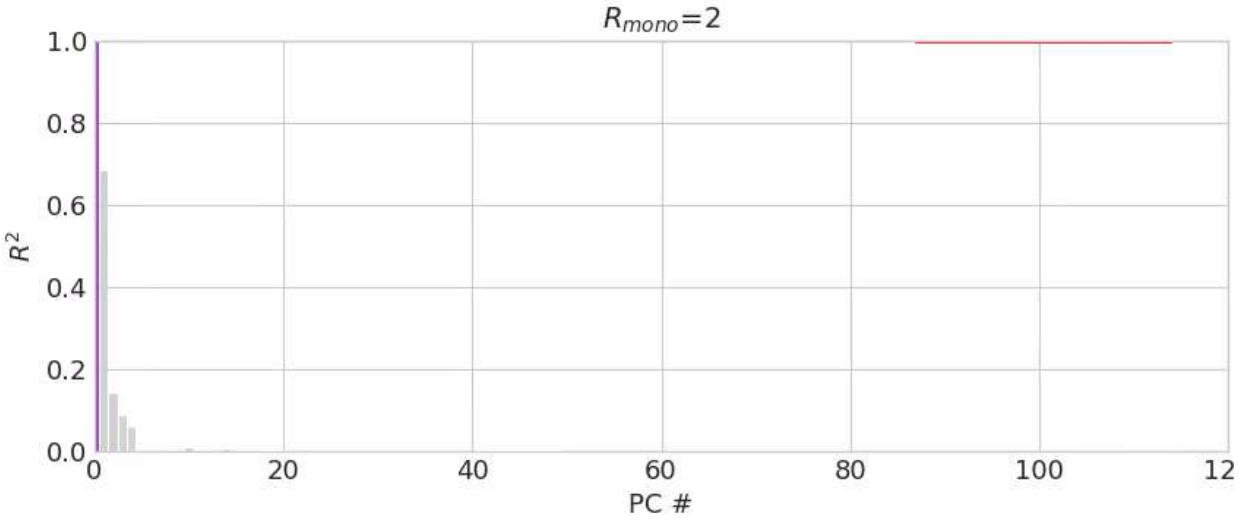


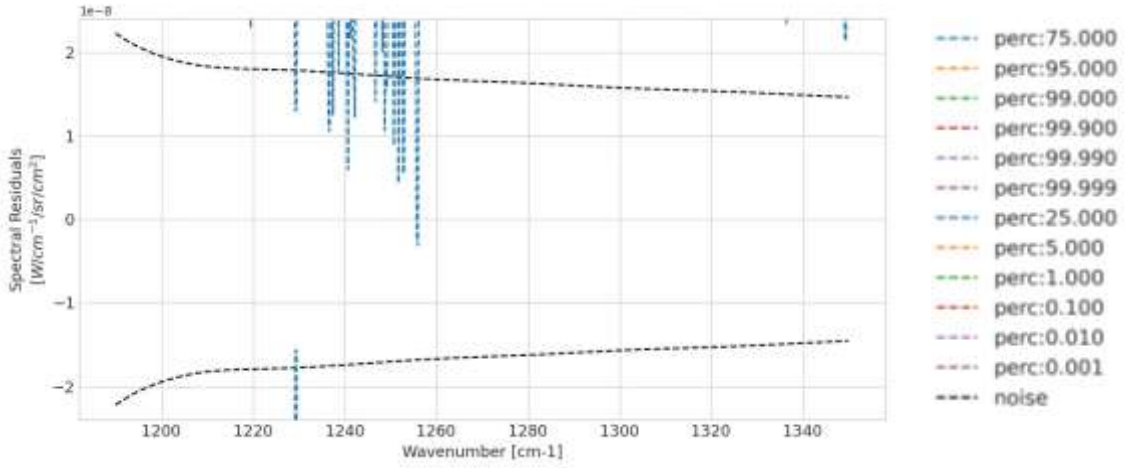
STEP 3

Choose the monochromatic features to best model the PC scores

How to aggregate the R_{mono}?

→ First: cycle through PCs adding a few (2) R_{mono} for each PC that best fit the data, aggregating the R_{mono}



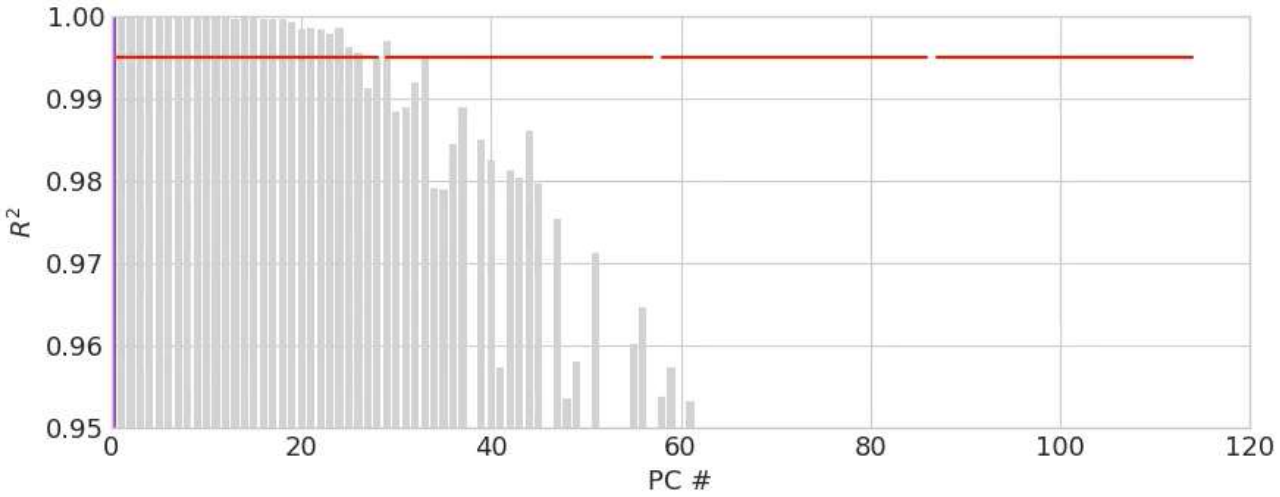


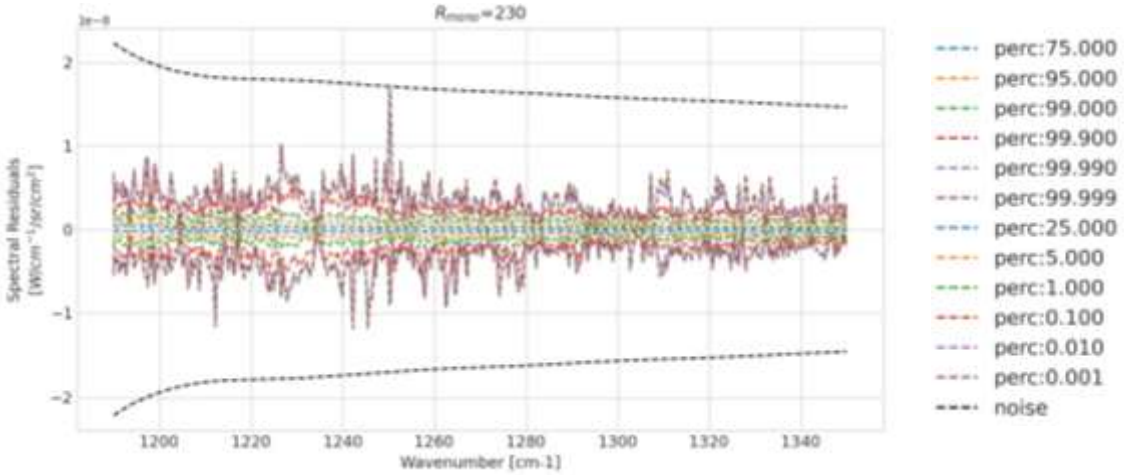
STEP 3

Choose the monochromatic features to best model the PC scores

How to aggregate the R_{mono}?

→ Second: cycle through PC adding a R_{mono} for each PC until R^2 threshold is reached





STEP 4 Jacobians for profile retrievals

Numerical Jacobians?

- For CH_4 retrievals: ~100 RTM calculations needed
- Only a 4x speed improvement compared with monochromatic RTM with analytical jacobians

STEP 4 Jacobians for profile retrievals

Numerical Jacobians?

- For CH_4 retrievals: ~100 RTM calculations needed
- Only a 4x speed improvement compared with monochromatic RTM with analytical jacobians

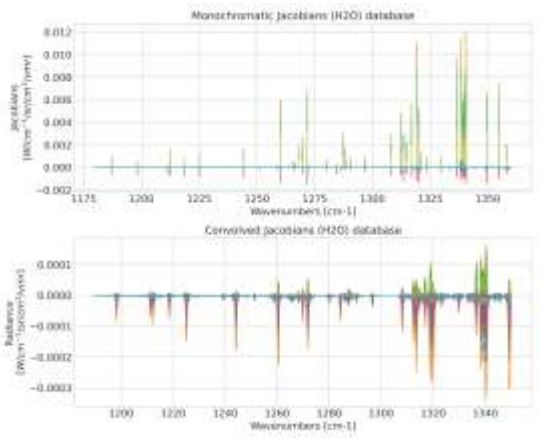
What is the alternative?

- Similar approach as the radiance
- Assume that the convolved jacobians can be calculated as a function of the monochromatic jacobians, independent of the layer
- Each molecular Jacobians will have its own set of PCs

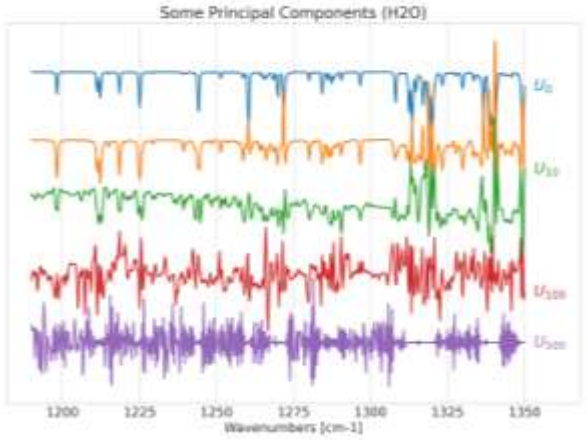
STEP 4 Jacobians

For each molecule:

Jacobians database



PC extraction (SVD)



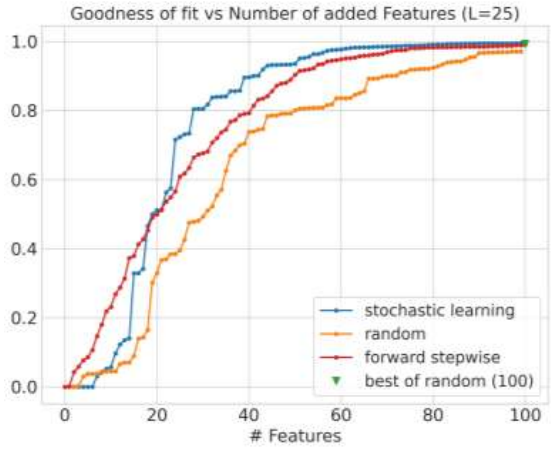
How many PC to keep?

Reconstruction of analytical Jacobians using $\boldsymbol{N_{PC}}$ in retrieval scheme until difference in retrieval results is minimal

$\Delta\chi^2 < 0.005$

$\Delta x < 0.1\%$

Rmono selection

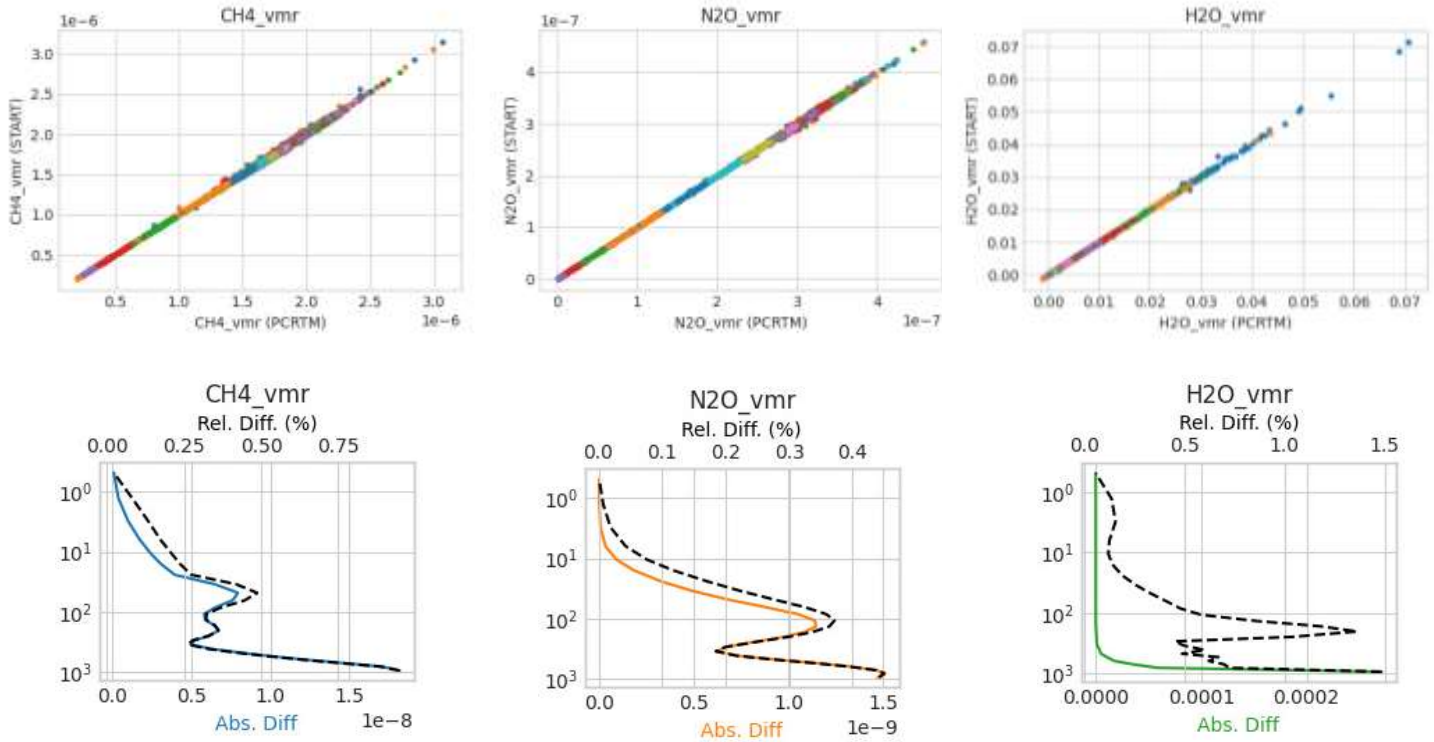


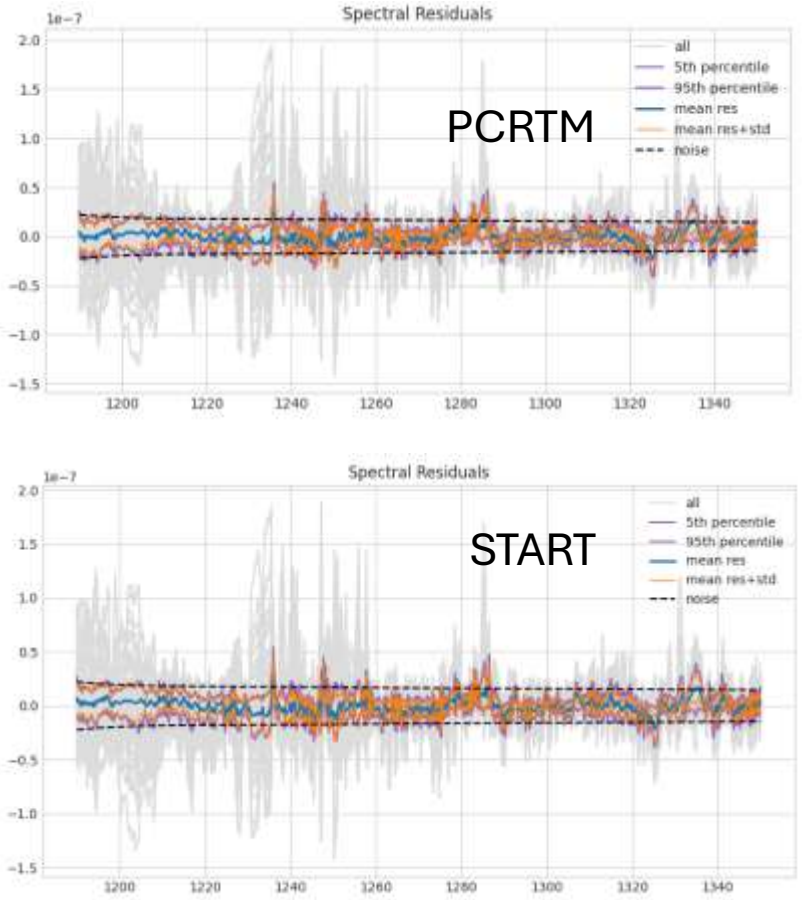
STEP 5

Finalize and test your model (radiance + jacobians) based on final ensemble of selected $\boldsymbol{R_{mono}}$

Retrievals Comparison: START vs PCRTM

→ For 500 random IASI observations





STEP 5

Finalize and test your model (radiance + jacobians) based on final ensemble of selected $\boldsymbol{R_{mono}}$

How long to build the PCRTM model?

→ ~ 1 day for radiance/jacobians generation

→ ~ a few hours for R_{mono} selection and PCRTM model parameter fits

Speed comparison: START vs PCRTM

→ $\Delta t_{START} / \Delta t_{PCRTM}$ (Radiance only) = 60

→ $\Delta t_{START} / \Delta t_{PCRTM}$ (rad + jacobians) = 95

Conclusions

→ Congrats! Now you can build your very own PCRTM model!

→ Increase your retrievals speed by a factor of 40 – 100 (depending on the problem)

→ You can use your own RTM set-up (model levels, spectroscopy, spectral resolution, etc)

→ Reconstruct Radiances and Jacobians for the entire spectral range from a handful of monochromatic simulations

→ A good fit for operational/NRT processing

THANK YOU!
MORE INFO?

iasi.aeronomie.be

charles.robert@aeronomie.be

This work has been supported by PRODEX Project Proposal: **HIRS**