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Advances in Gaussian Processes for Earth Sciences: Physics-aware, interpretability and consistency

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Earth observation from remote sensing satellites allows us to monitor the processes occurring on the land cover, water bodies and the atmosphere, as well as their interactions. In the last decade machine learning has impacted the field enormously due to the unprecedented data deluge and emergence of complex problems that need to be tackled (semi)automatically. One of the main problems is to perform estimation of bio-geo-physical parameters from remote sensing observations. In this model inversion setting, Gaussian processes (GPs) are one of the preferred choices for model inversion, emulation, gap filling and data assimilation. GPs do not only provide accurate predictions but also allow for feature ranking, deriving confidence intervals, and error propagation and uncertainty quantification in a principled Bayesian inference framework.

Here we introduce GPs for data analysis in general and to address the forward-inverse problem posed in remote sensing in particular. GPs are typically used for inverse modelling based on concurrent observations and in situ measurements only, or to invert model simulations. We often rely on forward radiative transfer model (RTM) encoding the well-understood physical relations to either perform model inversion with machine learning, or to replace the RTM model with machine learning models, a process known as emulation. We review four novel GP models that respect and learn the physics, and deploy useful machine learning models for remote sensing parameter retrieval and model emulation tasks. First, we will introduce a Joint GP (JGP) model that combines in situ measurements and simulated data in a single GP model for inversion. Second, we present a latent force model (LFM) for GP modelling that encodes ordinary differential equations to blend data and physical models of the system. The LFM performs multi-output regression, can cope with missing data in the time series, and provides explicit latent functions that allow system analysis, evaluation and understanding. Third, we present an Automatic Gaussian Process Emulator (AGAPE) that approximates the forward physical model via interpolation, reducing the number of necessary nodes. Finally, we introduce a new GP model for data-driven regression that respects fundamental laws of physics via dependence-regularization, and provides consistency estimates. All models attain data-driven physics-aware modeling. Empirical evidence of performance of these models will be presented through illustrative examples of vegetation/land monitoring involving multispectral (Landsat, MODIS) and passive microwave (SMOS, SMAP) observations, as well as blending data with radiative transfer models, such as PROSAIL, SCOPE and MODTRAN.

References

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