GPdoemd: Gaussian processes for design of experiments for model discrimination

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Abstract

This document describes how to install and use the GPdoemd python package.

1 Introduction

The GPdoemd package contains functionality for performing design of experiments for model discrimination. The idea is to hybridise analytical and data-driven approaches to design of experiments to exploit useful features of both approaches, mainly computational efficiency and the ability to accommodate black-box models.

The aim has been to develop a plug-and-play python package. Our hope is that the package will be easy to extend and build upon.

GPdoemd contains functionality for testing and comparing analytical, numerical and GP surrogate methods for design of experiments for model discrimination.

GPdoemd package contains a set of analytical and non-analytical case studies. Most case studies are taken from literature, and a few have been constructed in the process of developing this package.

2 Installation

The GPdoemd package has been tested and validated on OSX and Ubuntu. No guarantees are provided that GPdoemd works on Windows-based systems.

2.1 Requirements

Python 3.4+.

Required python packages are:

- numpy >= 1.7
- scipy >= 0.17
- GPy

GPy (at the time of writing this) requires the packages six and paramz >= 0.9.0.

2.2 Creating a virtual environment

The recommendation is to install GPdoemd in a virtual environment. To set up a new virtual environment called myenv (example name), run the command

```
python3 -m venv myenv
```

in the folder where you want to store the virtual environment. After the virtual environment has been created, activate it as follows

```
source myenv/bin/activate
```

It is recommended that you update the pip installation in the virtual environment

```
pip install --upgrade pip
```

2.3 Installing `GPdoemd`

To install `GPdoemd`, first install all required packages. They are listed in the file requirements.txt. Then run the following

```
pip install git+https://github.com/cog-imperial/GPdoemd
```

This should also take care of installing the pre-required packages.

It is also possible to clone into the `GPdoemd` git repository and install it using `setup.py`, but this is not recommended for most users.

2.4 Uninstalling `GPdoemd`

The `GPdoemd` package can be uninstalled by running

```
pip uninstall GPdoemd
```

Alternatively, the folder containing the virtual environment can be deleted. This will remove the entire virtual environment in one go. There is no need to uninstall all packages in the virtual environment prior to deleting it.

If `setup.py` has been used to install `GPdoemd`, then good luck!

3 License

The `GPdoemd` package is released under the MIT License. Details can be found in the file LICENSE included in the package, as well as online.

4 Using `GPdoemd`

4.1 Creating a surrogate model

To be written.

4.2 Learning surrogate model hyperparameters

To be written.

4.3 Approximating the model parameter distribution

To be written.

4.4 Computing approximate marginal predictive distribution

To be written.

4.5 Computing design criterion

To be written.