Statistical Emulator For Fast Uncertainty Quantification

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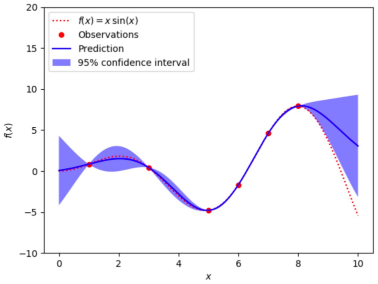
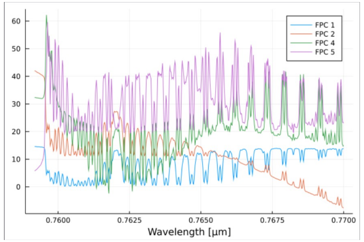
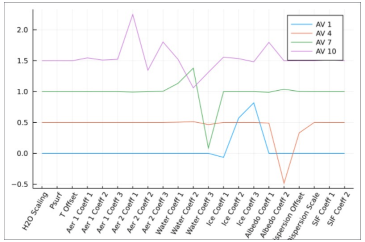
We propose a fast Gaussian process emulator for the OCO-2 retrieval problem. Idea is to predict radiances at unknown atmospheric states based on a model trained with known radiances y_i obtained at known states x_i



Dimension reduction:
Functional Principal Components for y,
Active Subspace for x





$$X \to X[O_2],\quad X[WCO_2],\quad X[SCO_2]$$

$$X_r^{O_2} = W_r^T X[O_2] \qquad X_r^{WCO_2} = W_r^T X[WCO_2] \qquad X_r^{SCO_2} = W_r^T X[SCO_2]$$

$$z_i = GP_i(X_r^{SCO_2}) \qquad z_j = GP_j(X_r^{SCO_2}) \qquad z_k = GP_k(X_r^{SCO_2})$$

$$y[O_2] = \mu_{O_2} + \sum_{i=1}^{N_{O_2}} \eta_i z_i \qquad y[WCO_2] = \mu_{WCO_2} + \sum_{j=1}^{N_{WCO_2}} \eta_j z_j \qquad y[SCO_2] = \mu_{SCO_2} + \sum_{k=1}^{N_{SCO_2}} \eta_k z_k \quad \to y$$

Final pipeline for an emulator predicting radiances y from atmospheric states x

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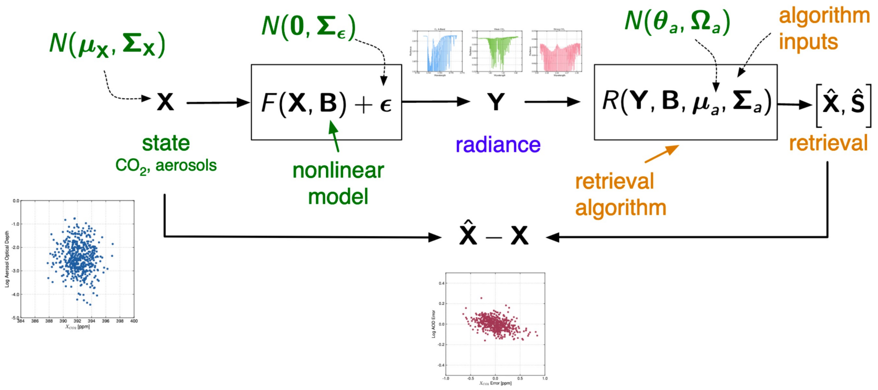
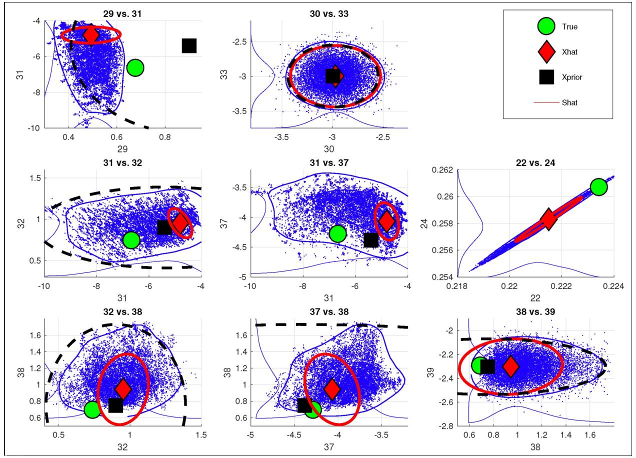
Motivation for an emulator

Rigorous Uncertainty Quantification (UQ) for remote sensing retrievals often relies on large amount of forward model evaluations, which becomes prohibitively expensive in the case of OCO-2 ACOS Full Physics model. We aim to replace the costly Full Physics model by a fast *Gaussian Process Emulator*.

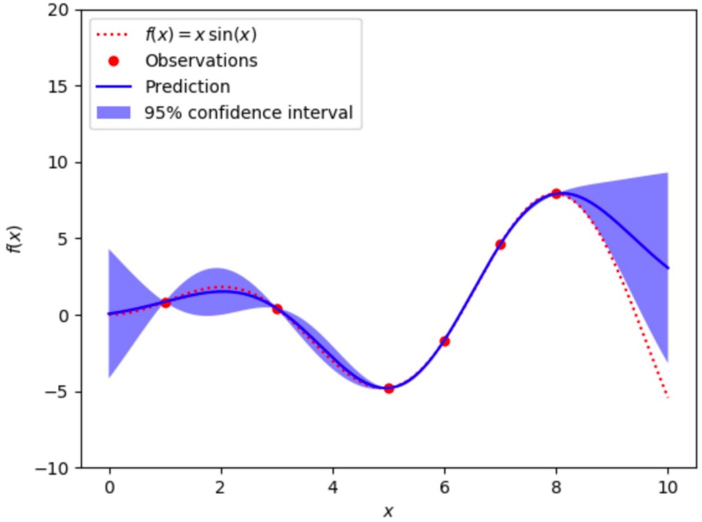




Simulation based UQ of Hobbs et al. (2017) utilizes a large amount of forward model evaluations to get radiances and consecutive retrievals to produce a distribution of true vs retrieved states.

Markov Chain Monte Carlo (MCMC) implemented for OCO-2 in Lamminpää et al. (2020) evaluates the Full Physics model numerous time to produce samples from exact posterior distribution of a retrieval.

Interpretable Machine Learning: Gaussian Processes



A *Gaussian Process* (GP) is a statistical method for learning a function *f* from a set of evaluations $y_i = f(x_i)$ at known points x_i . A GP is specified by training a Kernel function K by specifying its parameters θ. Predictions at new point x are obtained as

$$y = K(x,X)K(X,X)^{-1}Y$$

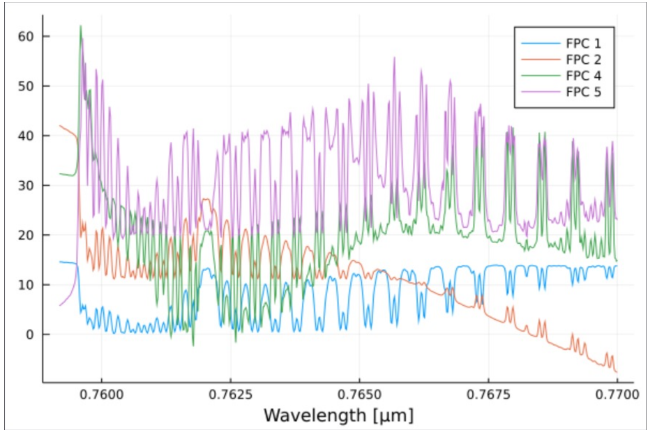
where X and Y represent all training points and corresponding training data.
A GP also provides confidence intervals for predictions, so the user can assess the credibility and performance of the predictions unlike in many other machine learning methods. The uncertainty is given by

$$\sigma = K(x,x) - K(x,X)K(X,X)^{-1}\,K(X,x)$$

Dimension Reduction

Using a spline basis, *Functional Principal Component Analysis* (FPCA) extracts a low dimensional decomposition for radiances. This approach is suited for OCO-2 output, which is obtained on a non-uniform wavelength grid

$$y_k(\omega) = \mu_k(\omega) + \sum_{i=1}^{p_k} \eta_{k,i}(\omega) z_{k,i}(x)$$



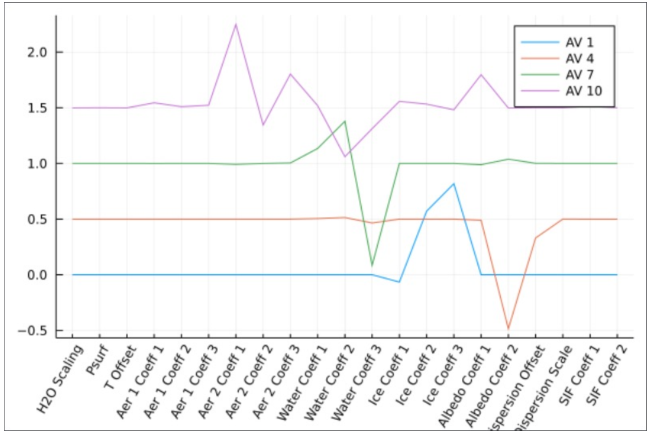
Example FPCA basis vectors for O_2 band

For each wavelength band, we find a gradient-based *Active Subspace* (AS), which captures the principal components of the state vector that the forward model is most sensitive to. This way we get a low-dimensional decomposition for the state.

$$\boldsymbol{C} = \mathbb{E}[(\nabla_x z_i(x))(\nabla_x z_i(x))^T]$$

$$\Rightarrow \boldsymbol{C} = \boldsymbol{W} \Lambda \boldsymbol{W}^T, \quad \boldsymbol{W} = [\boldsymbol{W}_r, \boldsymbol{W}_\perp]$$

$$\Rightarrow x_r = \boldsymbol{W}_r^T x, \quad x_\perp = \boldsymbol{W}_\perp^T x$$



Example AS basis vectors for O_2 band

Emulator Flowchart

X

$$X[O_2] \qquad X_r^{O_2} = W_r^T X[O_2] \qquad z_i = GP_i(X_r^{SCO_2}) \qquad y[O_2] = \mu_{O_2} + \sum_{i=1}^{N_{O_2}} \eta_i z_i$$

$$X[WCO_2] \qquad X_r^{WCO_2} = W_r^T X[WCO_2] \qquad z_j = GP_j(X_r^{SCO_2}) \qquad y[WCO_2] = \mu_{WCO_2} + \sum_{j=1}^{N_{WCO_2}} \eta_j z_j$$

$$X[SCO_2] \qquad X_r^{SCO_2} = W_r^T X[SCO_2] \qquad z_k = GP_k(X_r^{SCO_2}) \qquad y[SCO_2] = \mu_{SCO_2} + \sum_{k=1}^{N_{SCO_2}} \eta_k z_k$$

y

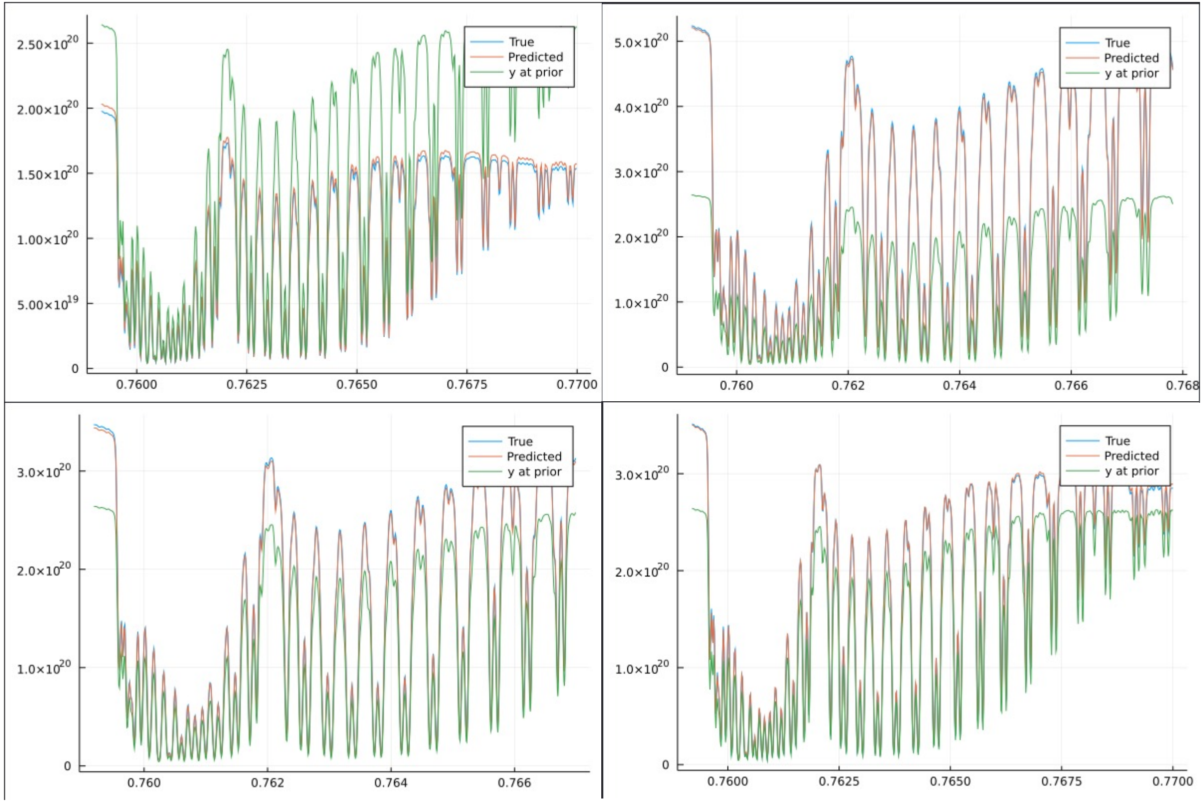
Partition X to components each band is sensitive to

Extract the AS component of X for each band

Predict FPCA coefficients z with independent Gaussian Processes

Assemble predicted coefficients, multiplied by FPCA basis functions, and mean vectors to output radiances

Results: O_2 band



Full Physics forward model evaluated at a known true state and at the prior mean, compared to the emulator evaluated at a known true state.

Our statistical emulator is thus shown to reproduce the output of the OCO-2 Full Physics model on the O_2 band with great accuracy. Although work is ongoing for WCO_2 and SCO_2 bands, these results show the potential of the emulator to be used in a retrieval setting.

The emulator is also computationally fast: an evaluation of Full Physics model takes minutes on a personal computer, while the emulator is evaluated in only milliseconds.