Active learning for efficiently constructing surrogate models

AA 222 | Engineering Design Optimization | Spring 2020

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Efficiently learning a surrogate model using adaptive sampling

Goal

Given an arbitrary objective function, efficiently construct a surrogate model

Approach

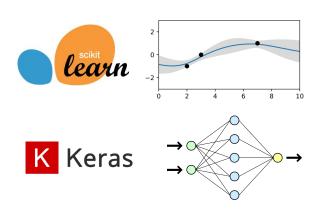
Utilize active learning (adaptive sampling) to improve sample efficiency

Consider only Gaussian process and neural network surrogates

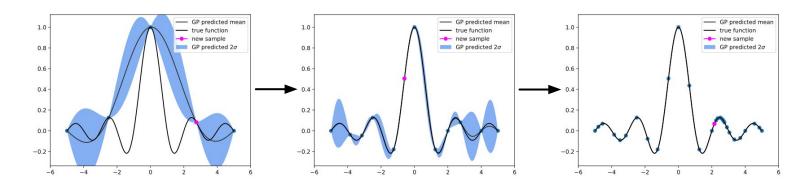
- Construct and fit GPs using scikit-learn
- Construct and fit NNs using tensorflow.keras

Select next sample based on:

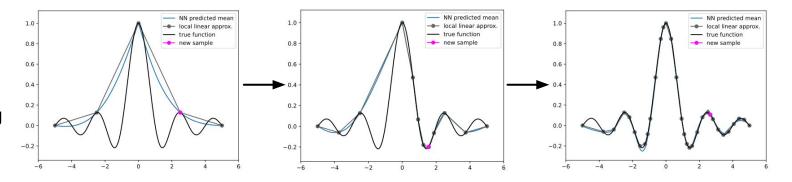
- Maximum variance estimator (GP only)
- Maximum k-fold cross-validation variance estimator
- Maximum linear approximation error using surrounding samples
- Random sampling and space-filling sequences



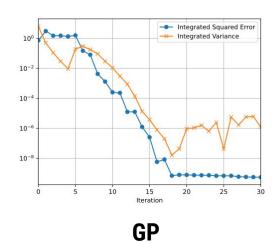




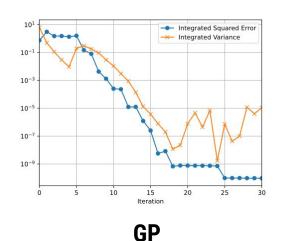
NN Local approximation error-based sampling



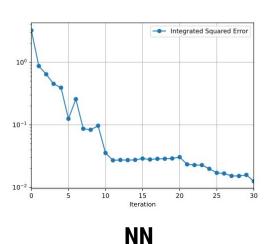
Compare model errors to examine sample efficiency



Variance-based sampling



Local approximation error-based sampling



Local approximation error-based sampling