You like scikit-learn? You like Stan? You love scikit-stan!

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Abstract

scikit-stan is a Python library of pre-compiled Bayesian models that adheres to the scikit-learn model philosophy and workflow. As such, this package provides a familiar API for fitting models, generating predictions, and scoring outcomes via a robust Stan backend. These design choices ensure that efficient probabilistic models are seamlessly integrated with the vast scikit-learn ecosystem while improving Stan’s accessibility and outreach.

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Introduction

- Since its 2012 release, Stan has demonstrated novel state-of-the-art algorithms with top, cutting-edge performance for Bayesian methods and garnered over 100k users as of June 2022
- Wrappers \texttt{RStan}, \texttt{CudaStan}, and \texttt{CmdStanPy} have introduced Bayesian methods to programming communities alongside libraries of models such as \texttt{rstanarm}, \texttt{brms} and industrial packages like Facebook’s \texttt{Prophet}
- scikit-learn is a classic Python library with an elegant API and off-the-shelf models embedded in a mature ecosystem of modular operations and natural compositions
- This promising project improves Stan’s accessibility via a familiar Python style and reduces required devtime by many provided true pre-compiled Stan models as a component crucial for the Bayesian workflow

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scikit-learn API Matching

- Stan is versatile and supports several inference algorithms:
  - NUTS-HMC for sampling the posterior
  - \texttt{L-BFGS} for performing an MLE (point estimate) of model parameters
  - ADVI for variational inference of the posterior
- scikit-stan models can perform any of the above inference methods to perform the role of a scikit-learn Estimator:
  - Estimator initialization and learning are separated \cite{1} between object instantiation and \texttt{fit(Xtrain, ytrain)}
  - Extend to a predictor with \texttt{predict(Xtest)}
  - Introspect performance with \texttt{score(Xtest, ytest)}
- One-to-one matching of scikit-learn class methods and functionality - models satisfy their respective validation suites

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Example Applications

- Fits results of package Gamma GLM on 9 data points from blood clotting data \cite{4}
- Integrates with scikit-learn optimization, such as GridSearchCV
  - Performs hyperprior optimization out of the box:
    - GridSearch on \( \alpha_1 \), the intercept prior’s error scale in
      \( y = \alpha_1 + \beta x, \alpha_j \sim N(\mu_j, \sigma_j^2), \ j = 1, 2, \ldots, 8 \)
      Score with Gridsearch on Prior Intercept \( \alpha_1 \) Parameter
- Optimize over Radon household data from \cite{5} to brute force \( \mu_0 \in [0.21, 0.38] \)

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References

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\[5\] A Primer on Bayesian Multilevel Modeling using PyStan - Fonnesbeck

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