

ModestPy

An Open-Source Python Tool for Parameter Estimation in
Functional Mock-up Units

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Introduction

Background

- Functional Mock-up Interface (FMI) is becoming a *de facto* standard co-simulation interface, already supported by over 100 simulation tools
- **FMI offers flexibility** in terms of modeling environments
- **FMI attracts generic tools** for co-simulation, system identification, and optimization
- There are several tools for **parameter estimation** in Functional Mock-up Units (FMUs), but most of them are tied to at least one of the following:
 - Specific optimization algorithms
 - Specific proprietary platforms
 - Large software environments

Objective

The objective was to develop a tool for parameter estimation in FMUs that would:

- be lightweight,
- support multiple optimization methods,
- support chaining of global and local methods,
- be easily deployable.

Software Description

Architecture

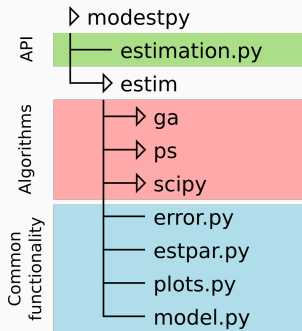


Figure 1: Package structure.

Dependencies:

`pyfmi`, `numpy`, `scipy`,
`pandas`, `matplotlib`

Available algorithms:

- Genetic Algorithm (GA)
- Generalized Pattern Search (GPS)
- SciPy:
 - Sequential Least Squares Programming (SLSQP)
 - Limited Memory Broyden-Fletcher-Goldfarb-Shanno with box constraints (L-BFGS-B)
 - Truncated Newton Method (TNC)

Error Metrics

Currently, two type of error metrics are implemented, the total mean-square error (MSE_{tot}) and the total normalized mean-square error ($NMSE_{tot}$). $NMSE_{tot}$ is suggested for multi-output models.

$$MSE_{tot} = \sum_i \frac{\sum_{t=1}^N (\hat{Y}_i^t - Y_i^t)^2}{N}$$
$$NMSE_{tot} = \sum_i \frac{MSE_i}{\bar{Y}_i^2}$$

where \hat{Y}_i^t is the measured value of variable i at time step t , Y_i^t is the simulated value of variable i at time step t , \bar{Y}_i is the mean measured value of variable i , N is the number of time steps, and MSE_i is the mean-square error for variable i .

Through conda (recommended):

```
conda config --add channels conda-forge  
conda install modestpy
```

Through pip:

```
python -m pip install modestpy
```

Installation through pip requires `pyfmi` to be installed separately.


```
from modestpy import Estimation

session = Estimation(workdir, fmu_path,
                    inputs, known_parameters,
                    estimated_parameters, measurements,
                    method=('GA', 'GPS'),
                    ga_opts={'maxiter': 5, 'tol': 1e-4},
                    gps_opts={'maxiter': 500, 'tol': 1e-6},
                    ftype='MSE')

estimates = session.estimate()
err, res = session.validate()
```

Example

Test Case: Thermal Zone Gray-Box Model

- Gray-box model is calibrated to mimic the dynamics of a white-box model implemented in **EnergyPlus**
- Model outputs used in the cost function: T, CO₂, verate, qrad
- Error metric: $NMSE_{tot}$

T – indoor temperature [°C], CO₂ – indoor CO₂ [ppm], verate – ventilation airflow rate [m³s⁻¹],
qrad – radiator heating rate [W]

Gray-Box Model

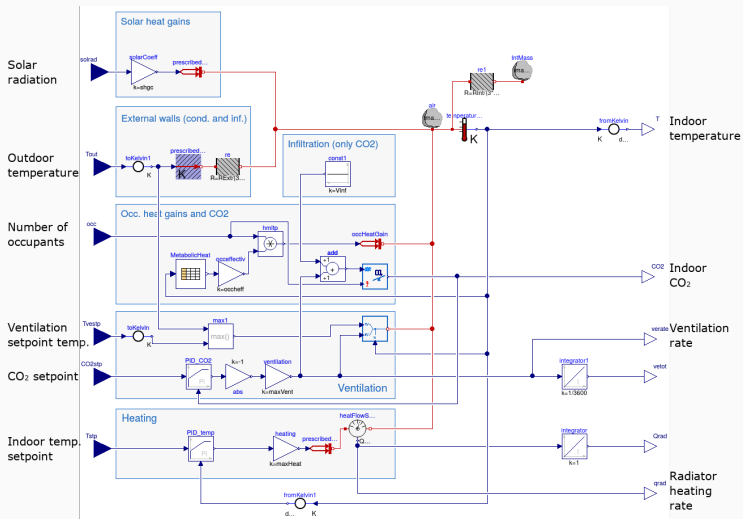


Figure 2: Gray-box zone model developed in Modelica (using Dymola).

Estimation Setup

Table 1: Setup of model parameters

| Parameter | Initial guess* | Lower bound | Upper bound |
|-----------|----------------|-------------|-------------|
| shgc | 5 | 0.1 | 10 |
| tmass | 50 | 1 | 100 |
| imass | 50 | 1 | 100 |
| RExt | 5 | 0.1 | 10 |
| RInt | 5 | 0.1 | 10 |
| Vinf | 5 | 0.1 | 10 |
| maxVent | 5 | 0.1 | 10 |

* Not used by GA

shgc – solar heat gain coefficient [-], tmass – indoor air thermal mass [$\text{JK}^{-1}\text{m}^{-3}$],
imass – internal thermal mass [$\text{JK}^{-1}\text{m}^{-2}$], RExt – external wall resistance [m^2WK^{-1}],
RInt – internal wall resistance [m^2WK^{-1}], Vinf – infiltration air change rate [h^{-1}],
maxVent – max. ventilation air change rate [h^{-1}]

Results

Table 2: CPU time and $NMSE_{tot}$ for validation and training, sorted in ascending order by validation error

| Method | Training $NMSE_{tot}$ | Validation $NMSE_{tot}$ | CPU Time [s] |
|-------------|--------------------------|----------------------------|-----------------|
| GA+SLSQP | 0.377 | 0.353 | 920 |
| GA+GPS | 0.351 | 0.371 | 1319 |
| GA+TNC | 0.393 | 0.372 | 801 |
| GA | 0.394 | 0.373 | 723 |
| GA+L-BFGS-B | 0.349 | 0.379 | 934 |
| GPS | 1.306 | 3.428 | 986 |
| TNC | 4.967 | 5.856 | 101 |
| L-BFGS-B | 4.929 | 6.808 | 38 |
| SLSQP | 5.040 | 6.920 | 12 |

Results

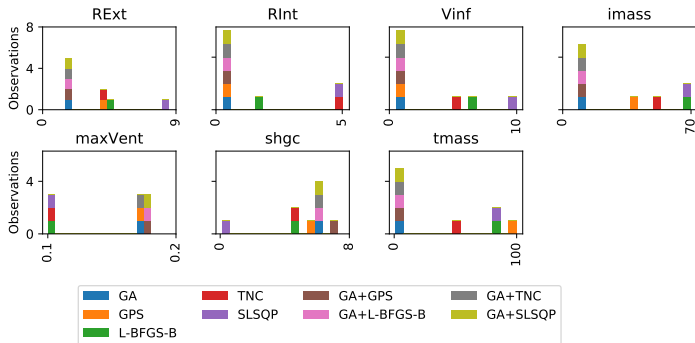


Figure 3: Histogram of estimates yielded by the 9 method sequences.

Results

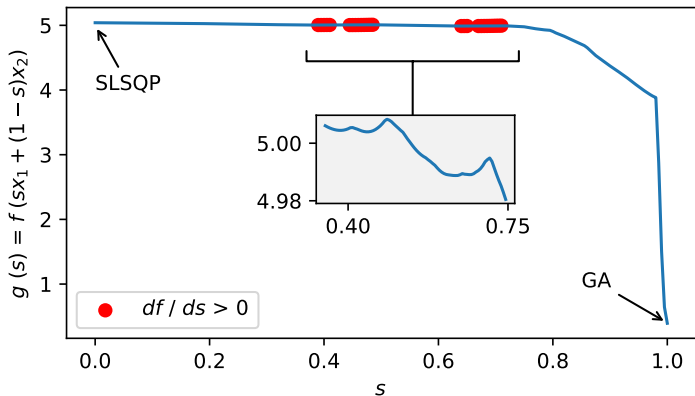


Figure 4: Cost function evaluated on the training data based on linear combinations of parameters yielded by GA (x_1) and SLSQP (x_2). Sections with positive derivatives with respect to s marked in red.

Results

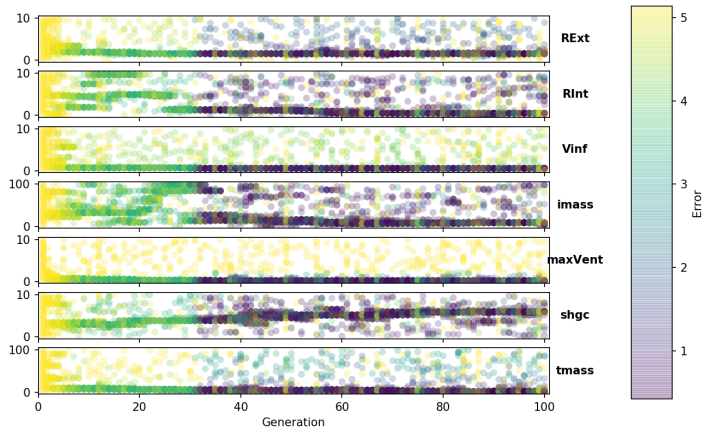


Figure 5: Parameter evolution in the genetic algorithm – color represents the training error (darker more accurate).

Results

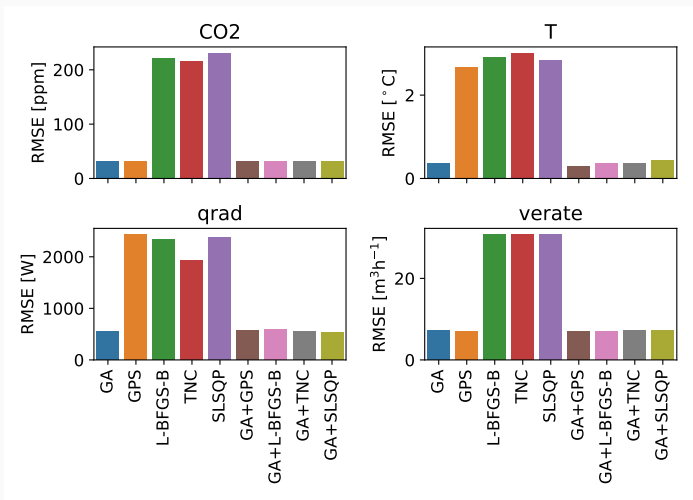


Figure 6: Validation root-mean-square error (RMSE) per output variable.

Results

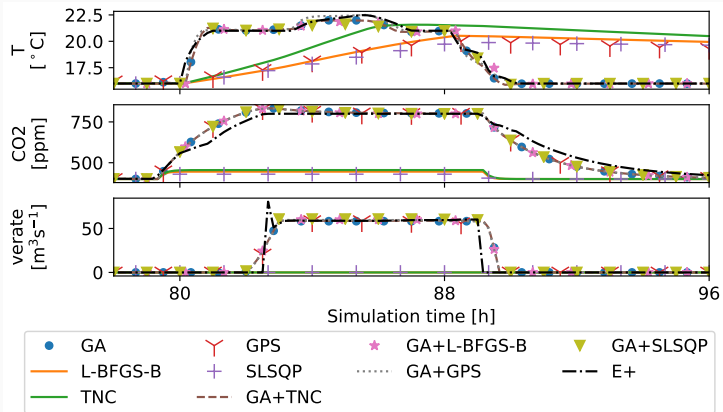


Figure 7: Validation results: temperature (T), CO₂ (CO₂), ventilation airflow rate (verate).

Results

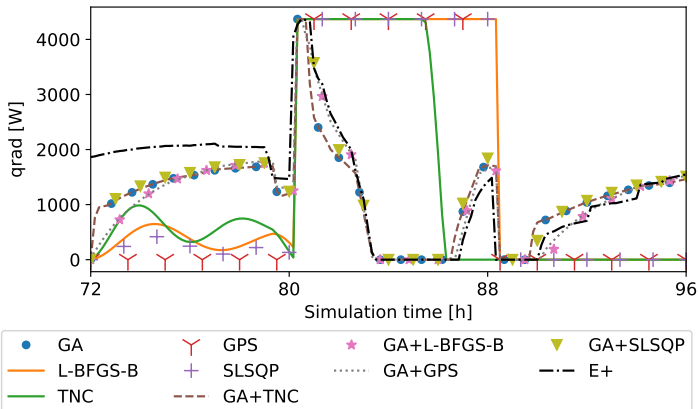


Figure 8: Validation results: radiator heating rate (q_{rad}).

Conclusions and Future Work

Conclusions

- The in-house algorithms (GA, GPS) were validated.
- Using GA for a preliminary global search significantly improved the model accuracy in the test case.¹
- The current functionality of the tool is already sufficient for a general use. It is used by the authors for calibrating gray-box models of buildings and HVAC systems for the use in MPC.

¹It should be noted, that the initial global search would not be needed if the approximate initial values of parameters were known. In such a case the gradient-based methods would easily outperform GA. Another solution could be to run gradient-based methods with multiple initial guesses.

The development work continues and there are plans to include the following functionality:

- a simple graphical user interface to attract users less experienced in the Python programming language,
- support for on-line estimation methods (e.g. Kalman filter),
- support for multi-period stochastic gradient descent training,
- support for parallel processing methods.

Project repository:

<https://github.com/sdu-cfei/modest-py>