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Grama: A Grammar of Model Analysis

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Software

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Summary

`Grama` is a Python package implementing a *functional grammar of model analysis* emphasizing the quantification of uncertainties. In `Grama` a *model* contains both a function mapping inputs to outputs as well as a distribution characterizing uncertainties on those inputs. This conceptual object unifies the engineer/scientist's definition of a model with that of a statistician. `Grama` provides an *implementation* of this model concept, as well as *verbs* to carry out model-building and model-analysis.

Statement of Need

Uncertainty Quantification (UQ) is the science of analyzing uncertainty in scientific problems and using those results to inform decisions. UQ has important applications to building safety-critical engineering systems, and to making high-consequence choices based on scientific models. However, UQ is generally not taught at the undergraduate level: Many engineers leave their undergraduate training with a purely deterministic view of their discipline, which can lead to probabilistic design errors that negatively impact safety (del Rosario, Fenrich, & Iaccarino, 2020). To that end, I have developed a grammar of model analysis—`Grama`—to facilitate rapid model analysis, communication of results, and the teaching of concepts, all with quantified uncertainties. Intended users of `Grama` are scientists and engineers at the undergraduate level and upward, seeking to analyze computationally-lightweight models.

Differentiating Attributes

Packages similar to `Grama` exist, most notably Sandia National Lab's `Dakota` (Adams, 2017) and `UQLab` (Marelli & Sudret, 2014) out of ETH Zurich. While both of these packages are mature and highly featured, `Grama` has several differentiating attributes. First, `Grama` emphasizes an explicit but flexible *model object*: this object enables sharp decomposition of a UQ problem into a model-building stage and a model-analysis stage. This logical decomposition enables simplified syntax and a significant reduction in boilerplate code. Second, `Grama` implements a functional programming syntax to emphasize operations against the model object, improving readability of code. Finally, `Grama` is designed from the ground-up as a pedagogical and communication tool. For learnability: Its *verb-prefix* syntax is meant to remind the user how functions are used based solely on their name, and the package is shipped with fill-in-the-blank Jupyter notebooks (Kluyver et al., 2016) to take advantage of the pedagogical benefits of active learning (Freeman et al., 2014). For communication: The model object and functional syntax abstract away numerical details for presentation in a notebook, while preserving tracability and reproducibility of results through the inspection of source code.

Inspiration and Dependencies

`Grama` relies heavily on the SciKit package ecosystem for its numerical backbone (Hunter, 2007; McKinney, 2010; Pedregosa et al., 2011; van der Walt, Colbert, & Varoquaux, 2011; Virtanen et al., 2020). The functional design is heavily inspired by the `Tidyverse` (Wickham et al., 2019), while its implementation is built upon `dfply` (Katovich, 2019). Additional functionality for materials data via an optional dependency on Matminer (Ward et al., 2018).

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