National Aeronautics and Space Administration

UQ-aware Machine Learning for Uncertainty Quantification

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Program: FY22 R&TD Topics
Strategic Focus Area: Uncertainty Quantification

Objective:

Implement a computationally efficient emulator for the Surface Biology and Geology (SBG) Earth System Observatory mission's forward model.

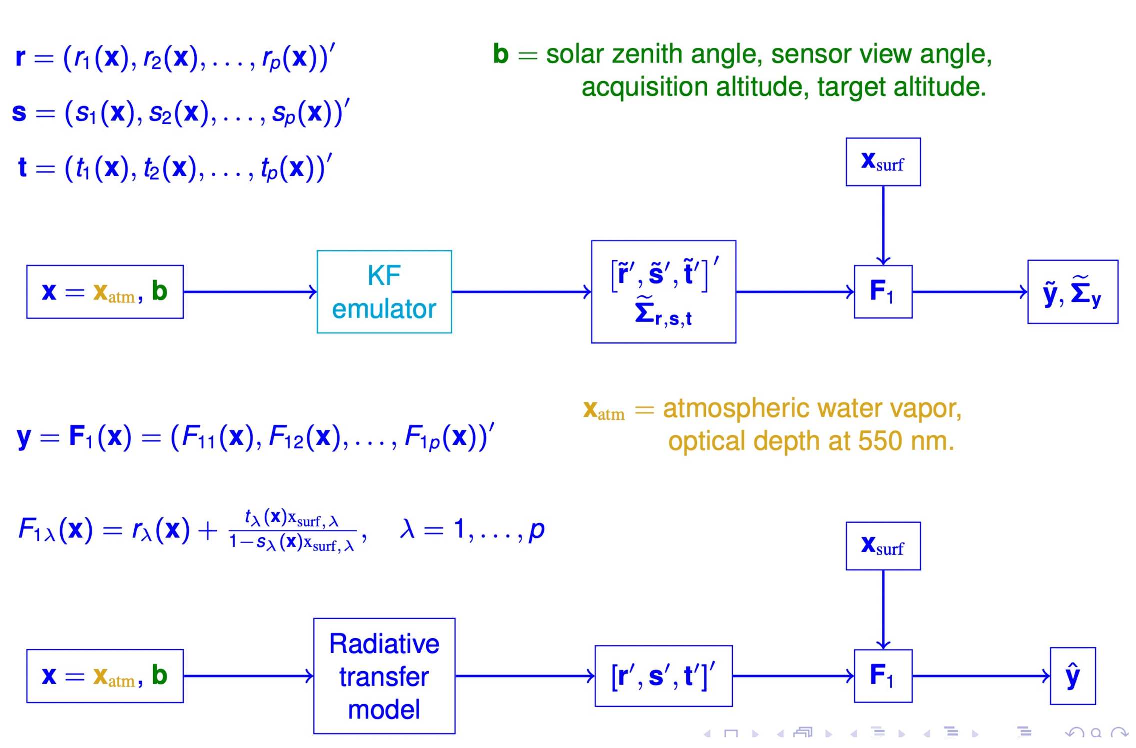
Background:

SBG and other missions' data processing will need to perform evaluations of physical forward models that predict radiances instruments will see for given atmospheric and surface states.

Forward model evaluation requires complex radiative transfer calculations, that are computationally expensive.

Our task was to build a statistical emulator that can predict radiative transfer outputs from a given set of inputs, quickly and with quantified uncertainties.

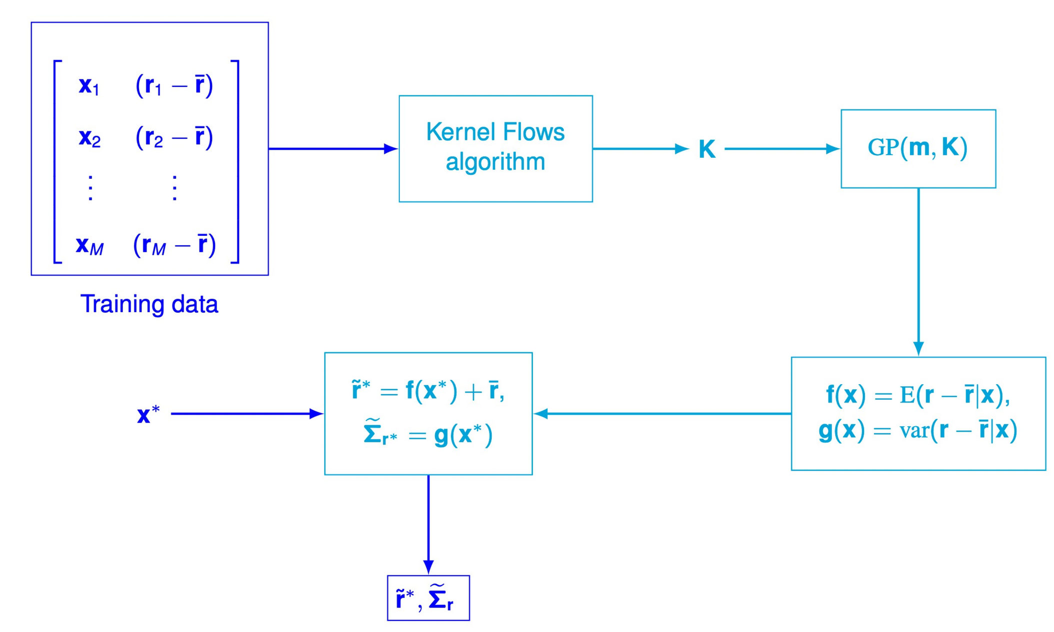
The **current state-of-the-practice** is to pre-compute a look-up table (LUT) that provides output on a grid of inputs, and use linear interpolation to obtain approximate outputs at intermediate input values. However, **LUTs must be very dense, and therefore expensive to produce, in order to provide necessary accuracy**, and LUTs provides no measure of uncertainty on predictions.



Forward model emulation approach for SBG. The SBG forward model, F_1, produces radiance vectors, y, from an input state vector, x. x is partitioned into an atmospheric part, containing water vapor and aerosol optical depth, and a surface part, containing a 425-dimensional vector of surface reflectances. We emulate the radiative transfer required to convert the atmospheric variables into path reflectance (**r**), spherical albedo (**s**), and transmissivity (**t**).

Approach and Results:

We build a Gaussian Process (GP) emulator for radiative transfer. **Kernel Flows is an algorithm for estimating the covariance matrix of the GP**, and propagating the uncertainty of that estimate through to the GP predictions.



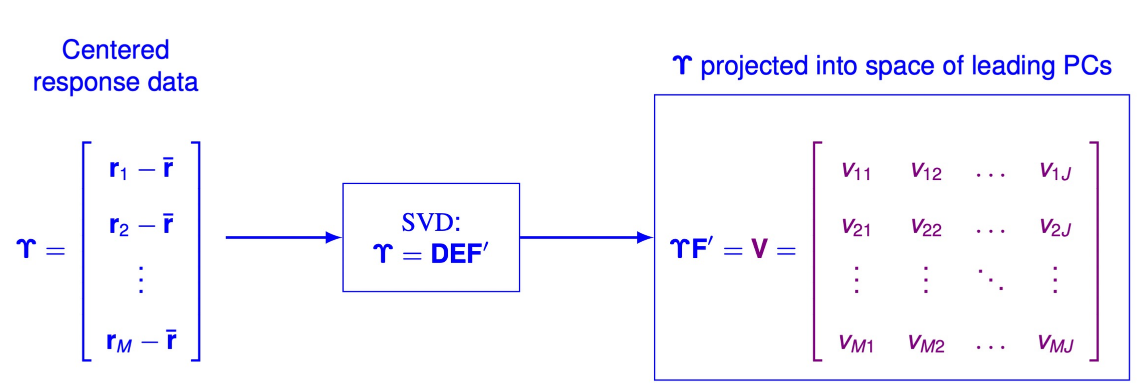
Emulator is two functions, f and g, that produce point estimates of parameter (**r** shown here, same for **s** and **t**) and prediction uncertainties, respectively. Predictors, x, are seven-dimensional inputs shown below.

Full data set generated by running radiative transfer model (MODTRAN; Berk et al., 2014) at 29,993 Sobol sequence points in a seven-dimensional hypercube:

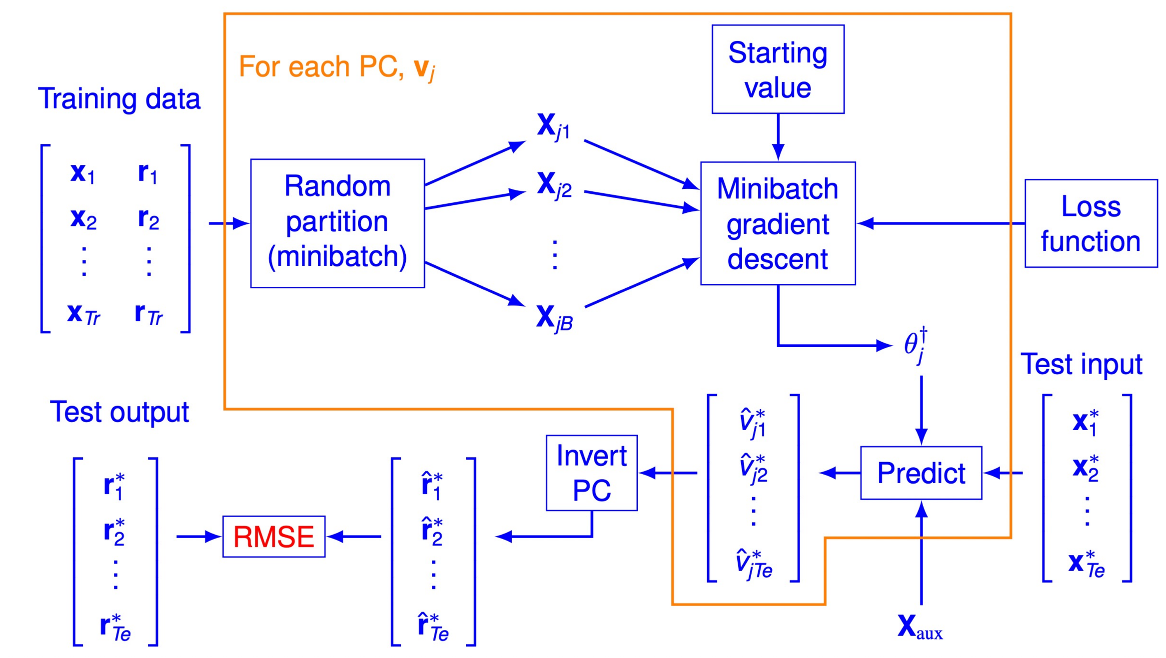
Input variables (x)	Range	Units	Element
Solar azimuth angle	[0, 89.7]	Degrees	**b**
Solar zenith angle	[0.4069, 79.9985]	Degrees	**b**
Sensor zenith angle	[130.0008, 179.7325]	Degrees	**b**
Sensor altitude	[0.01, 99.886]	km	**b**
Target altitude	[0.001, 8.8451]	km	**b**
Water vapor	[0.1, 4.4998]	g/cm^2	$\mathbf{x}_{atm}$
Aerosol fraction	[0.01, 0.9999]	NA	$\mathbf{x}_{atm}$

Output variables: **r**, **s**, and **t**; each is a $p = 425$-dimensional vector. Build separate emulators for them.

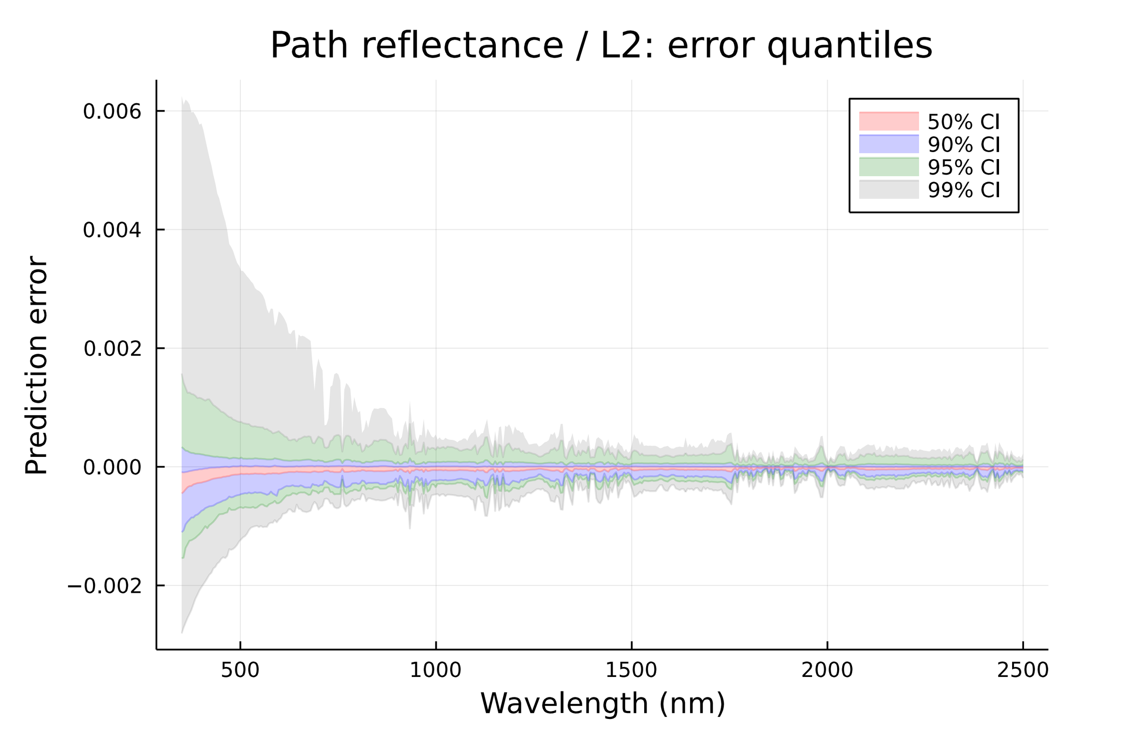
KF currently implemented for univariate response variable, but r is vector-valued. So, we project **r** into the space of leading principal components, and apply KF to each component independently.



Then, we reconstruct our estimates by inverting the principal component transformation.



We use minibatch gradient descent with L_2 loss to estimate parameters of the principal component emulators. Figure of merit for our predictions is RMSE.



Representative results (over ~900 test set members) for emulating path reflectance, **r**.

Significance/Benefits to JPL and NASA:

1) Provides proof-of-concept implementation showing that the KF emulator can replace computationally expensive forward models and achieve accuracies needed for science.
2) Already used for experimental emulators for the Microwave Limb Sounder (MLS) and OCO-2, as well as the upcoming Investigation of Convective Updrafts (INCUS) mission. Demonstrates the wide applicability of KF emulators and the importance of enabling fast data processing of very large remote sensing data sets.
3) Increase JPL's competitiveness in winning new missions by enabling efficient utilization of more data.
4) We have established a strong, productive, synergistic relationship with Caltech in which new computational and statistical research motivated by JPL problems is collaboratively addressed, and new practical solutions returned to JPL.

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Publications:

Jouni Susiluoto, Houman Owhadi, Amy Braverman, and Otto Lamminpaa, "Cross-validated radiative transfer emulation for imaging spectroscopy retrievals," in preparation for submission to the *Journal of Computational Physics*.

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