Uncertainty estimation via Neural Networks: Retrieval of the atmospheric CO_2 and the associated uncertainties

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The context

The retrieval of geophysical parameters from satellite missions plays an important role in the knowledge of Earth's physical phenomenon, such as greenhouse gases, which are responsible for important effects on our atmosphere such as Earth reheating.

In this context, methods based on deep learning algorithms have gained an important place in the scientific community. Multi-Layer Perceptron (MLP) Neural Networks (NN) have proven to provide good estimates of atmospheric parameters and to be more performant than classical retrieval methods – e.g. Optima Estimation Method (OEM) – in terms of computational cost and processing of non-lineal models.

The problem

Classical NN techniques do not provide uncertainty information on the retrieved parameters.

Uncertainty information is essential for the exploitation of scientific products, for example; its utilization in analyse/forecasting systems of the atmospheric composition or dynamics.

The objective

Understand and estimate the potential of the retrieval of the atmospheric CO_2 from infrared hyperspectral sounding instruments such as IASI, IASI-NG or OCO-2 and its associated uncertainty via Neural Networks based methods in order to prepare future missions – e.g. Microcarb –.

The solution

Implementation of a Quantile Regression Neural Network (QRNN)

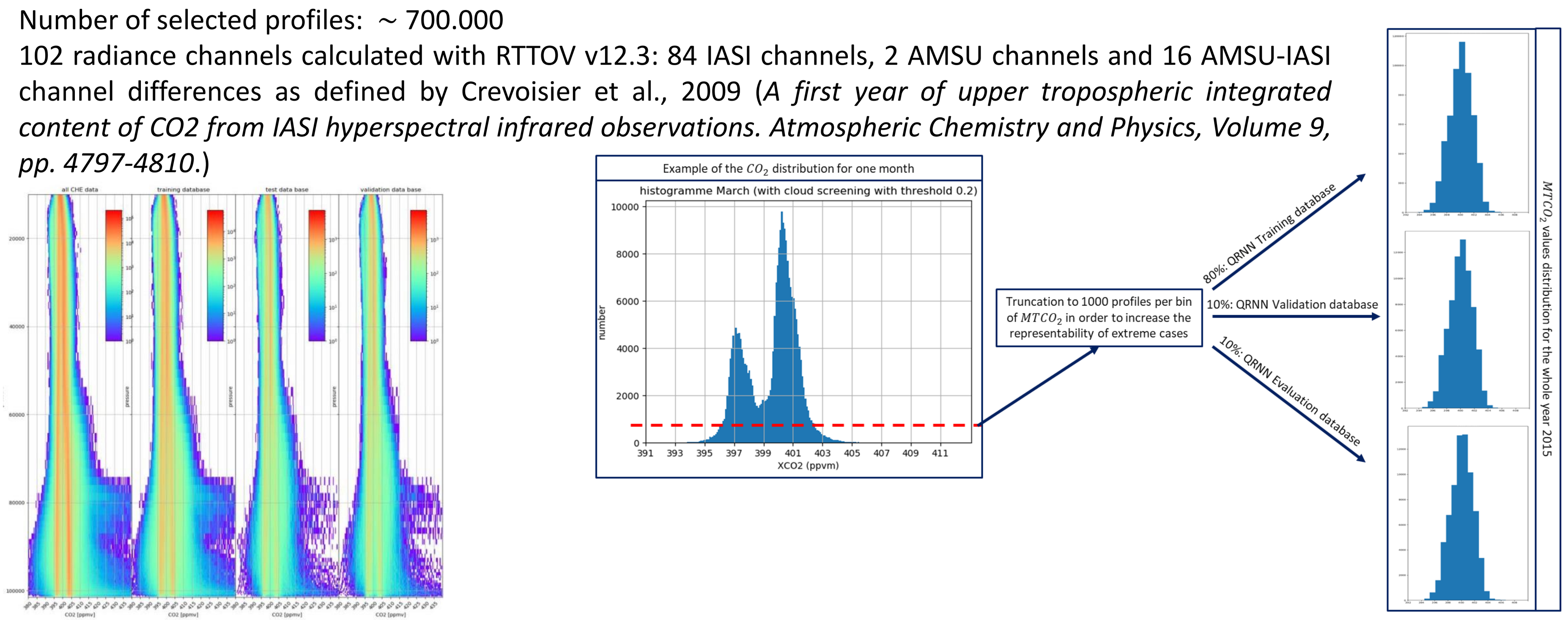
The data: Synthetic radiances in agreement with IASI and AMSU

The data used in this study consists of a series of synthetic [radiance, $MTCO_2$] couples of values corresponding to selected IASI and AMSU channels. These series are representative of a wide range of atmospheric situations in the tropical zones of the globe, including extreme events.

Database characteristics:

Database created from CHE (*Agusti-Panareda & McNorton (2019): CHE Tier 2 Global Nature Run (CHE-D2.6 report)*) high resolution state-of-the-art simulations of CO_2:

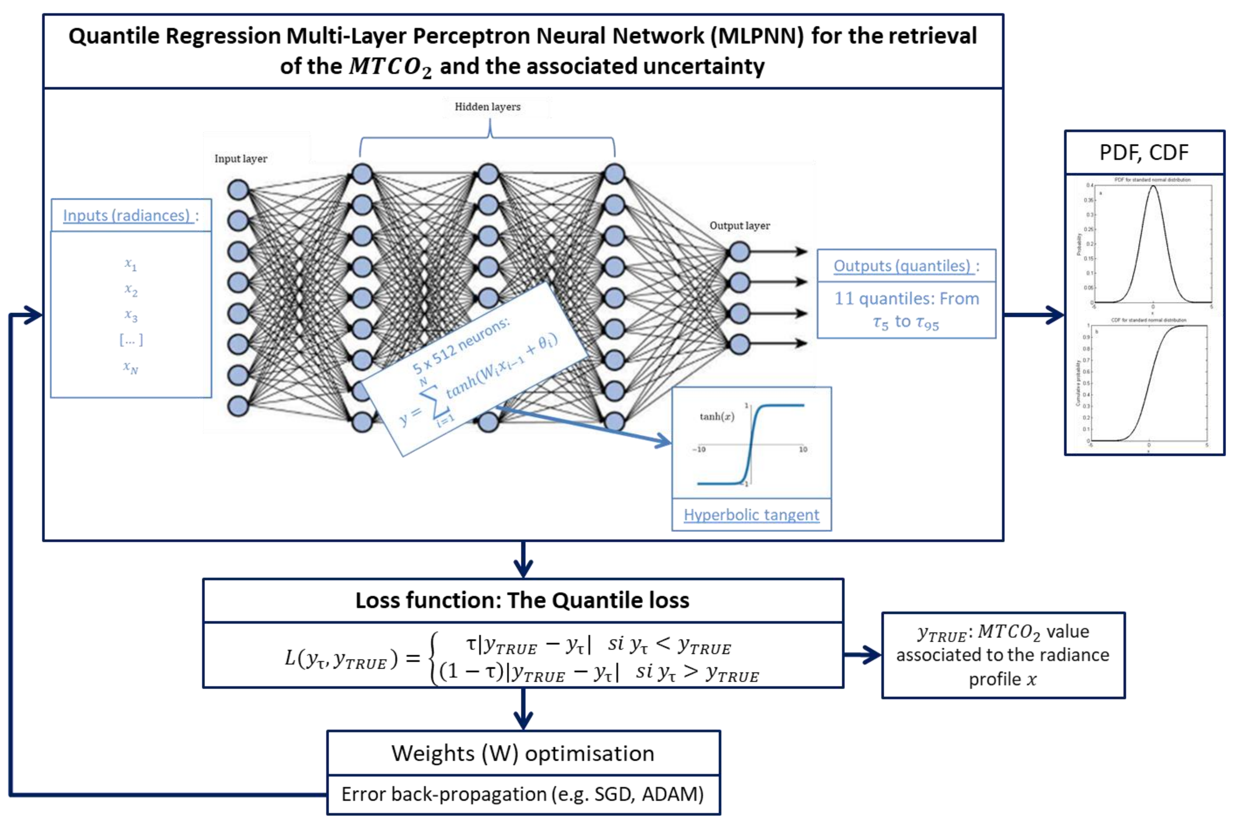
- Type of profiles extracted : Profiles corresponding to the tropical zones – i.e. 25N-25S –, clear sky, for both land and ocean areas and for each month of the year 2015.
- Further subsampling (per month) in order to increase the number of profiles with extreme values of CO_2 columns.
- Number of selected profiles: ~ 700.000
- 102 radiance channels calculated with RTTOV v12.3: 84 IASI channels, 2 AMSU channels and 16 AMSU-IASI channel differences as defined by Crevoisier et al., 2009 (*A first year of upper tropospheric integrated content of CO2 from IASI hyperspectral infrared observations. Atmospheric Chemistry and Physics, Volume 9, pp. 4797-4810.*)



The Quantile Regression Neural Network (QRNN)

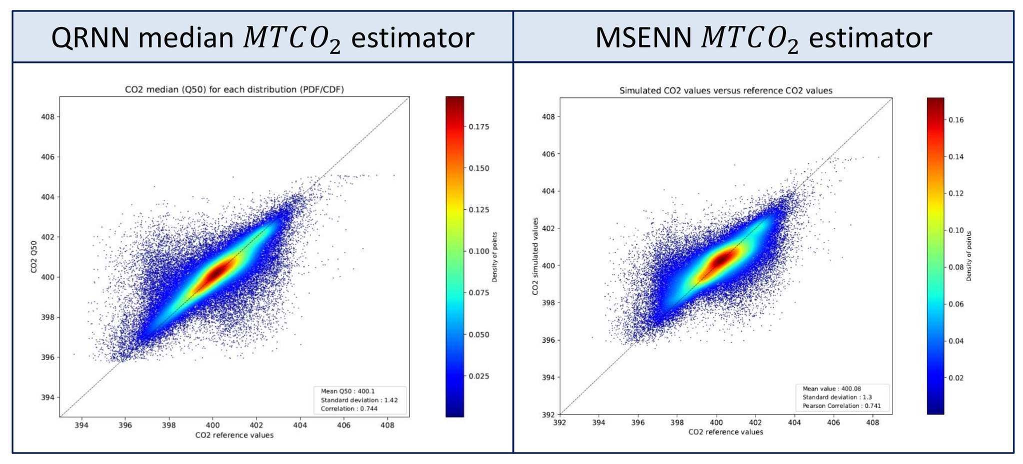
The QRNN has the particularity to be able to learn how to **predict a probability distribution** from a single truth value by using a **quantile regression loss function**. The estimation of such probability distribution – i.e. Cumulative Distribution Function (CDF) or Probability Distribution Function (PDF) – gives exploitable information about the uncertainty associated to the retrieved parameter.

A Quantile Regression MLP has therefore been implemented in order to estimate the predicted probability intervals of the mid-tropospheric CO_2 ($MTCO_2$) – 11 quantiles positions ranging from 0,05 to 0,95 –.



Validation of the QRNN $MTCO_2$ retrieval (I): The τ_{50} estimator

The median (τ_{50}) $MTCO_2$ estimator of the QRNN is compared against the $MTCO_2$ prediction from a classical MLP – i.e. Mean Squares Error (MSE) loss function – in order to analyse and validate the QRNN behaviour. The comparison is carried out using the $MTCO_2$ ground truth values as the reference.



As observed, the median estimator is equivalent – even slightly better – to the prediction of a classical neural network → **The QRNN is** therefore **a valid model for the retrieval of $MTCO_2$ values.**
For the majority of the scenes, the QRNN estimator is close to the ground truth $MTCO_2$ value.
The presence of considerable biases on the estimations – i.e. (τ_{50} $-reference$) – can be explained by the representability and nature of the learning dataset.
It is important to mention that the **objective** of the study at this point is to **implement a QRNN model which is able to provide consistent uncertainties associated to the retrieved $MTCO_2$ values** – but not having an optimised model providing "perfect" retrievals – .
Results show that **most of the $MTCO_2$ biased estimations have a large value of uncertainty associated**, meaning that the QRNN model is not certain about the validity of the estimation.

Validation of the QRNN $MTCO_2$ retrieval (II): Quantiles validation

Once the median estimator is validated, it is also important to make sure that the remaining predicted quantiles are coherent with the characteristics and the definition of a probability distribution:

- The Cumulative Distribution Function (CDF) – i.e. the estimated quantiles – must be strictly increasing, which means that:
- The Probability Density Function (PDF) is also strictly positive

$\forall \tau_{CO_2}, \tau_i > \tau_{i+1}$	$f(x)_{CO_2} < 0$
0 %	0 %

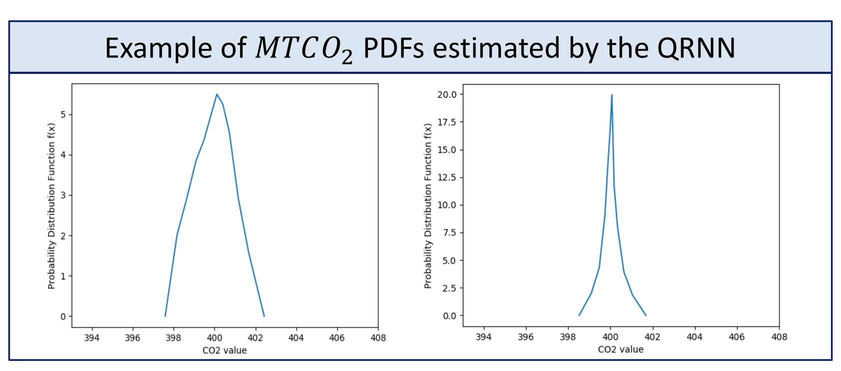
All the retrieved CDF/PDF conform with the imposed constraints

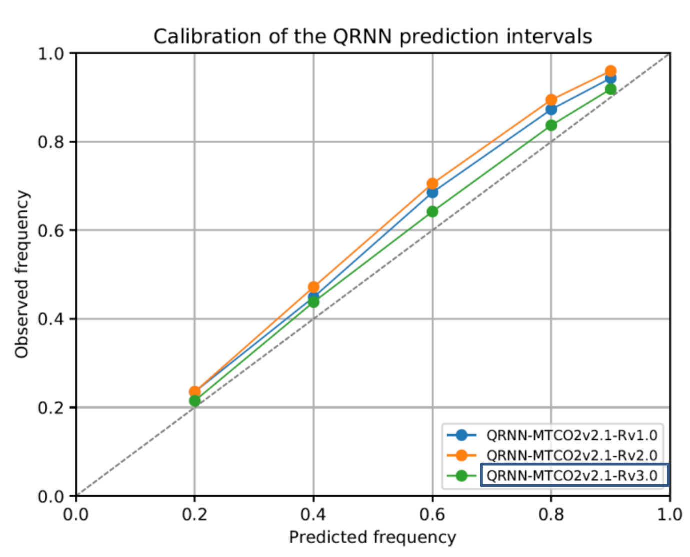
In addition, less than 3% of the evaluated scenes present a $MTCO_2$ ground truth value which lies outside the predicted quantile envelope – i.e. there cannot exist a ground truth value lower than the estimated quantile 0 or higher than the estimated quantile 100 – .

$CO_{2_{VT}} < \tau_0\ CO_2$	$CO_{2_{VT}} > \tau_{100}\ CO_2$
2,16 %	1,52 %

Finally, the predicted quantiles intervals must be representative for the observed $MTCO_2$ ground truth intervals:

- The calibration plot shows a robust and well-calibrated QRNN with a slightly over-estimation of the uncertainties → As agreed with the presence of the restitution biases.

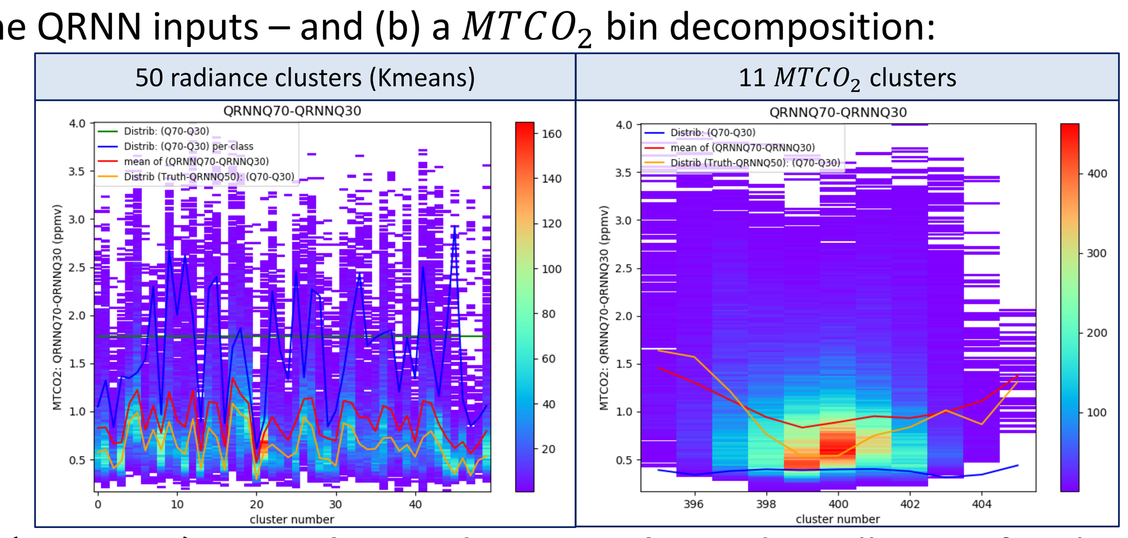




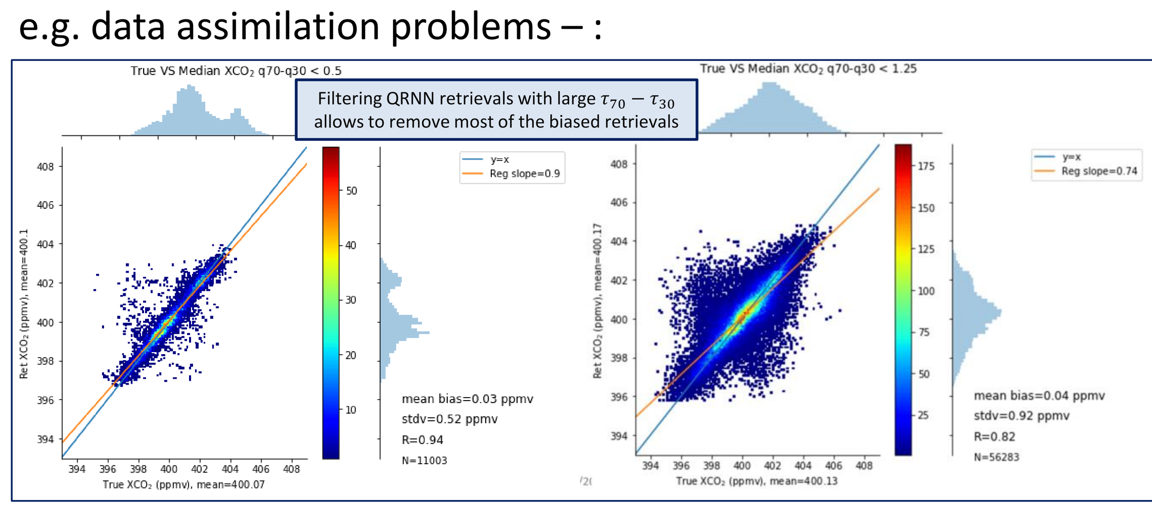
Validation of the QRNN uncertainty estimation

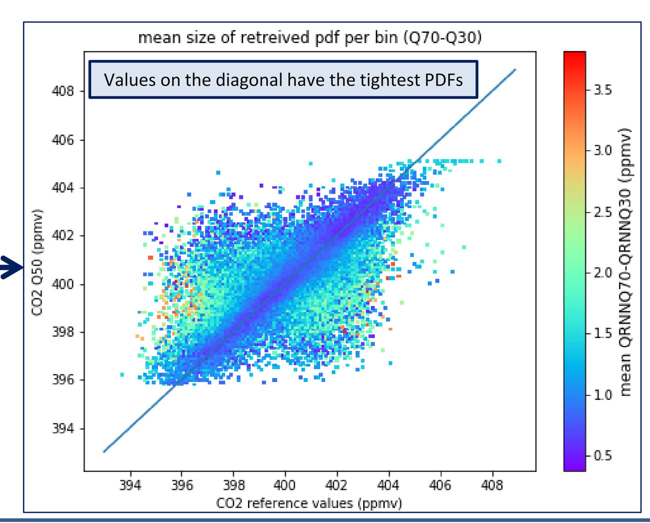
The validation of the uncertainty estimates is carried out by the comparison of the QRNN predictions ($\tau_{50}$$-Truth$) – i.e. reference – against the mean distribution of the PDFs derived from the estimated quantiles. This exercise is performed in bins, using : (a) A bin decomposition via a K-Means method in the radiance space – i.e. same information as the QRNN inputs – and (b) a $MTCO_2$ bin decomposition:

- There is a **good correlation between the estimated uncertainty** (red lines) **and the reference/empirical uncertainty** (orange lines).
- There is a slightly over-estimation of the uncertainties → As agreed with the calibration curve.
- Both the reference and the estimation have a higher uncertainty for the $MTCO_2$ extreme values, these values corresponding to the most biased retrievals for which **the model correctly predicts higher uncertainty**.



The QRNN uncertainty estimation – e.g. ($\tau_{70} - \tau_{30}$) – **can be used as a quality index**, allowing for the filtering of the $MTCO_2$ most uncertain retrievals, and therefore preventing their use in latter applications – e.g. data assimilation problems – :





Acknowledgements

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