UQ-PyL User Manual (Version 1.1)

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1 Introduction

1.1 A Quick Start

UQ-PyL (**U**ncertainty **Q**uantification **Py**thon **L**aboratory) is a software platform for performing various uncertainty quantification (UQ) activities such as Design of Experiments (DoE), Statistical Analysis, Sensitivity Analysis (SA), Surrogate Modeling and Parameter Optimization. This document describes how to set up problems and use these UQ methods to solve them through UQ-PyL. The mathematics of those UQ methods can be found in the separate theory manual.

We request that you cite the following paper when you report the results obtained by using the UQ-PyL software platform:

C. Wang, Q. Duan, Charles H. Tong, (2015), UQ-PyL – A GUI platform for uncertainty quantification of complex models. Under review for Environmental Modeling & Software.

1.2 Available UQ-PyL Capabilities

1.2.1 Design of Experiment

Full-Factorial design, Fractional-Factorial design, Plackett-Burman design, Box-Behnken design, Central-Composite design, Monte Carlo design, Latin Hypercube design (random, center, maxmin, center maxmin, correlate), Symmetric Latin Hypercube design, Improved Distributed Hypercube design, Sobol' sequence, Halton sequence, Faure sequence, Hammersley sequence, Good Lattice Point.

1.2.2 Statistical Analysis

Statistical moments, Confidence interval, Hypothesis test.

1.2.3 Sensitivity Analysis

Morris One at A Time (MOAT), Derivative-based Global Sensitivity Measure (DGSM), Sobol' Sensitivity Analysis, Fourier Amplitude Sensitivity Test (FAST), Metamodel-based Sobol', Correlation analysis, Delta Moment-Independent Measure (Delta), Multivariate Adaptive Regression Splines (MARS) based sensitivity analysis.

1.2.4 Surrogate Modeling

Generalized Linear Model (Ordinary Least Squares, Ridge Regression, Lasso, Least Angle Regression, LARS Lasso, Bayesian Regression, and Elastic Net), Regression

Tree, Random Forest, Nearest Neighbors, Support Vector Machine, Gaussian Process, MARS, Stochastic Gradient Descent.

1.2.5 Parameter Optimization

Shuffled Complex Evolution (SCE), Dynamically Dimensional Search (DDS), Adaptive Surrogate Modeling based Optimization (ASMO), Particle Swarm Optimization (PSO), Simulated Annealing (SA), and Monte Carlo Markov Chain (MCMC).

1.3 Overview about functionality of the UQ-PyL package

```
__init__.py
DoE/
    __init__.py              # Ensure all needed files are loaded
    __main__.py              # For GUI uses
    box_behnken.py           # Box-behnken design
    central_composite.py     # Central-composite design
    fast_sampler.py          # FAST sensitivity analysis design
    faure.py                 # Faure design
    ff2n.py                  # Factorial design
    finite_diff.py           # DGSM sensitivity analysis design
    frac_fact.py             # Factorial design
    full_fact.py             # Full Factorial design
    GLP.py                   # Good Lattic Point design
    halton.py                # Halton Quasi-Monte Carlo design
    hammersley.py            # Hammersley Quasi-Monte Carlo design
    lhs.py                   # Latin Hypercube design
    monte_carlo.py           # Monte Carlo design
    morris_oat.py            # Morris One at A Time design
    plackett_burman.py       # Plackett Burman design
    saltelli.py              # Sobol' sensitivity analysis design
    sobol.py                 # Sobol' Quasi-Monte Carlo design
    symmetric_LH.py          # Symmetric Latin Hypercube design
analysis/
    __init__.py              # Ensure all needed files are loaded
    __main__.py              # For GUI uses
    confidence.py            # Confidence Interval
    correlations.py          # Correlation analysis
    delta.py                 # Delta sensitivity analysis
    dgsm.py                  # DGSM sensitivity analysis
    extended_fast.py         # FAST sensitivity analysis
    hypothesis.py            # Hypothesis Test
```

```
    moments.py              # Statistics moments method
    morris.py               # MOAT sensitivity analysis
    sobol_analyze.py        # Sobol' sensitivity analysis
    sobol_svm.py            # Metamodel based sobol' sensitivity analysis
RSmodel/
    __init__.py             # Ensure all needed files are loaded
    __main__.py             # For GUI uses
    BayesianRidge.py        # GLP-Bayesian Ridge regression
    DT.py                   # Decision Tree regression
    ElasticNet.py           # GLP-Elastic Net regression
    gp.py                   # Gaussian Process regression
    kNN.py                  # k-nearest neighbor regression
    LAR.py                  # GLP-LAR regression
    Lars.py                 # GLP-Lars regression
    Lasso.py                # GLP-Lasso regression
    MARS.py                 # MARS regression
    OrdinaryLeastSquares.py    # GLP-Ordinary Least Squares regression
    RF.py                   # Random Forest regression
    Ridge.py                # GLP-Ridge regression
    SGD.py                  # Stochastic Gradient Descent regression
    SVR.py                  # Support Vector Machine regression
optimization/
    __init__.py             # Ensure all needed files are loaded
    __main__.py             # For GUI uses
    ASMO.py                 # ASMO optimization
    DDS.py                  # DDS optimization
    MCMC.py                 # Monte Carlo Markov Chain optimization
    PSO.py                  # Particle Swarm Optimization
    SA.py                   # Simulated Annealing optimization
    SCE.py                  # Shuffled Complex Evolution optimization
util/
    __init__.py             # Ensure all needed files are loaded
    discrepancy.py          # Compute discrepancy of design
    spyderlib/              # Spyder package
    spyderplugins/          # Spyder package
```

2 Installation

2.1 Dependencies

UQ-PyL is an open-source package written in Python language. It runs on all major platforms (Windows, Linux, MacOS). It requires some pre-installed standard Python packages:

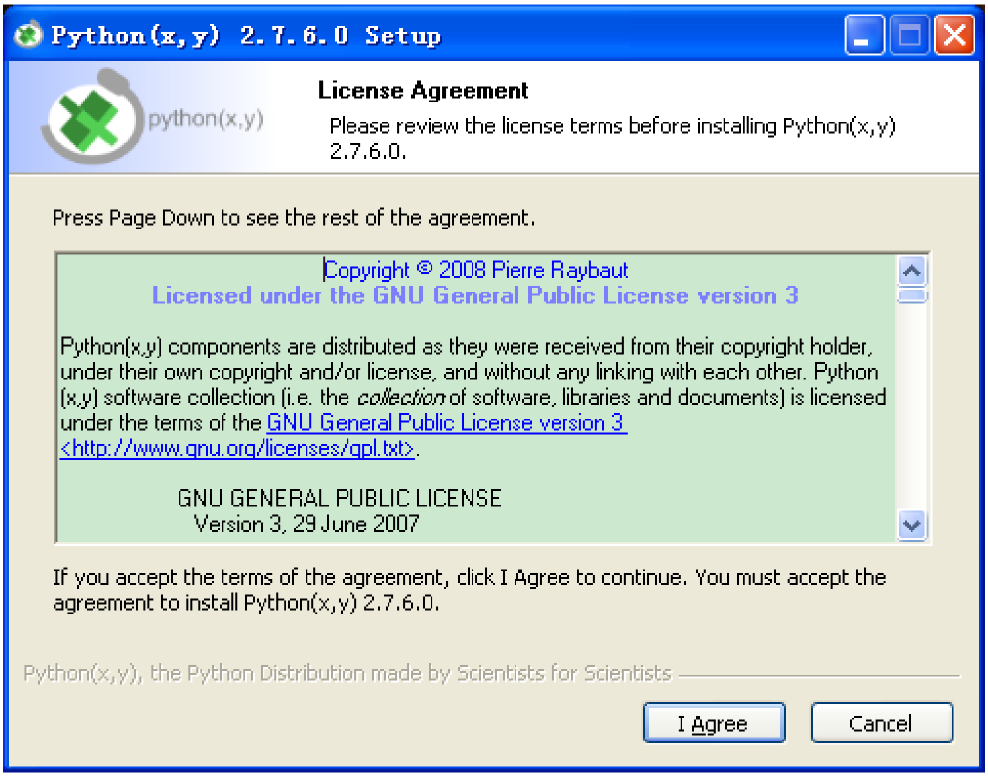
- Python version >= 2.7.6
- Numpy >= 1.7.1
- Scipy >= 0.16.0
- Matplotlib >= 1.4.3
- PyQt4 (If you use graphic user interface)
- Scikit-learn = 0.14.1

2.2 Detailed Installation

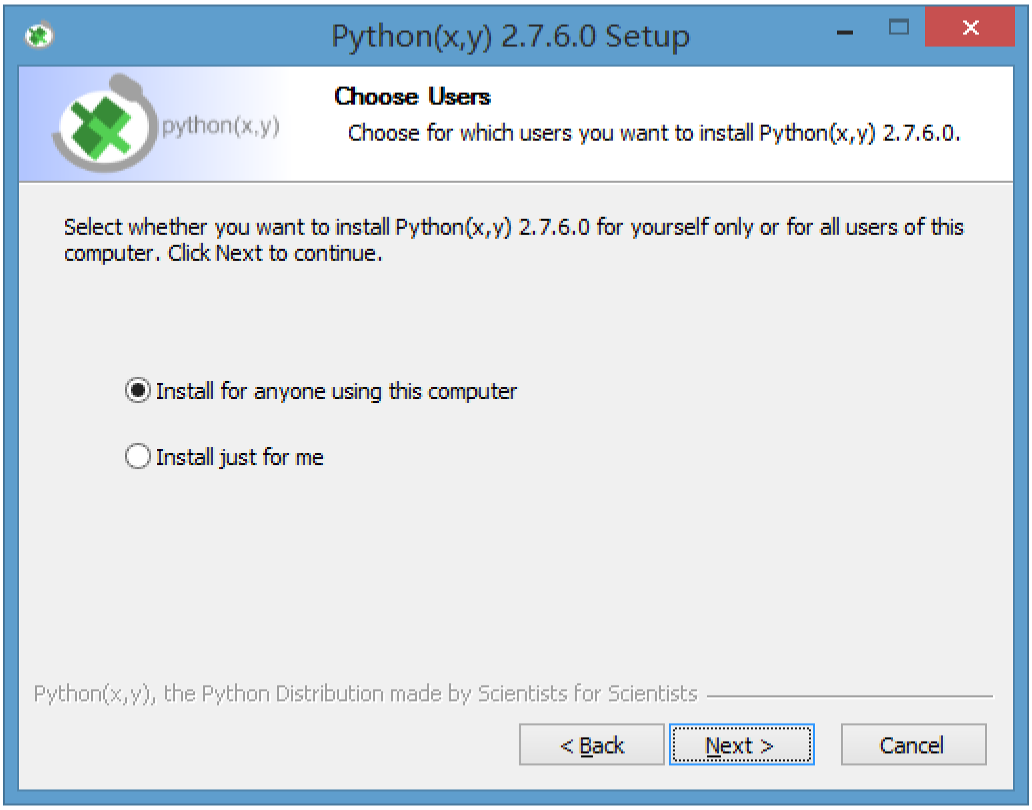
2.2.1 Windows platform

For Windows platform, there is a software integrate Python and some common packages called Python(xy). It contains all the packages UQ-PyL needed. You can just install Python(xy) and UQ-PyL to run UQ analysis.

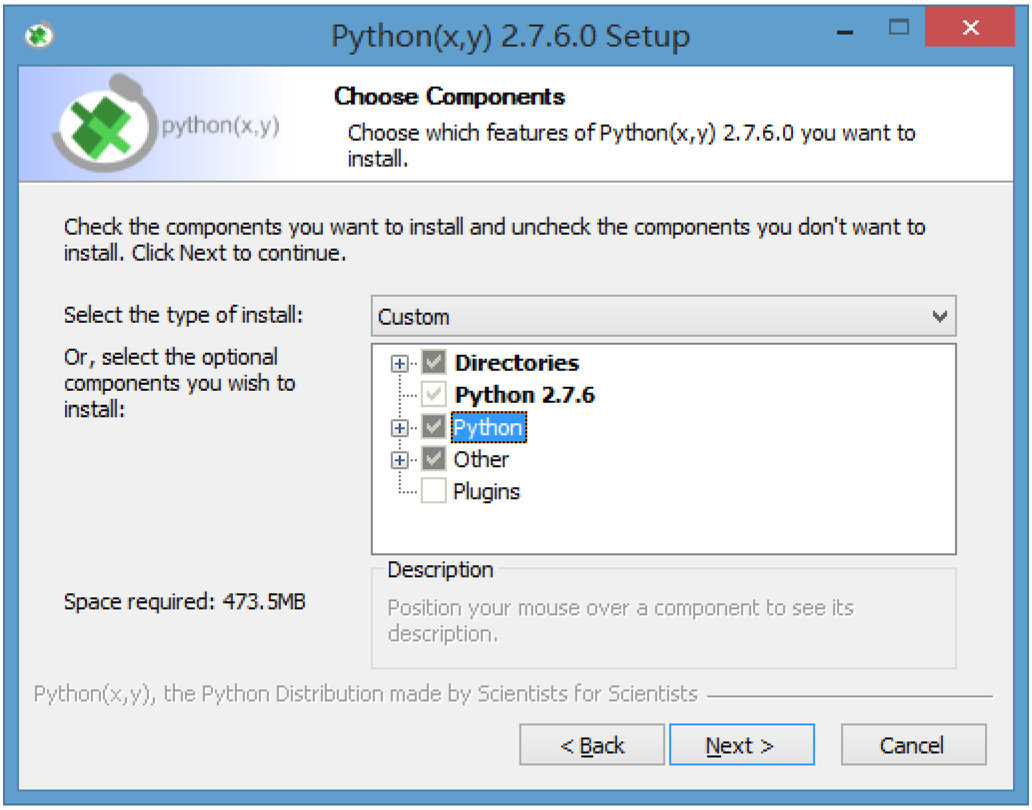
Step 1. Install Python(xy) software.
You can download “Python(xy)” from our website. Double click the Installation file to start installation.



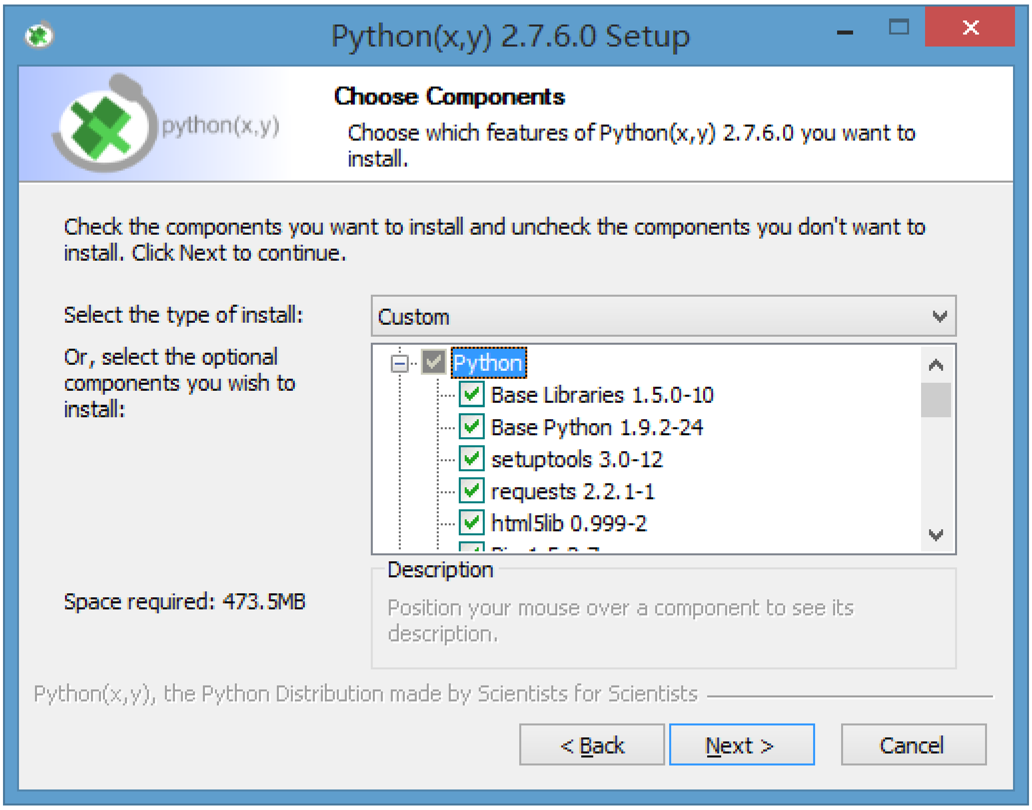
Click “I Agree” to continue.



Click “Next” to continue.



Choose "Custom" type to install.

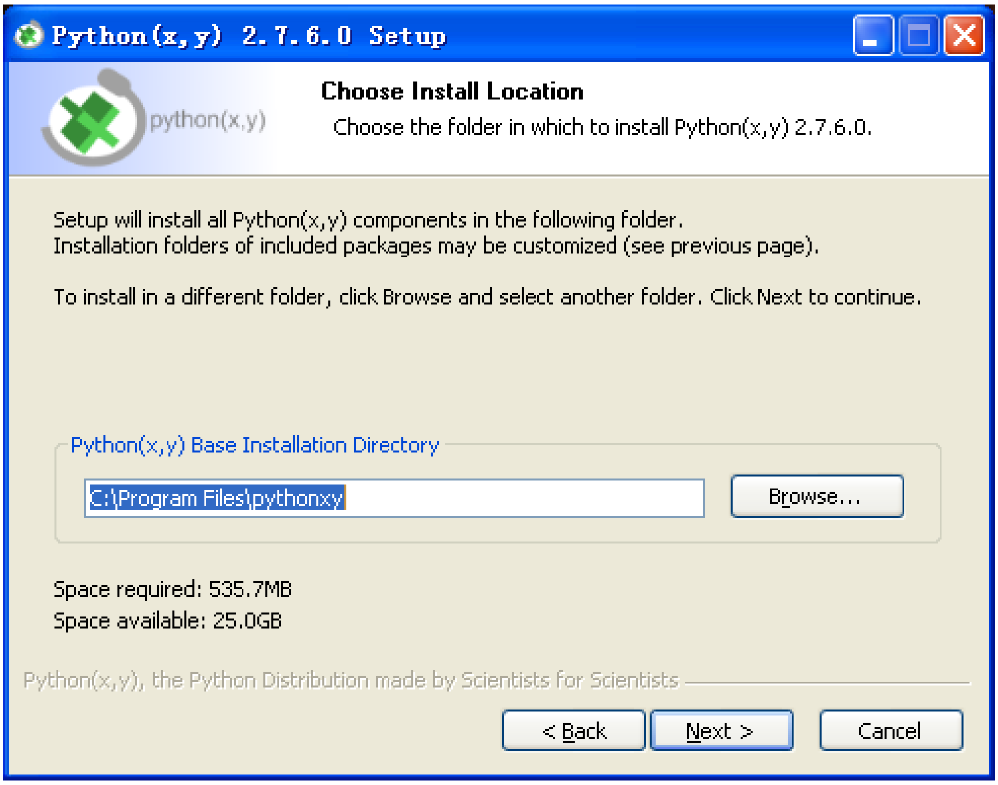


For "Python" option, you must check all the package UQ-PyL needed.
"

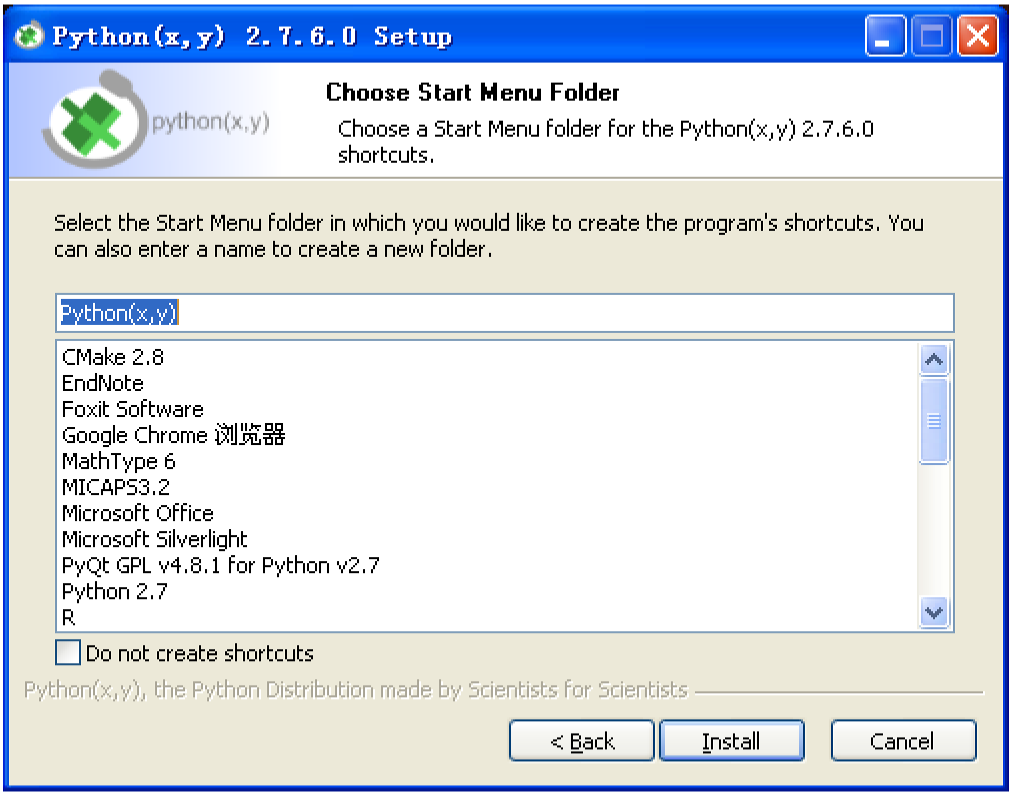
PyQt 4.9.6-4

NumPy 1.8.0-5
Scipy 0.13.3-6
Matplotlib 1.3.1-4
Scikit-learn 0.14.1-4 **(Please note: this one is not checked by default)**
"

Click "Next" to continue.



Click "Next" to continue.

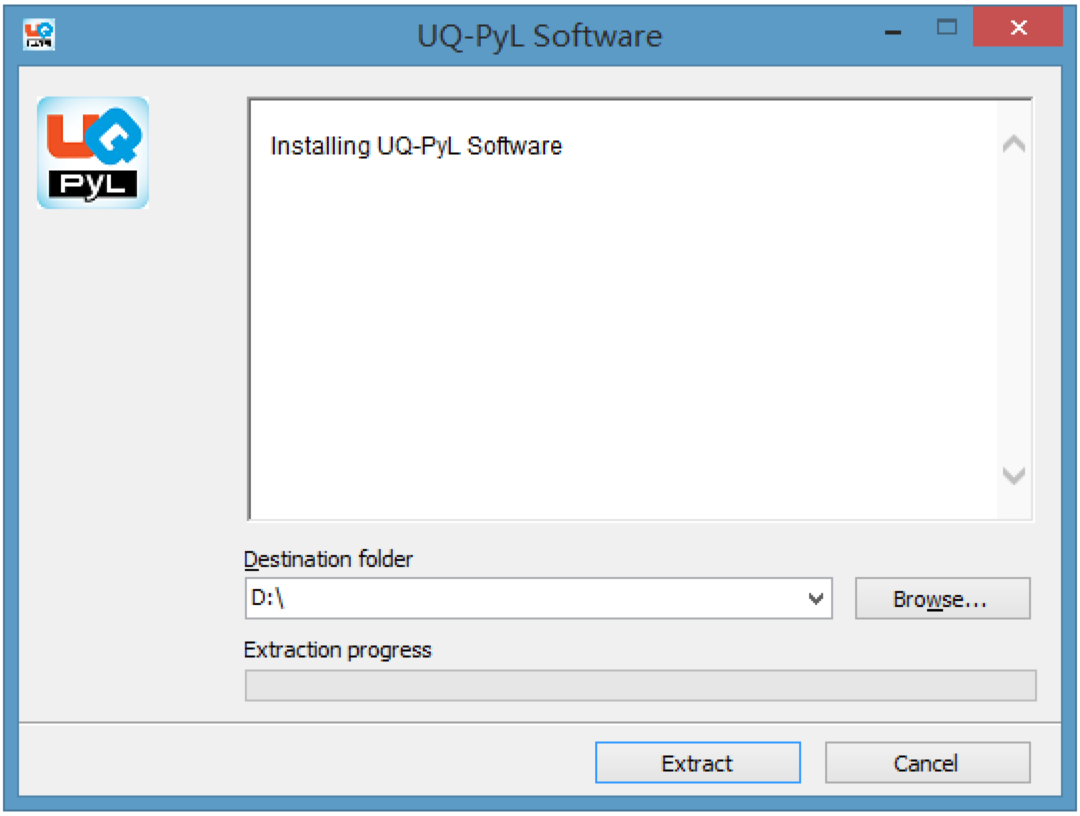


Click “Install”, then waiting for the installation process.

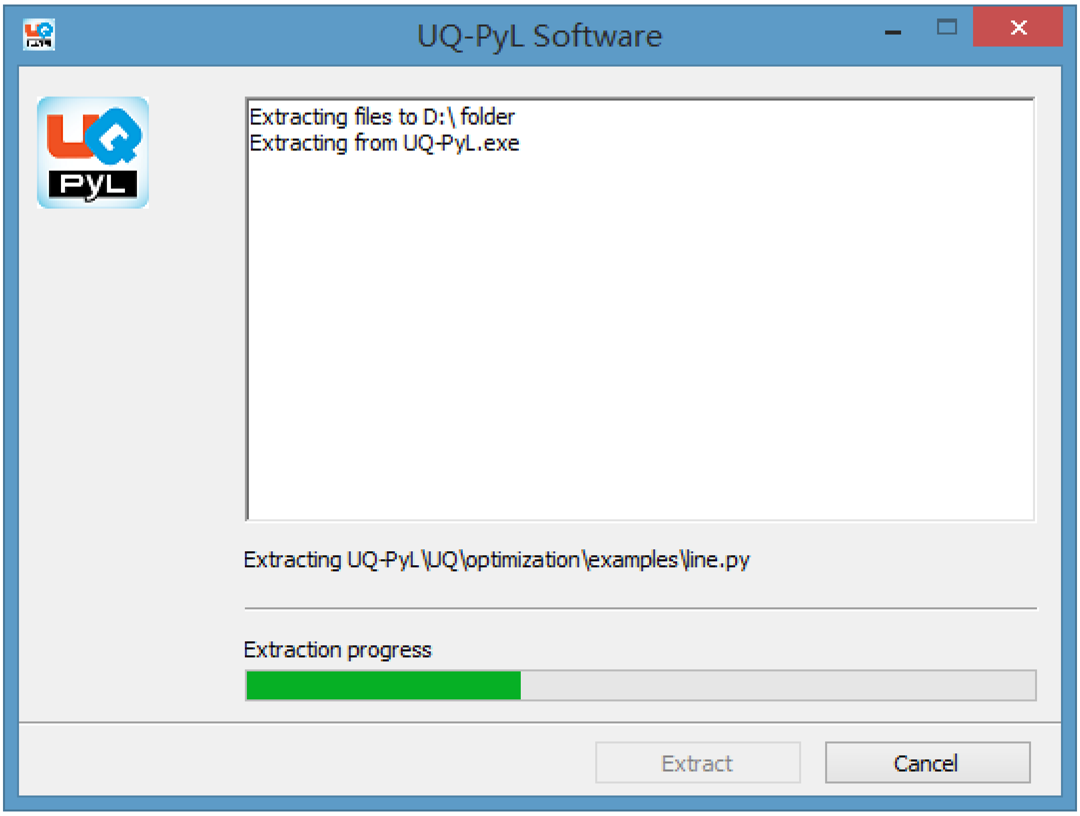
After installation, you executable python.exe file will be C:\Python27\python.exe. All the package will be in the C:\Python27\Lib\site-packages directory.

Step 2. Install UQ-PyL software

Please download UQ-PyL Windows version, double click to run the installation file.

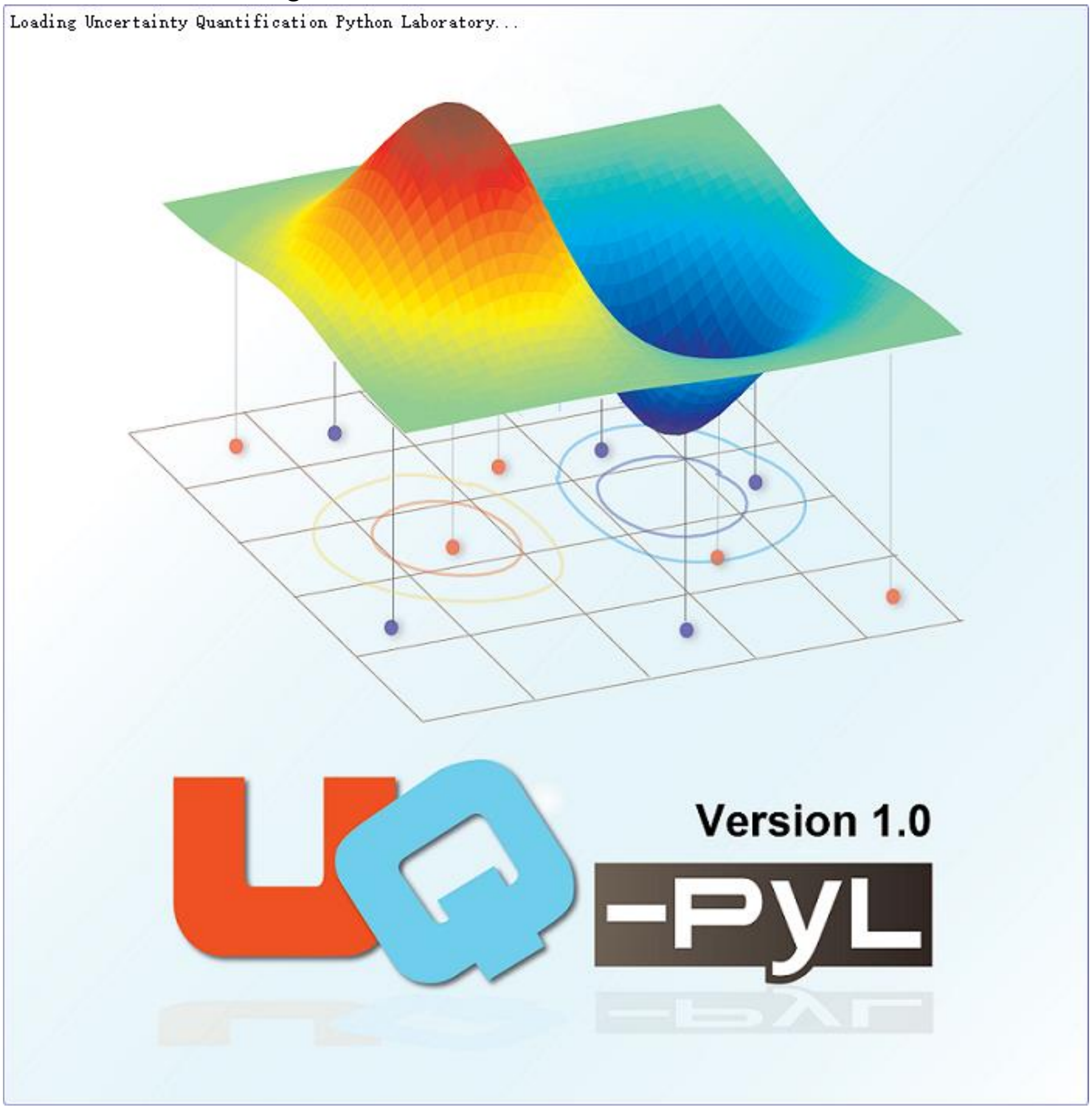


Choose the default directory D:\ or your own path, then click "unzip" to continue.

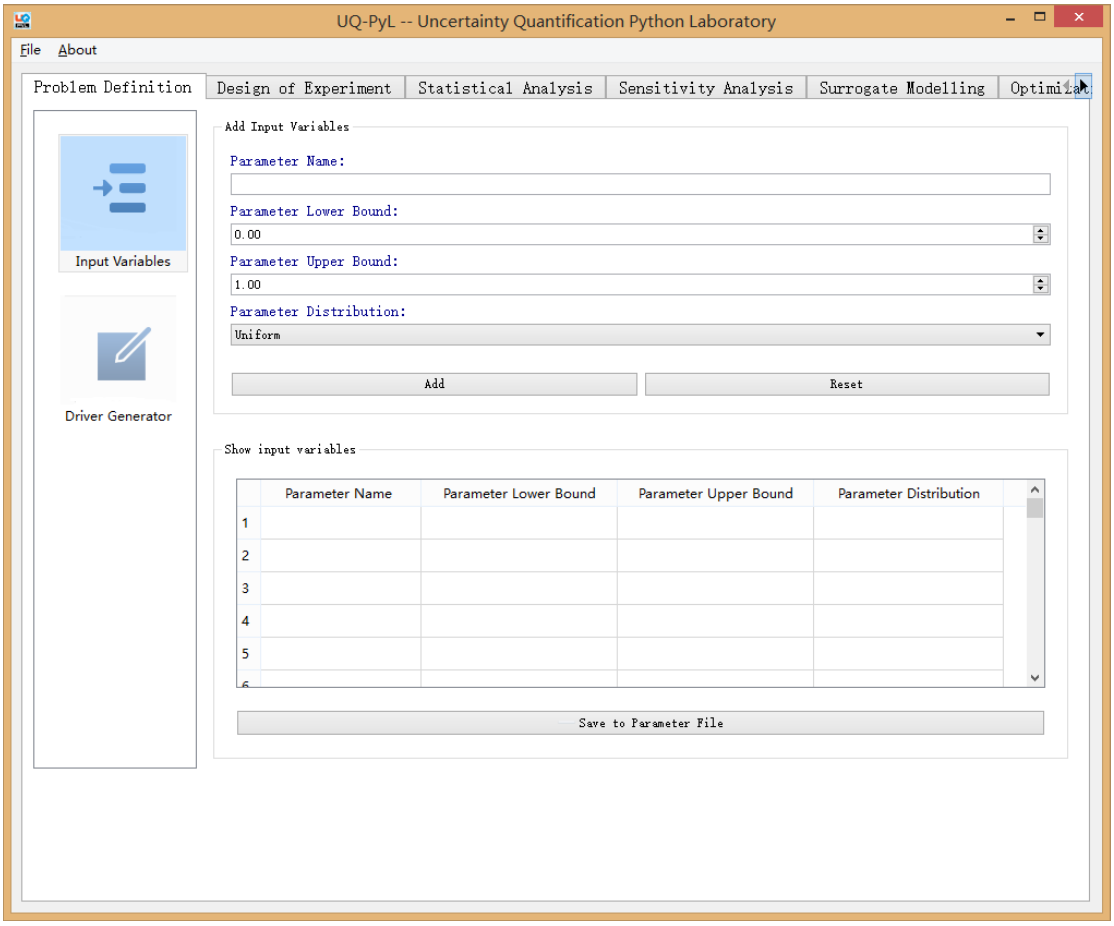


After unzip, there will be two shortcut on the desktop, one is refer to UQ-PyL software main page, the other is refer to interactive version of UQ-PyL software. Double click the shortcuts can start the UQ-PyL software. If the shortcut doesn't work, please go to your install path, double click the “main.pyw” file or “main_interactive.pyw” file to start these.

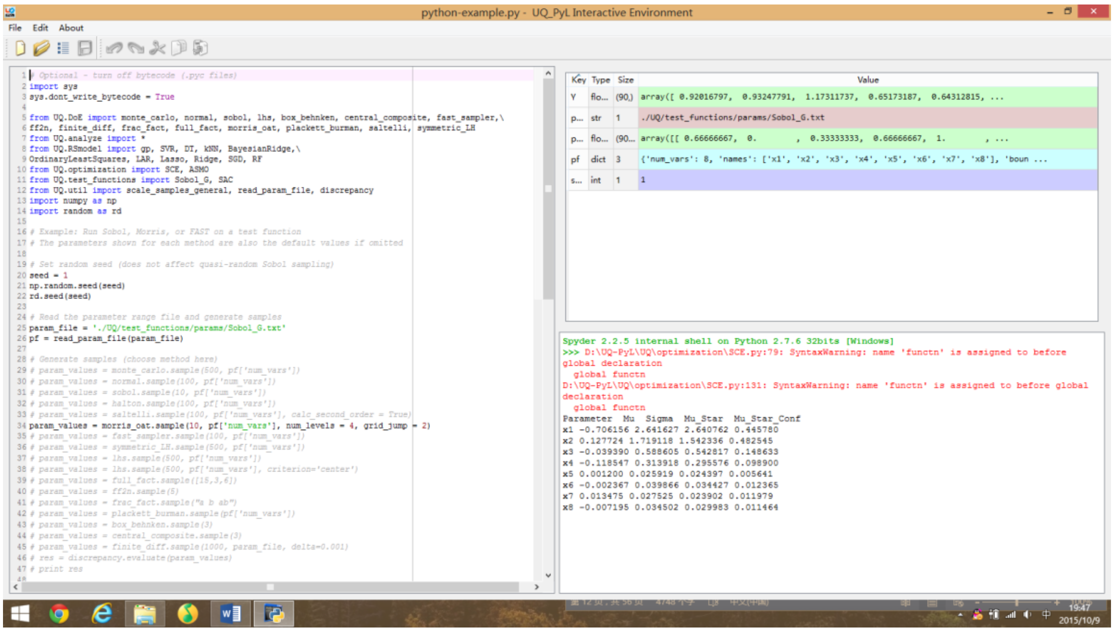
In UQ-PyL main page, you can do uncertainty quantification analysis through pull-down menus. In interactive version of UQ-PyL software, you can write python script to run uncertainty quantification analysis and can see output results and internal variables’ values through the software’s interface.



UQ-PyL Splash Page



UQ-PyL Software Main Page



Interactive UQ-PyL Software

2.2.2 Linux platform

Canopy is a globally recommended Python distribution. It contains Python and 100+ common built-it packages. It also contains all the package UQ-PyL used in one software. So you can install Canopy for all the dependences UQ-PyL needed. Please go to the official website (https://www.enthought.com/products/canopy/) for more information.

Step 1. Install Canopy software.
Canopy is a commercial software. However, it provide free use for academic usage. If you use Canopy for education or academic, you can download canopy-1.5.5-full-rh5-64.sh from our website or from Canopy official website. After downloading, you should install Canopy by steps below:

chmod 755 canopy-1.5.5-full-rh5-64.sh
./canopy-1.5.5-full-rh5-64.sh

```
Welcome to the Canopy 1.5.5 installer!

To continue the installation, you must review and approve the license term
agreement.
Press Enter to continue
>>>
```

If you approve the license term, press Enter to continue

```
====================   ========================================
Canopy Product         License
Express                Canopy Express Software License Agreement
Basic & Professional   Canopy Subscription License Agreement
Academic               Canopy Software License for Academic Use
====================   ========================================

Please review your applicable license carefully.
By installing or using a Canopy product you
signify  your assent to and acceptance of the
terms of the  applicable license to Canopy.  If
you do not accept the terms of the applicable
license, then you must  not use the Canopy
products.  Should you have any  questions
regarding licensing, please contact us at
support@enthought.com.

ENTHOUGHT CANOPY EXPRESS

Software License Agreement

This Enthought Canopy Express Software License
Agreement (the ? . greement? .  is between Enthought,
Inc., a Delaware corporation (? . nthought? . , and
the licensee subscriber who accepts the terms of
this Agreement (the ? . ustomer? . .  The effective

Do you approve the license terms? [yes|no]
[no] >>> yes
```

Type “yes” then press Enter to continue.

```
Canopy will be installed to this location:
/home/quanjp/Canopy

  * Press Enter to accept this location
  * Press CTRL-C to abort
  * or specify an alternate location.  Please ensure that your location
    contains only ASCII letters, numbers, and the following punctuation
    chars: '.', '_', '-'

[/home/quanjp/Canopy] >>> /home/quanjp/swgfs/software/Canopy
```

Type the path you want to install Canopy, then press Enter to continue.

```
Installing to /home/quanjp/swgfs/software/Canopy ... please wait
Must specify the vendor namespace for these files with --vendor
No directories in update-desktop-database search path could be processed and updated.
***
* Updating MIME database in /home/quanjp/.local/share/mime...
Wrote 2 strings at 20 - 44
Wrote aliases at 44 - 48
Wrote parents at 48 - 4c
Wrote literal globs at 4c - 50
Wrote suffix globs at 50 - 108
Wrote full globs at 108 - 10c
Wrote magic at 10c - 118
Wrote namespace list at 118 - 11c
***
done.

    You can run the Canopy graphical environment by running the script:

        /home/quanjp/swgfs/software/Canopy/canopy

    or by selecting 'Canopy' in your Applications menu.

    On your first run, your Canopy User Python environment will be initialized,
    and you will have the opportunity to make Canopy be your default Python
    at the command line. Details at support.enthought.com/forums

    Thank you for installing Canopy!
```

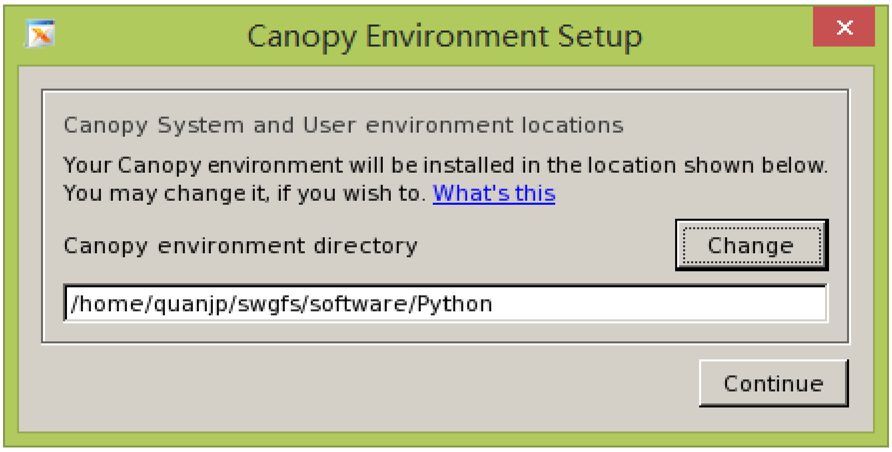
Complete to install Canopy.

Step 2: Setting up Canopy environment

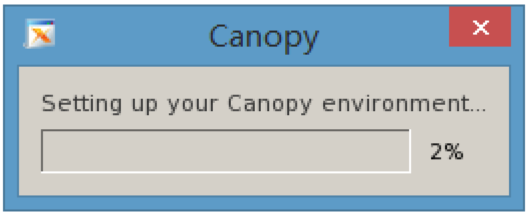
Enter into the Canopy directory, for me is "/home/quanjp/swgfs/software/Canopy", you can see the file inside it.

```
[quanjp@login02 Canopy]$ ll
total 336
drwxrwxr-x 3 quanjp quanjp 32768 Jul  4 07:23 appdata
drwxrwxr-x 2 quanjp quanjp 32768 Jul  4 07:23 bin
-rw-rw-r-- 1 quanjp quanjp 27157 Jul  4 06:41 __boot__.py
-rwxr-xr-x 1 quanjp quanjp    92 Jul  4 06:41 canopy
-rwxr-xr-x 1 quanjp quanjp    92 Jul  4 06:41 canopy_cli
-rwxrwxr-x 1 quanjp quanjp   401 Jul 31 14:06 canopy.desktop
-rw-rw-r-- 1 quanjp quanjp   394 Jul 31 14:06 canopy-mime.xml
-rw-rw-r-- 1 quanjp quanjp  9704 Jul  4 06:42 canopy.png
drwxrwxr-x 2 quanjp quanjp 32768 Jul  4 07:23 EXTRA-REPO
drwxrwxr-x 3 quanjp quanjp 32768 Jul  4 07:23 lib
```

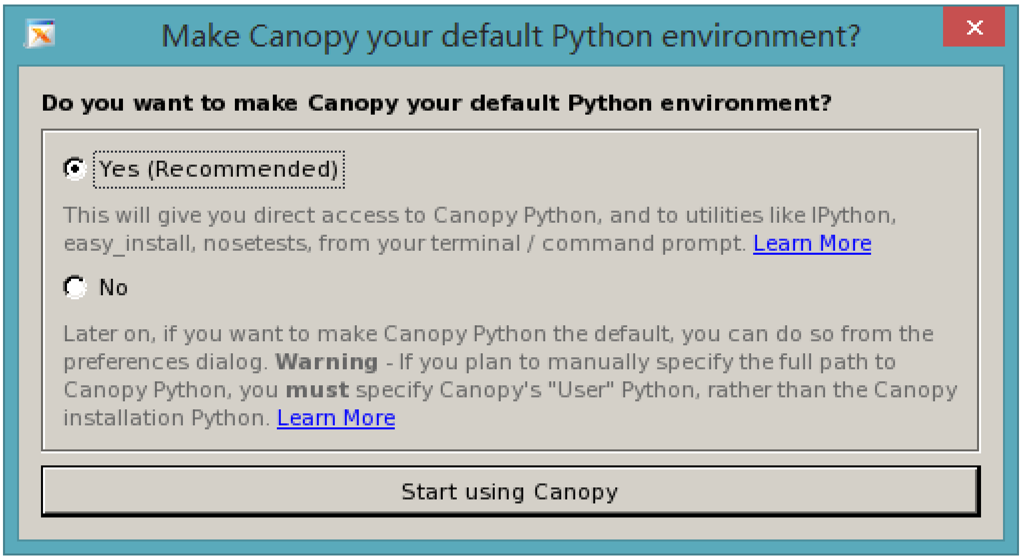
Run "./canopy" to setting up Canopy software



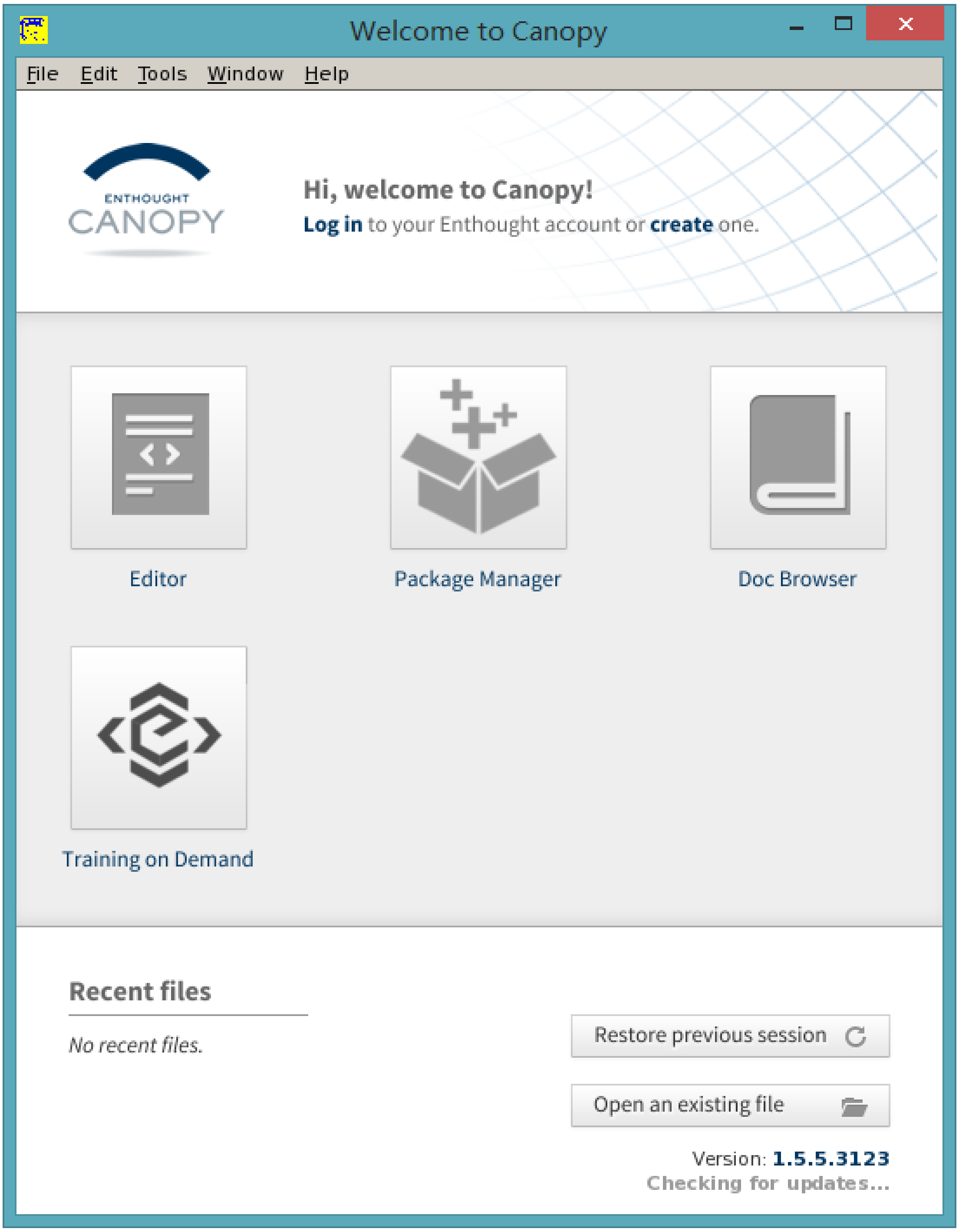
Enter the Canopy environment directory, for me is "/home/quanjp/swgfs/software/Python", click "Continue" to continue. Your python installation will in this directory.



After that, a dialogue will display,



Choose "Yes", then click "Start using Canopy".



In "Package Manager" section, you can check what packages in your Python library now.

Actually, you can check your python installation in your python installation path. All files are in "*YourPythonPath*/User/" (for me is /home/quanjp/swgfs/software/Python/User/). The python executable file is in "YourPythonPath/User/bin/" and all the packages are installed in "YourPythonPath/User/lib/python2.7/site-packages/".

Step 3: Test your Python installation

If you have multiple python environment, please specific one. Usually, modify

your .bashrc file can do it.
Add two sentence into your .bashrc file:

export PYTHON=/home/quanjp/swgfs/software/Python/User/bin
export PATH=$PATH:$PYTHON:

Then enter command “source .bashrc” to make your .bashrc file renew.

Type “python” or “python2.7” command, if you can see “Enthought Canopy Python” that means you already accomplished the installation.

```
Enthought Canopy Python 2.7.9 | 64-bit | (default, Jun 30 2015, 22:40:22)
[GCC 4.1.2 20080704 (Red Hat 4.1.2-55)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> 
```

You can check if all the packages UQ-PyL needed are already installed. Using “import” command, if no error messages that means you already have all the packages.

```
Enthought Canopy Python 2.7.9 | 64-bit | (default, Jun 30 2015, 22:40:22)
[GCC 4.1.2 20080704 (Red Hat 4.1.2-55)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy
>>> numpy.__version__
'1.9.2'
>>> import scipy
>>> scipy.__version__
'0.15.1'
>>> import matplotlib
>>> matplotlib.__version__
'1.4.3'
>>> import sklearn
>>> sklearn.__version__
'0.16.1'
>>> import PyQt4
>>> 
```

Step 4. Install UQ-PyL software
Download UQ-PyL Linux version, unzip the source code using command

tar –zxvf UQ-PyL_Linux.tar.gz

Then enter into the UQ-PyL directory

cd UQ-PyL_Linux

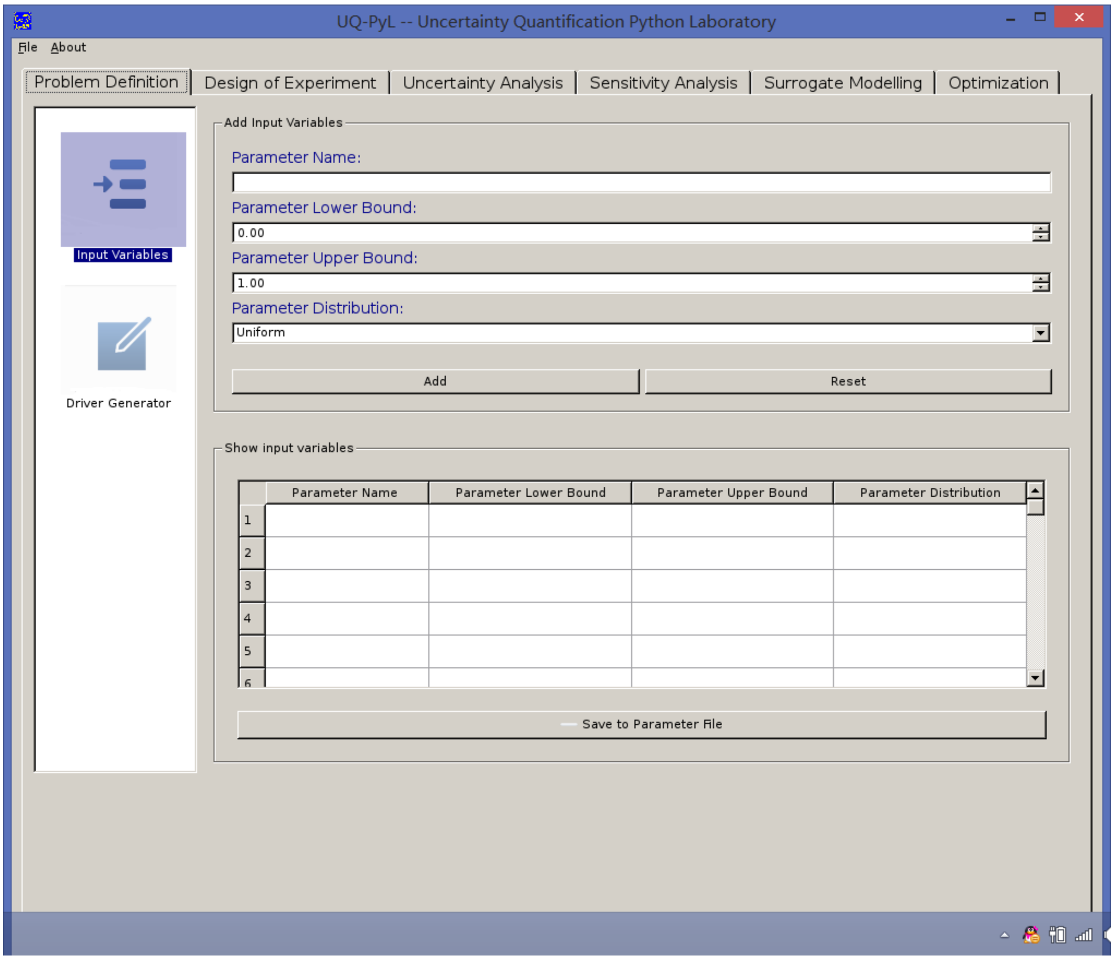
Enter command to run UQ-PyL main page

python main.pyw (or python2.7 main.pyw)

Or Interactive UQ-PyL Software

python main_interactive.pyw (or python2.7 main_interactive.pyw)

You can see the main page of UQ-PyL software.



2.2.3 MacOS platform

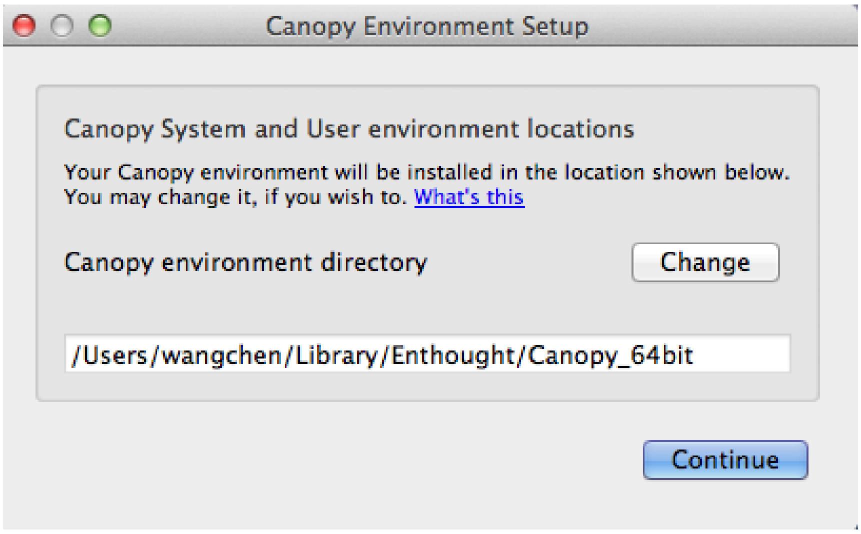
For MacOS platform, Canopy also has a MacOS version. You can download Canopy software and UQ-PyL MacOS version from our website. The installation process is very similar with Linux platform.

Step 1. Install Canopy software.
First, double click the .dmg file to start the installation.

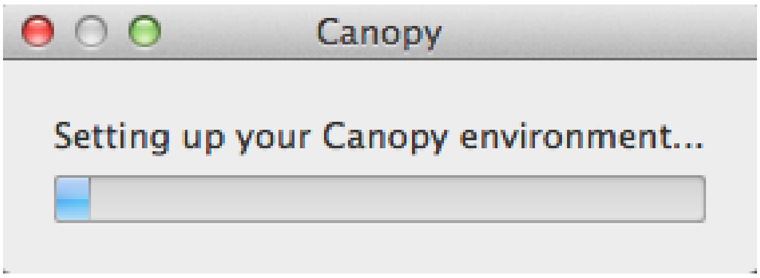
Pull Canopy icon to Application folder.

Step 2: Setting up Canopy environment

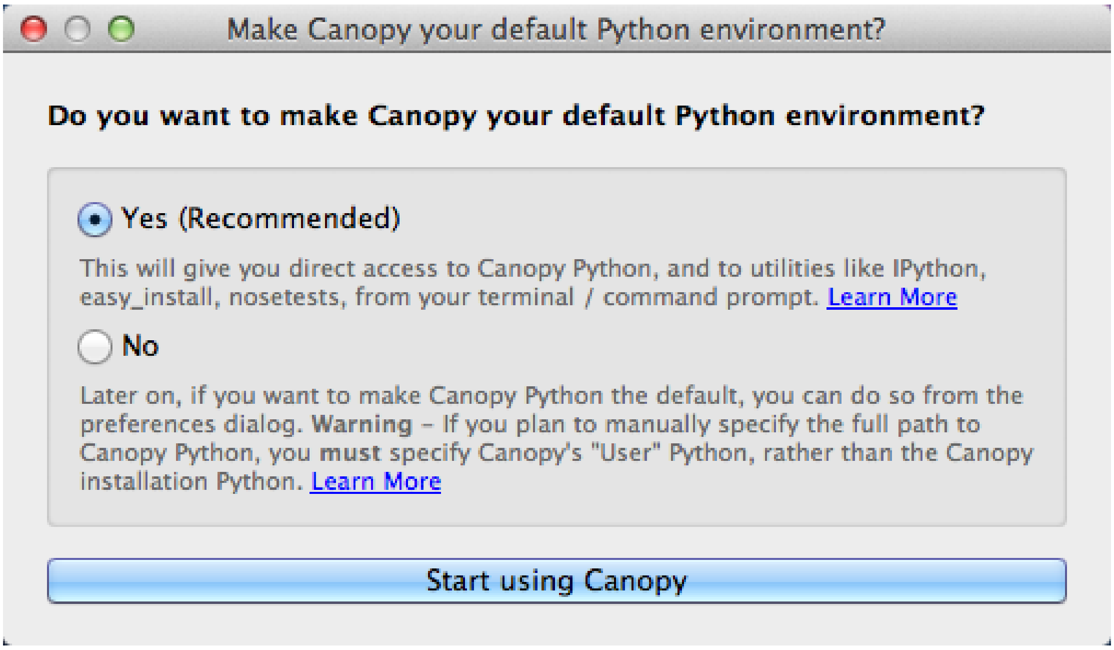
Double click “Canopy” icon to start setting Canopy environment.



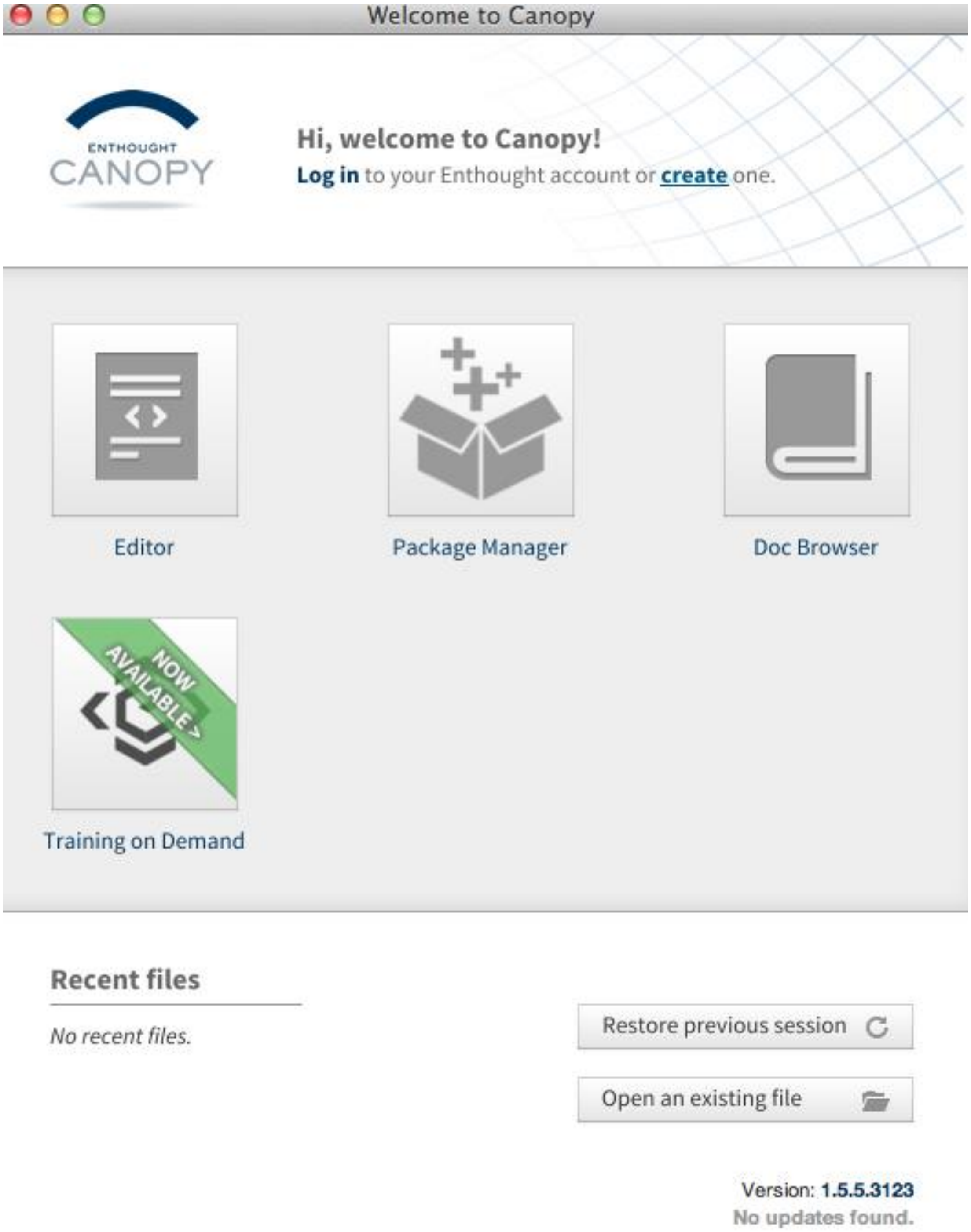
Write Canopy environment directory, click “Continue” to continue. Your python installation will be in this directory.



After that, a dialogue will display,



Choose “Yes”, then click “Start using Canopy”.



Also, you can check your python installation in your python installation path. All files are in "*YourPythonPath*/User/" (for me is /Users/wangchen/Library/Enthought/Canopy_64bit/User/). The python executable file is in "YourPythonPath/User/bin/".

Step 3: Test your Python installation

If you have multiple python environment, please specific one. For MacOS you could add a line like this to the /etc/launchd.conf file

export PYTHONPATH=/Users/wangchen/Library/Enthought/Canopy_64bit/User/bin

Then enter command "source launchd.conf" to make your launchd.conf file renew.

Type "python" or "python2.7" command, if you can see "Enthought Canopy Python" that means you already accomplished the installation.

```
ouchenmatoMacBook-Pro:UQ-PyL_Linux wangchen$ python
Enthought Canopy Python 2.7.9 | 64-bit | (default, Jun 30 2015, 19:41:21)
[GCC 4.2.1 (Based on Apple Inc. build 5658) (LLVM build 2335.6)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> 
```

Step 4. Install UQ-PyL software

Download UQ-PyL MacOS version, unzip the source code using command

tar –zxvf UQ-PyL_Mac.tar.gz

Then enter into the UQ-PyL directory

cd UQ-PyL_Mac

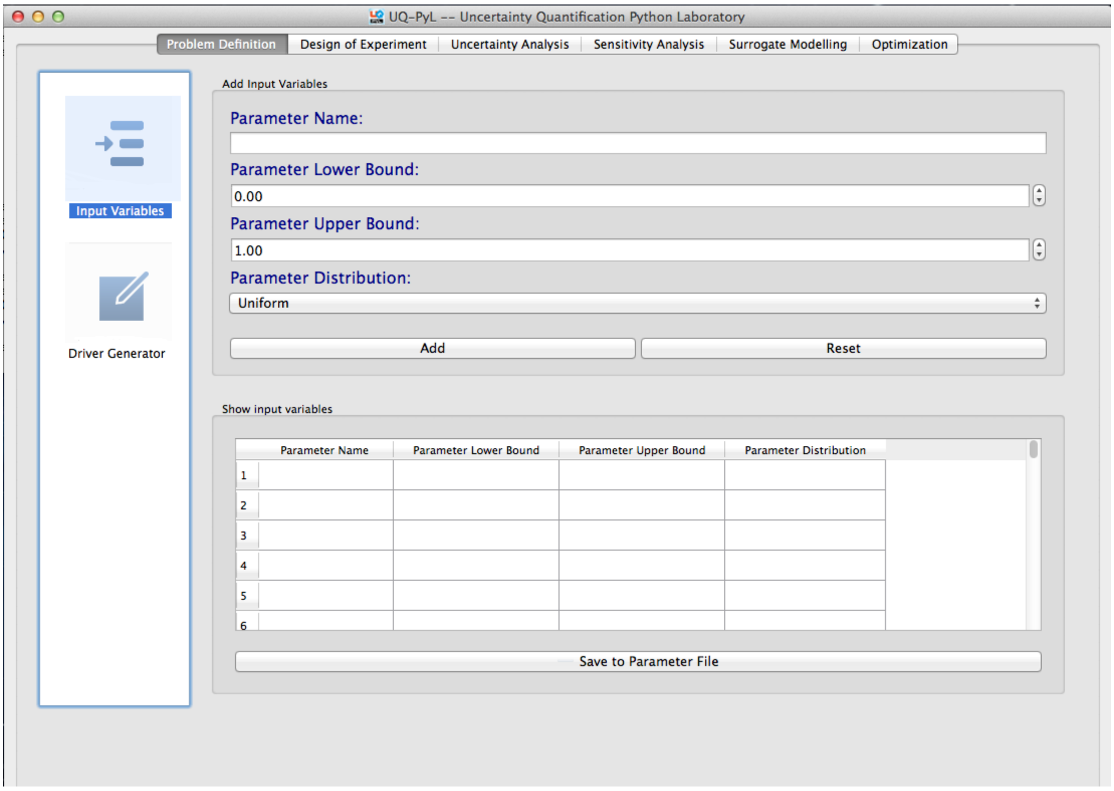
Enter command to run UQ-PyL main page

python main.pyw (or python2.7 main.pyw)

Or run Interactive UQ-PyL Software

python main_interactive.pyw (or python2.7 main_interactive.pyw)

You can see the main page of UQ-PyL software.



3 Using UQ-PyL

3.1 UQ-PyL Flowchart

Fig. 1 is the flowchart illustrating how UQ-PyL executes an UQ task. A typical task is carried out in three major steps: (1) model configuration preparation; (2) uncertainty propagation; and (3) UQ analysis. In the first step, the user specifies the model configuration information (i.e., parameter names, ranges and distributions), and the DoE information (i.e., the sampling techniques and sample sizes) to prepare for UQ exercise for a given problem. In the second step, the different sample parameter sets generated in the last step are fed into the simulation model (or mathematical function) to enable the execution of simulation model (function calculation). In the third step, a variety of UQ exercises are carried out, including statistical analysis, SA, surrogate modelling and parameter optimization.

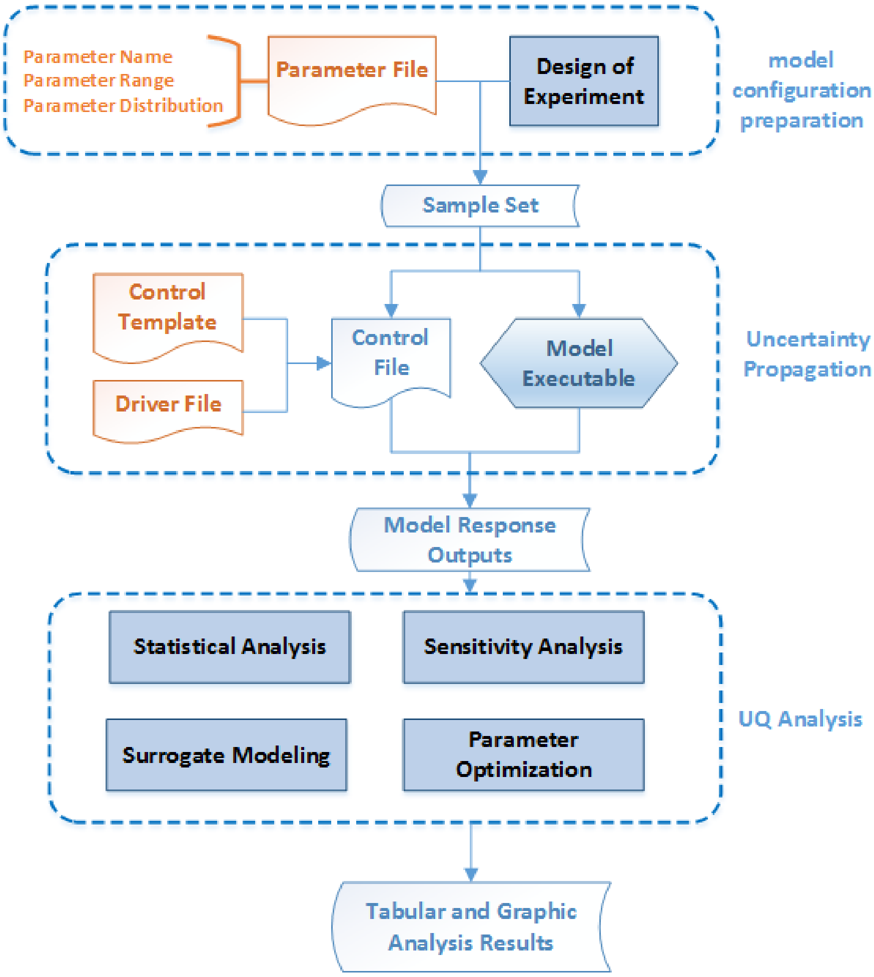


Fig 1. UQ-PyL flowchart

3.2 UQ-PyL Main Frame

UQ-PyL is equipped with a Graphic User Interface (GUI) to facilitate execution of various functions, but it can also run as a script program in a batch mode. Fig. 2 shows the main page of UQ-PyL. Different tab widgets allow user to execute different steps of UQ process, including problem definition, DoE, Statistical Analysis, SA, Surrogate Modeling and Parameter Optimization. One may click on the desired tab by mouse and/or enter the required information via keyboard to perform various tasks. After a task is completed, the software generates tabular results and/or graphical outputs. The graphical outputs can be saved in a variety of formats, including .png, .bmp, .tiff or .pdf formats, among others. Fig. 3 shows the interactive version of UQ-PyL software. In this page, you can write down python script to achieve UQ analysis and run the script to obtain the results. You can see the output results and internal variables' values through the page.

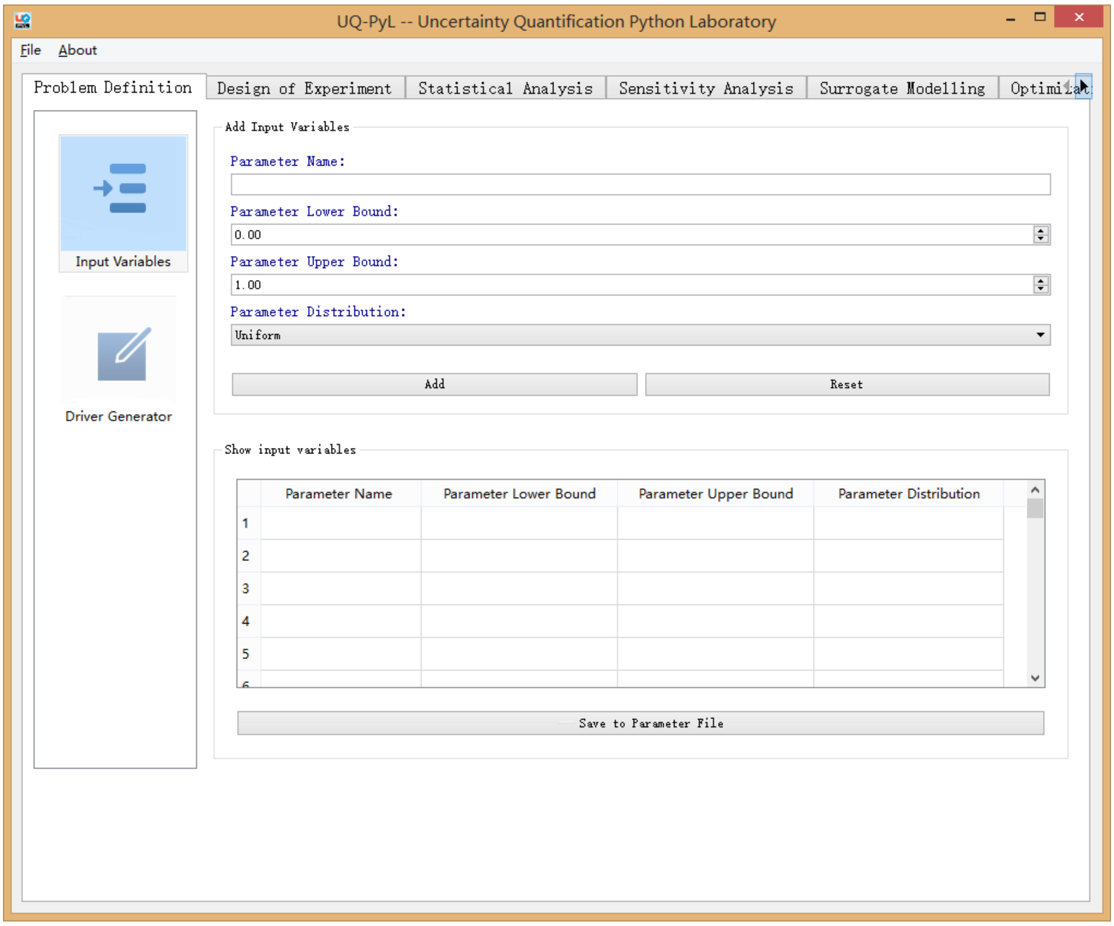


Fig 2. Graphic User Interface of UQ-PyL Main Page

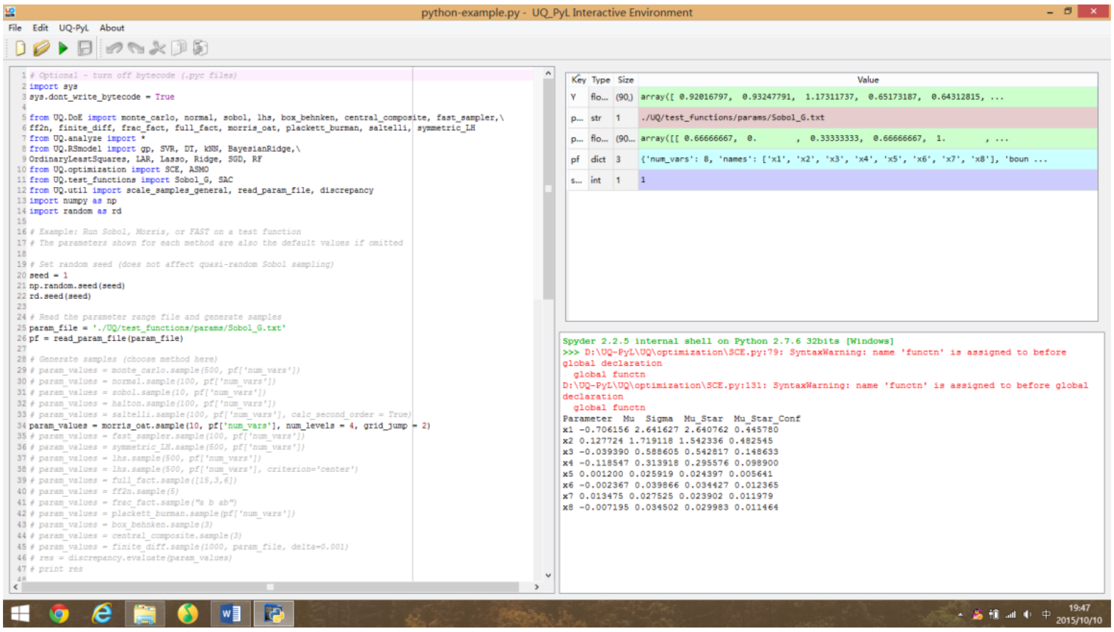


Fig 3. Interactive Version of UQ-PyL Software

4 Examples

4.1 Sobol' g-function

4.1.1 Problem Definition

The expression of sobol' g-function is:

$$f(x) = \prod_{i=1}^{n} g_i(x_i)$$

where

$$g_i(x_i) = \frac{|4x_i - 2| + a_i}{1 + a_i}$$

The input parameter x_i is uniformly distributed within (0, 1), $a_i = \{0, 1, 4.5, 9, 99, 99, 99, 99\}$.

The model is implemented using Python and the parameter file is shown below:

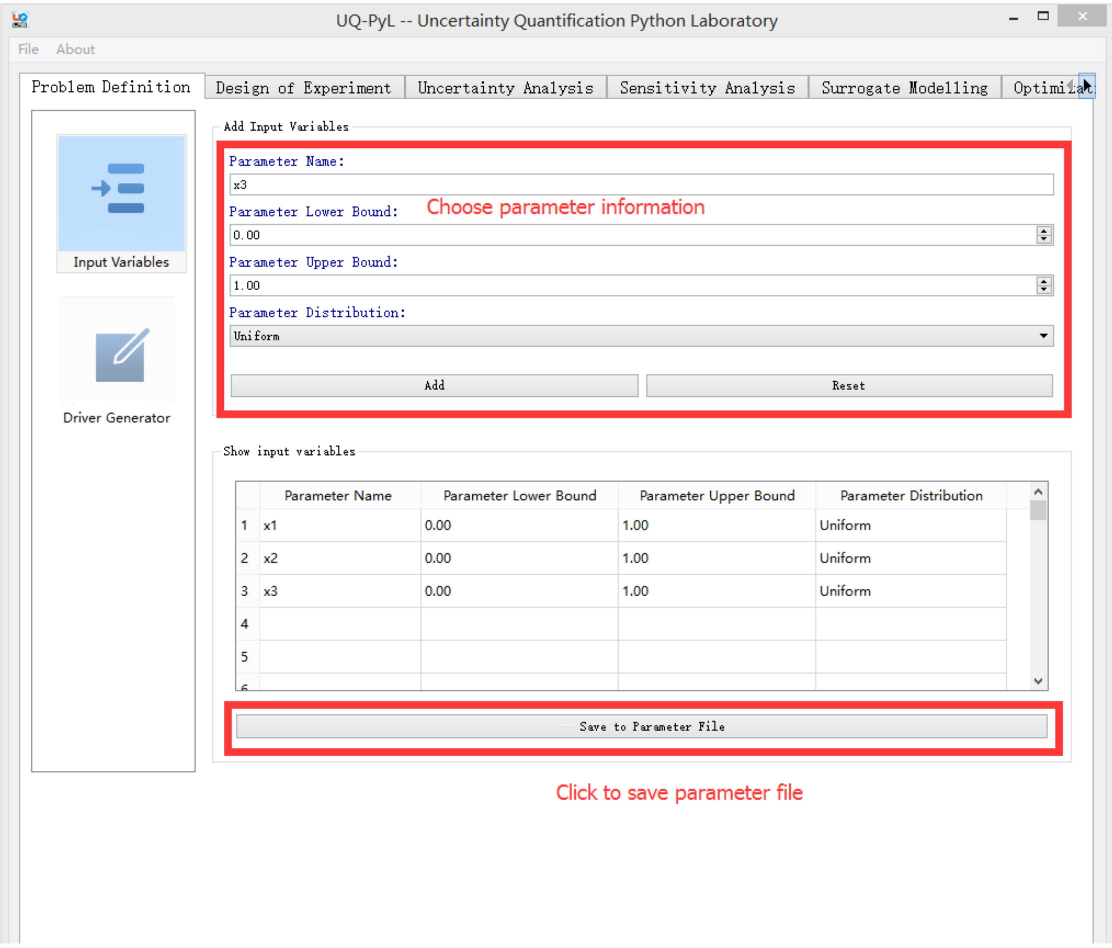
Model file (UQ-PyL/UQ/test_functions/Sobol_G.py)

```
from __future__ import division
import numpy as np

# Non-monotonic Sobol' G Function (8 parameters)
# First-order indices:
# x1: 0.7165   77.30%
# x2: 0.1791   19.32%
# x3: 0.0237   2.56%
# x4: 0.0072   0.78%
# x5-x8: 0.0001   0.01%

def predict(values):
    a = [0, 1, 4.5, 9, 99, 99, 99, 99]
    Y = np.empty([values.shape[0]])

    for i, row in enumerate(values):
        Y[i] = 1.0

        for j in range(8):
            x = row[j]
            Y[i] *= (abs(4*x - 2) + a[j]) / (1 + a[j])

    return Y
```

Parameter file (UQ-PyL/UQ/test_functions/params/Sobol_G.txt)

```
x1 0.0 1.0
x2 0.0 1.0
x3 0.0 1.0
x4 0.0 1.0
x5 0.0 1.0
x6 0.0 1.0
x7 0.0 1.0
x8 0.0 1.0
```

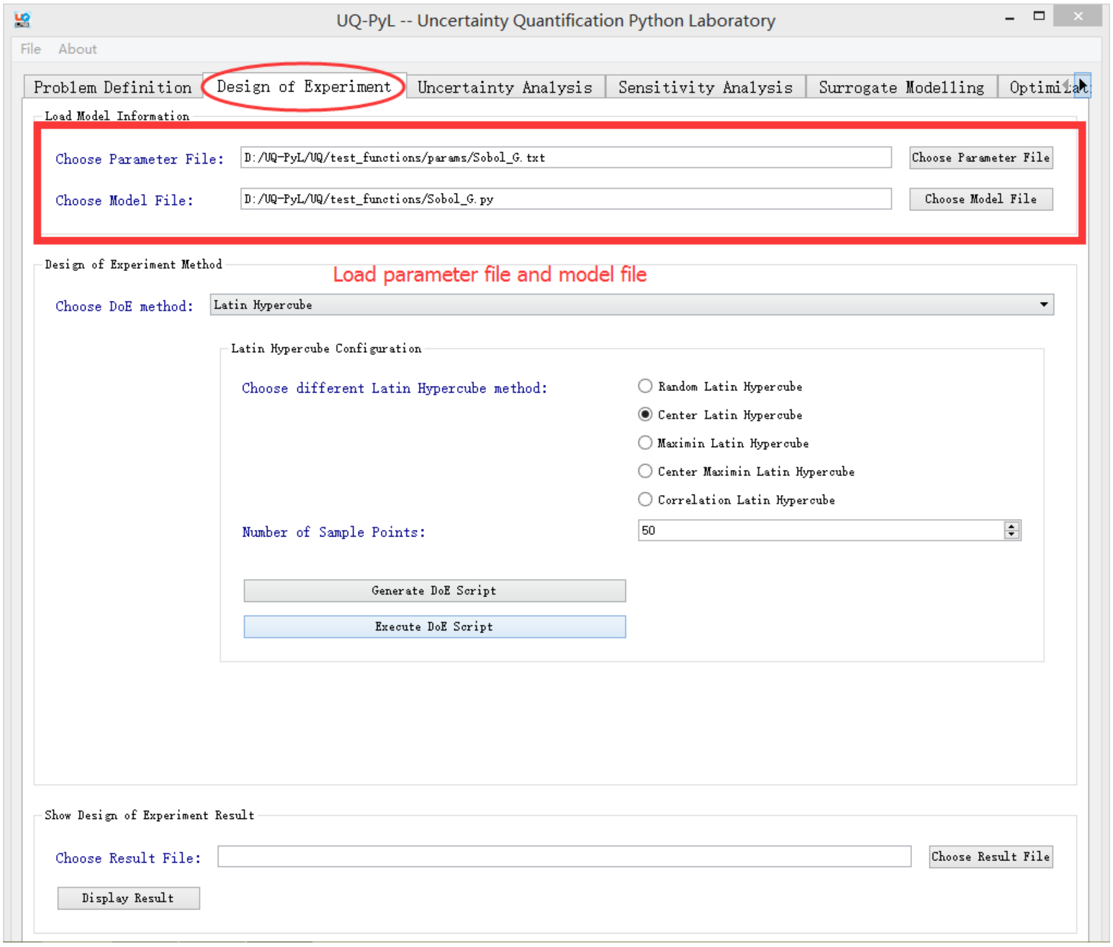
Parameter file can also be generated from GUI of UQ-PyL:
Step 1: Enter "Parameter Name", "Parameter Lower Bound" and "Parameter Upper Bound", choose "Parameter Distribution";
Step 2: Click "Add" button to save this parameter information to table widget;
Step 3: Enter every parameter's information, click "Save to Parameter File" button, choose the save path "UQ-PyL/UQ/test_functions/params/Sobol_G.txt".



4.1.2 Design of Experiment

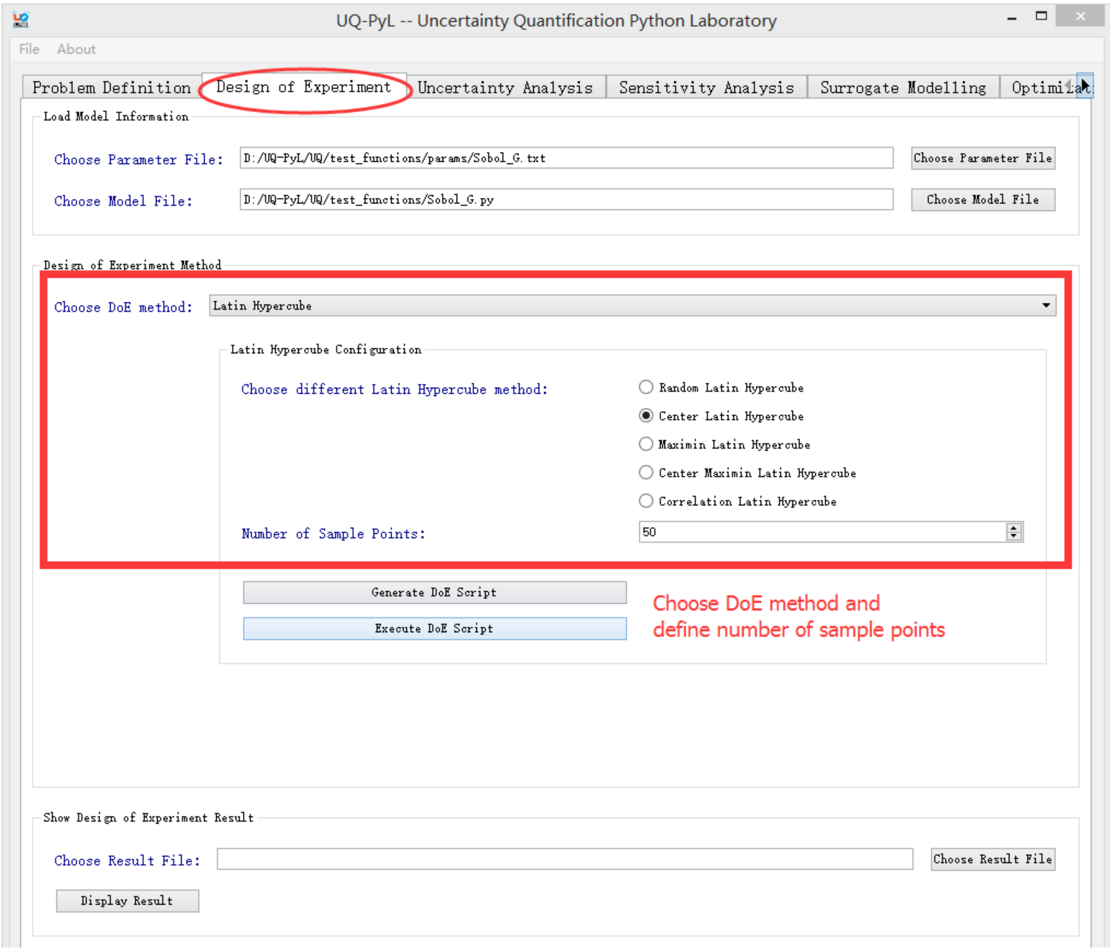
After problem definition, we do Design of Experiment, the experiment has three steps:

1) Define parameter and model information;
2) Choose Design of Experiment method;
3) Generate script and run the script.



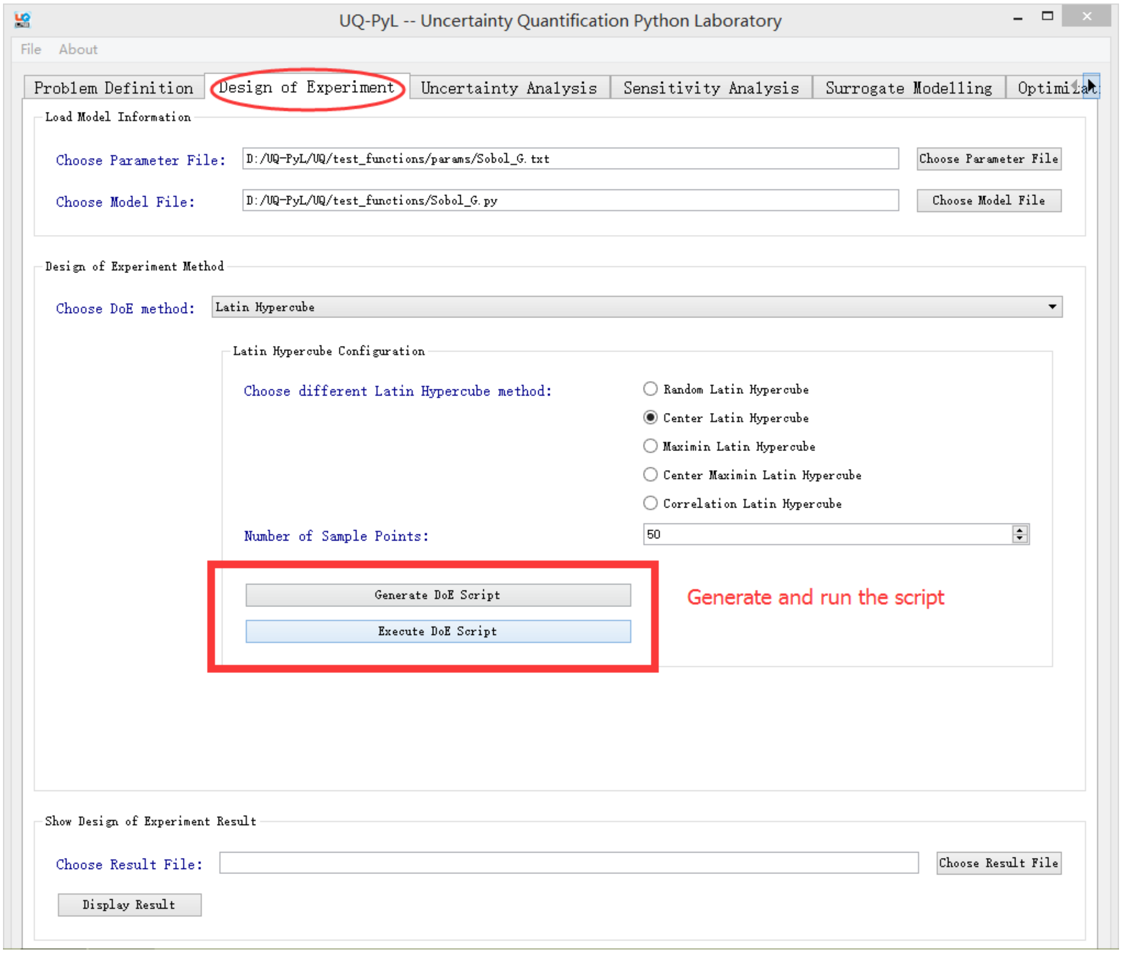
Step 1: Define parameter and model information

- ✧ Switch to "Design of Experiment" tab;
- ✧ Click "Choose Parameter File" button to choose "UQ-PyL/UQ/test_functions/params/Sobol_G.txt" file;
- ✧ Click "Choose Model File" button to choose "UQ-PyL/UQ/test_functions/Sobol_G.py" file.



Step 2: Choose DoE method

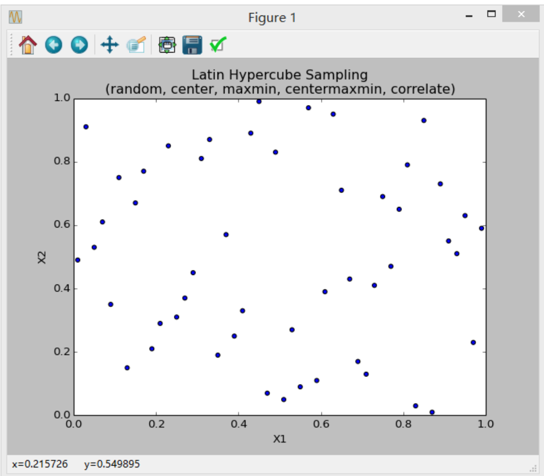
- ✧ Choose DoE method, like “Latin Hypercube”, choose one specific Latin Hypercube method, like “Center Latin Hypercube”;
- ✧ Set “Number of Sample Points”, like: 50.

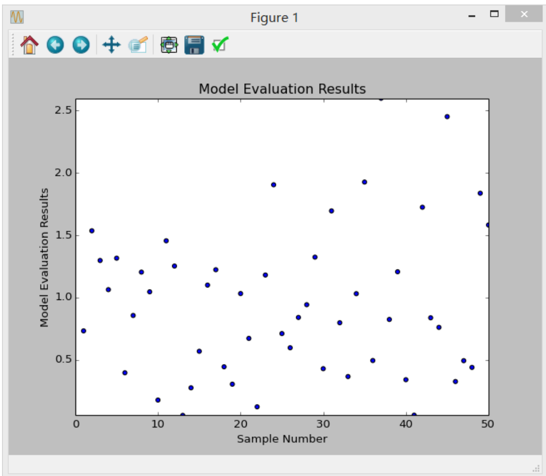


Step 3: Run for DoE results

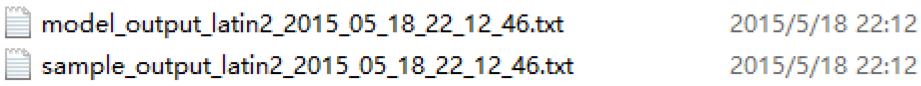
- ✧ Click "Generate DoE Script" button to generate DoE script which contains information you just choose;
- ✧ Click "Execute DoE Script" button to run DoE script.

Then, UQ-PyL gives the tabular and graphic results of DoE:





The result automatically save in text files, the name of files including DoE method used and current time.



This step can also implemented using python script:

Python script file (Sobol_G_DoE.py)

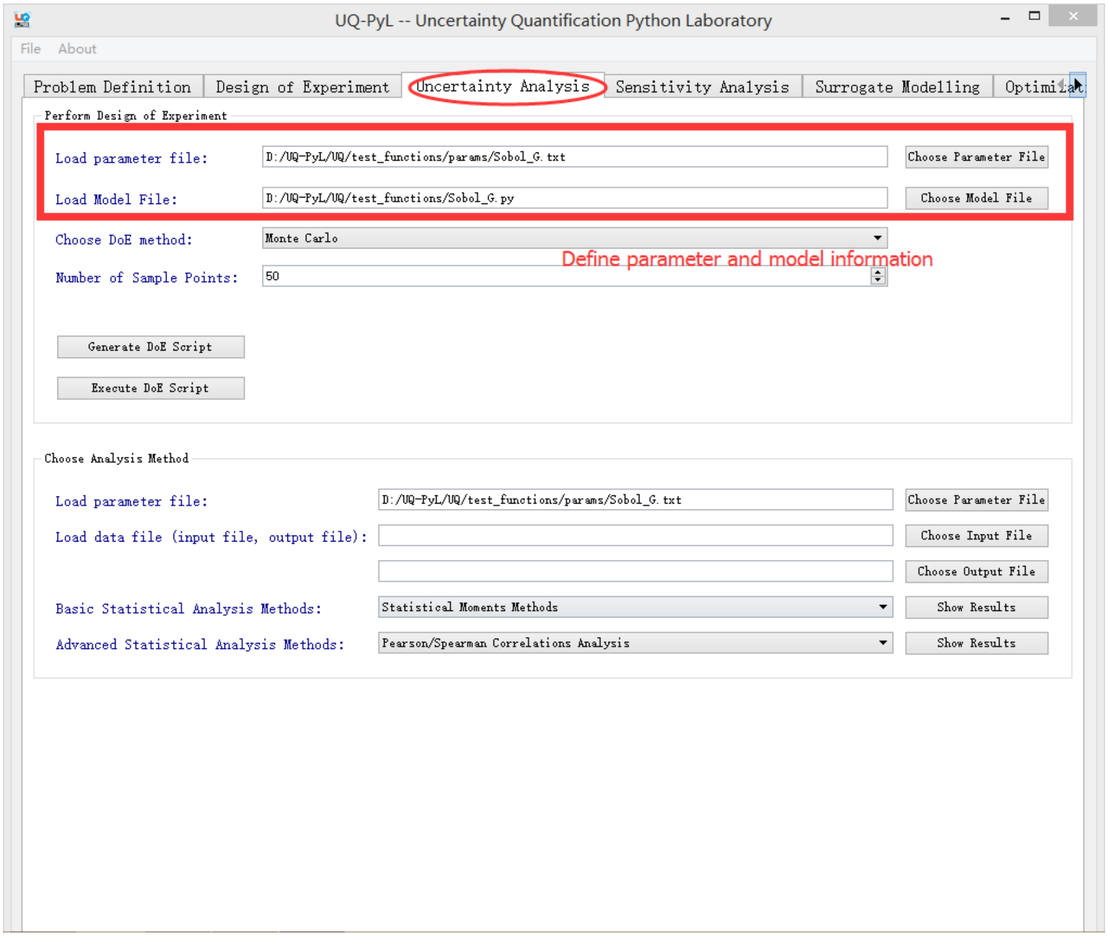
```
# Optional - turn off bytecode (.pyc files)
import sys
sys.dont_write_bytecode = True

from UQ.DoE import lhs
from UQ.test_functions import Sobol_G
from UQ.util import scale_samples_general, read_param_file, discrepancy
import numpy as np
import random as rd

# Set random seed (does not affect quasi-random Sobol sampling)
seed = 1
np.random.seed(seed)
rd.seed(seed)

# Read the parameter range file and generate samples
param_file = './UQ/test_functions/params/Sobol_G.txt'
pf = read_param_file(param_file)

# Generate samples (choose method here)
param_values = lhs.sample(50, pf['num_vars'], criterion='center')
res = discrepancy.evaluate(param_values)
print res

# Samples are given in range [0, 1] by default. Rescale them to your
parameter bounds.
scale_samples_general(param_values, pf['bounds'])
np.savetxt('Input_Sobol\'.txt', param_values, delimiter=' ')

# Run the "model" and save the output in a text file
# This will happen offline for external models
Y = Sobol_G.predict(param_values)
np.savetxt("Output_Sobol\'.txt", Y, delimiter=' ')
```

4.1.3 Statistical Analysis

In this section, we do statistical analysis using UQ-PyL.

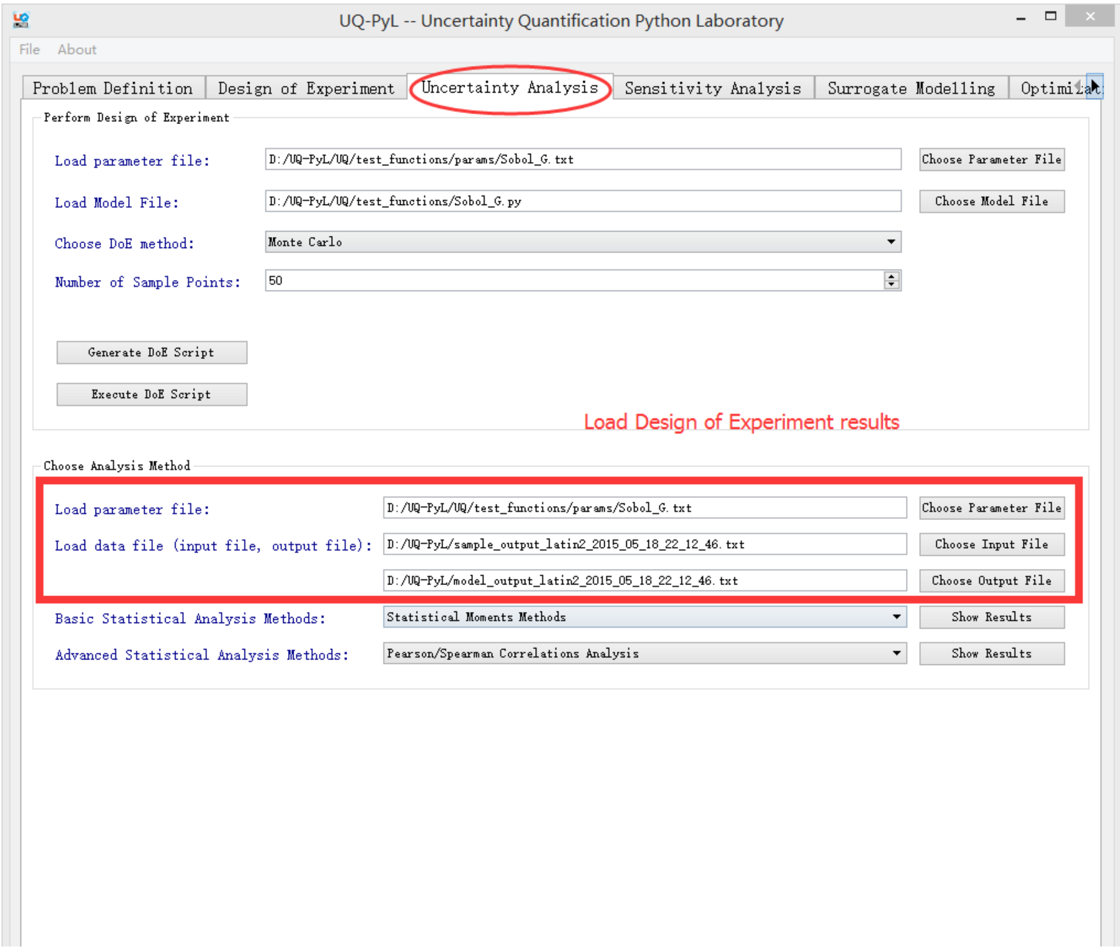
There are also three steps:

1) Define parameter and model information;
2) Do Design of Experiment or load Design of Experiment results;
3) Choose statistical analysis method and show the results.



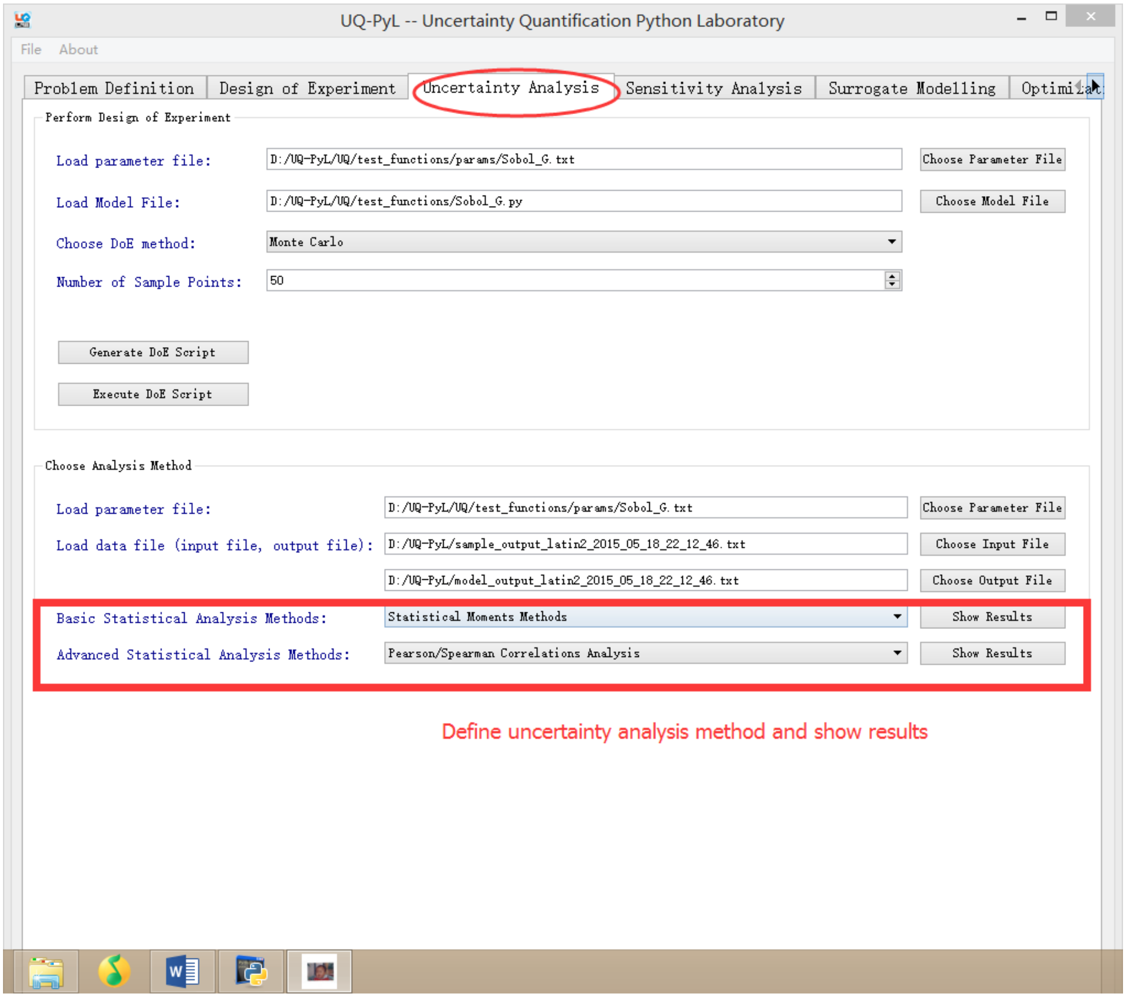
Step 1: Define parameter and model information

✧ Switch to "Statistical Analysis" tab;
✧ Click "Choose Parameter File" button to choose "UQ-PyL/UQ/test_functions/params/Sobol_G.txt" file;
✧ Click "Choose Model File" button to choose "UQ-PyL/UQ/test_functions/Sobol_G.py" file.



Step 2: Load DoE results

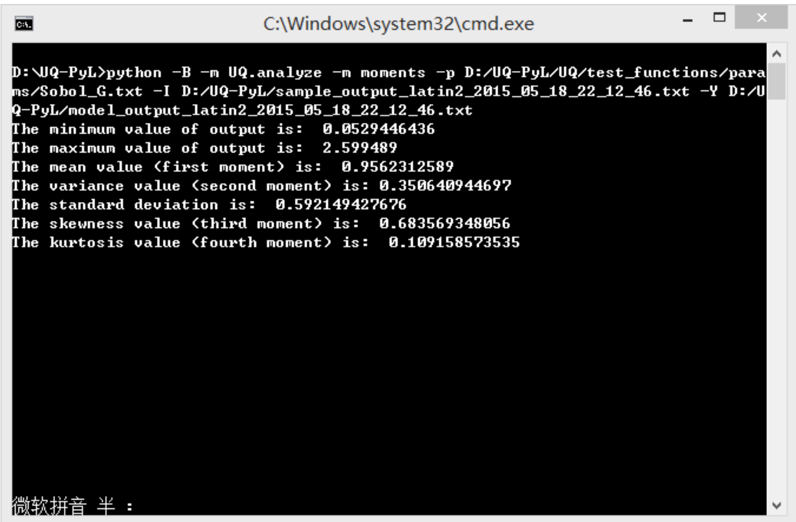
- Click "Choose Input File" button to choose sample file you just generated, for example: "sample_output_latin2_2015_05_18_22_12_46.txt";
- Click "Choose Output File" button to choose model output file you just generated, for example: "model_output_latin2_2015_05_18_22_12_46.txt".

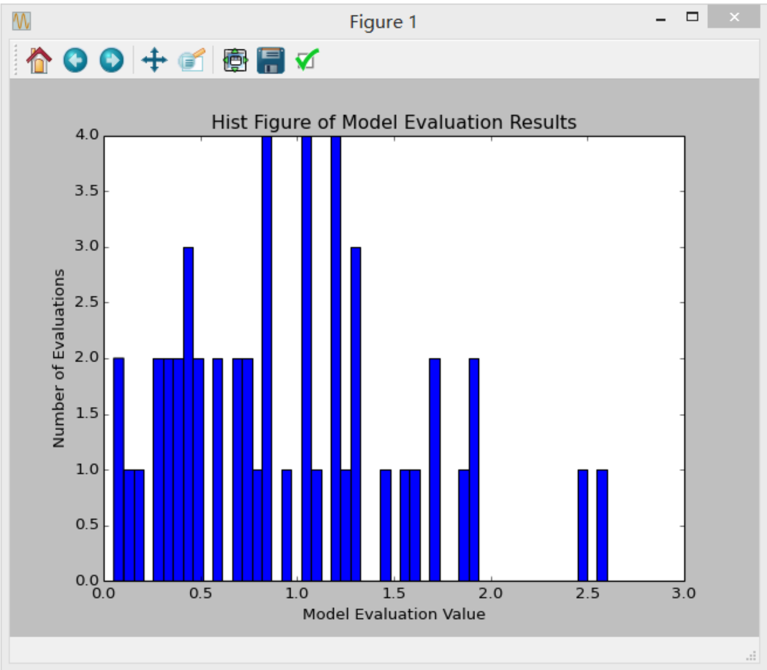


Step 3: Choose statistical analysis method and show results

- ✧ Choose statistical analysis method, like “Statistical Moments Methods”;
- ✧ Click “Show Results” button to show statistical analysis results.

UQ-PyL gives the tabular and graphic results:





This step can also implemented using python script:

Python script file (Sobol_G_UA.py)

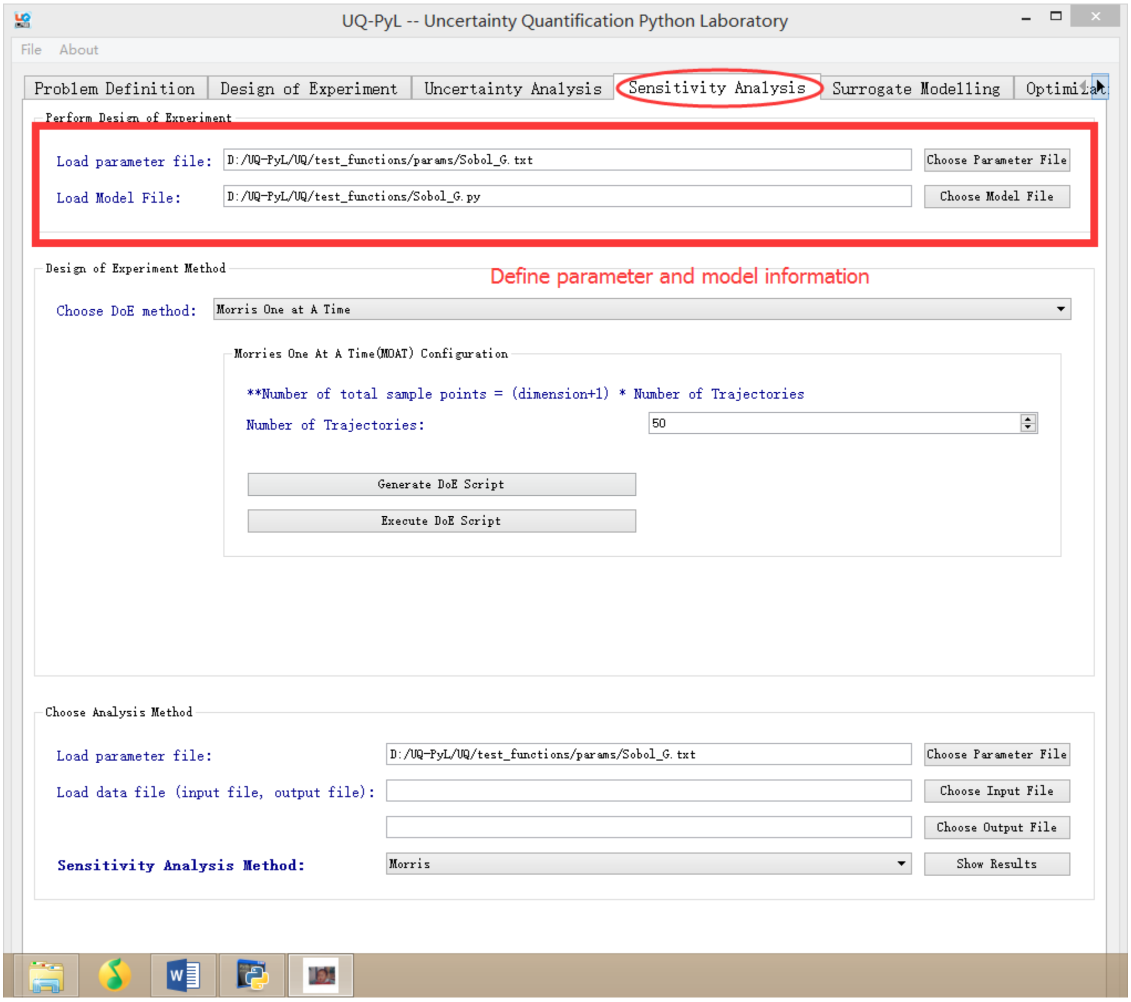
```
# Optional - turn off bytecode (.pyc files)
import sys
sys.dont_write_bytecode = True

from UQ.DoE import lhs
from UQ.analyze import *
from UQ.test_functions import Sobol_G
from UQ.util import scale_samples_general, read_param_file, discrepancy
import numpy as np
import random as rd

# Set random seed (does not affect quasi-random Sobol sampling)
seed = 1
np.random.seed(seed)
rd.seed(seed)

# Read the parameter range file and generate samples
param_file = './UQ/test_functions/params/Sobol_G.txt'
pf = read_param_file(param_file)

# Generate samples (choose method here)
param_values = lhs.sample(50, pf['num_vars'], criterion='center')
res = discrepancy.evaluate(param_values)
print res
```

```
# Samples are given in range [0, 1] by default. Rescale them to your
parameter bounds.
scale_samples_general(param_values, pf['bounds'])
np.savetxt('Input_Sobol\'.txt', param_values, delimiter=' ')

# Run the "model" and save the output in a text file
# This will happen offline for external models
Y = Sobol_G.predict(param_values)
np.savetxt("Output_Sobol\'.txt", Y, delimiter=' ')

# Perform the sensitivity analysis/uncertainty analysis using the model
output
# Specify which column of the output file to analyze (zero-indexed)
moments.analyze('Output_Sobol\'.txt', column=0)
```

4.1.4 Sensitivity Analysis

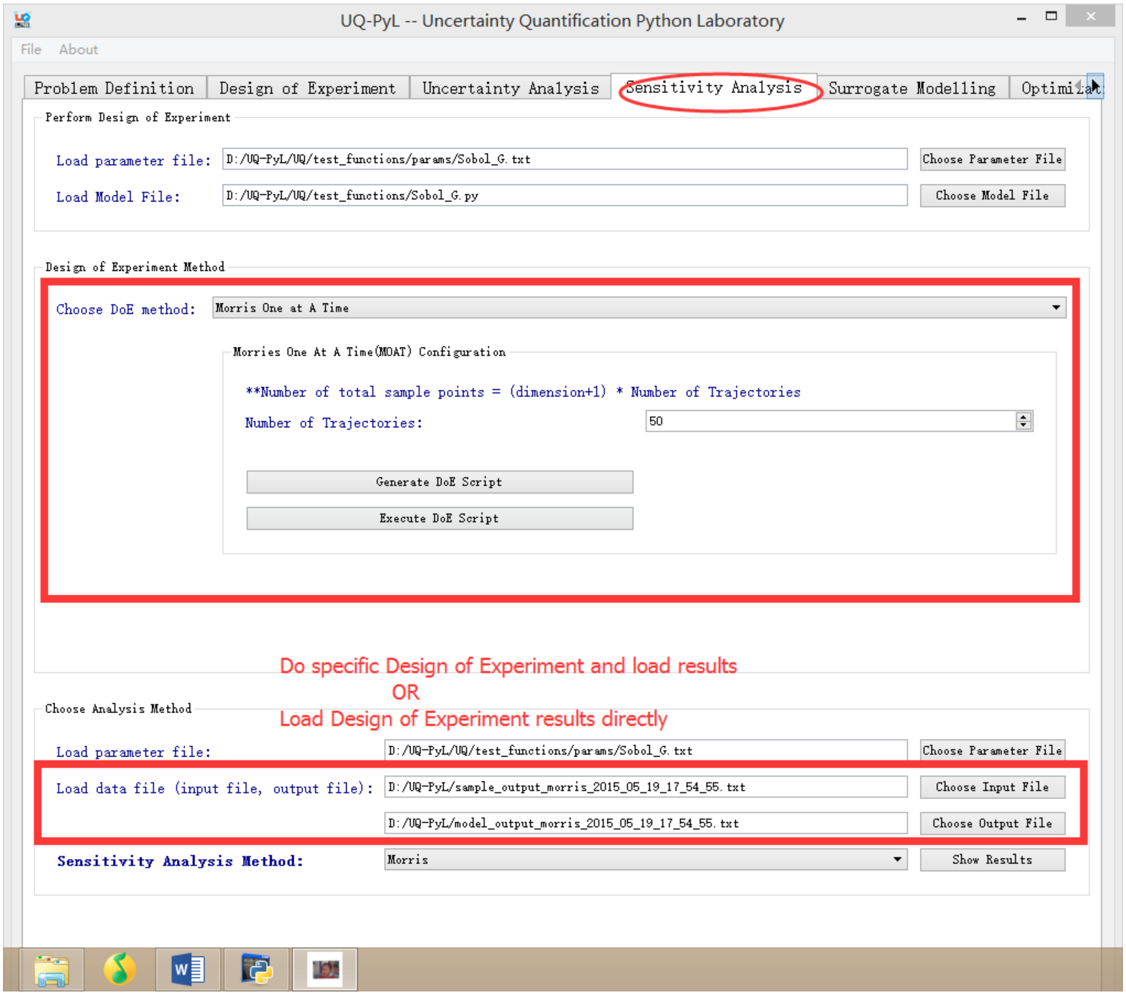
Next, we do sensitivity analysis using UQ-PyL. There are three steps:

1) Define parameter and model information;
2) Do specific Design of Experiment or load Design of Experiment results (Different sensitivity analysis method need different Design of Experiment method);
3) Choose sensitivity analysis method and show the results.



Step 1: Define parameter and model information

- ✧ Switch to “Sensitivity Analysis” tab;
- ✧ Click “Choose Parameter File” button to choose “UQ-PyL/UQ/test_functions/params/Sobol_G.txt” file;
- ✧ Click “Choose Model File” button to choose “UQ-PyL/UQ/test_functions/Sobol_G.py” file.



Step 2: Do specific DoE for specific sensitivity analysis method. For example, we do Morris analysis in this chapter. Then load DoE results.

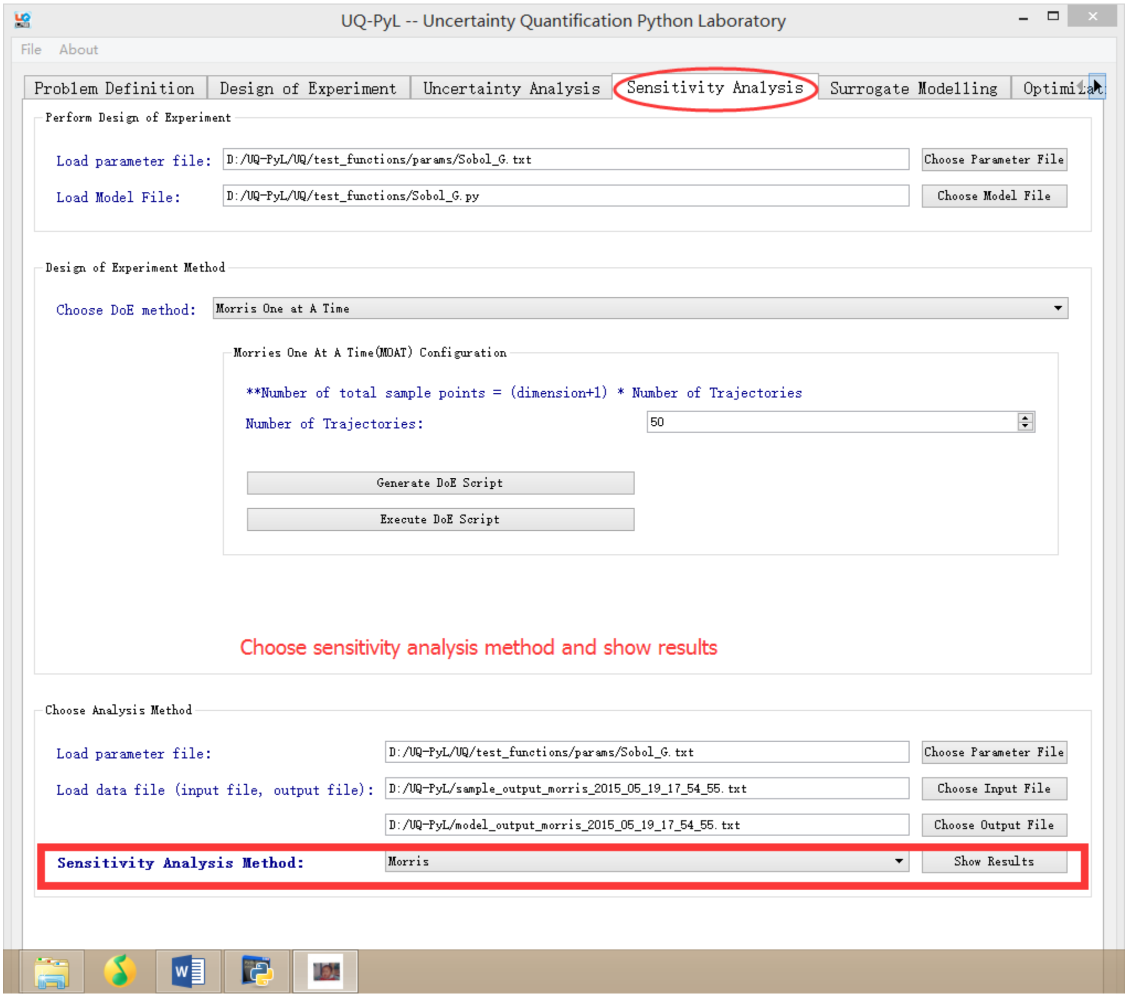
✧ Choose DoE method, for this experiment is "Morris One at A Time";

✧ Set "Number of Trajectories", for example: 50;

✧ Click "Generate DoE Script" button to generate script;

✧ Click "Execute DoE Script" button to run script and acquire DoE result;

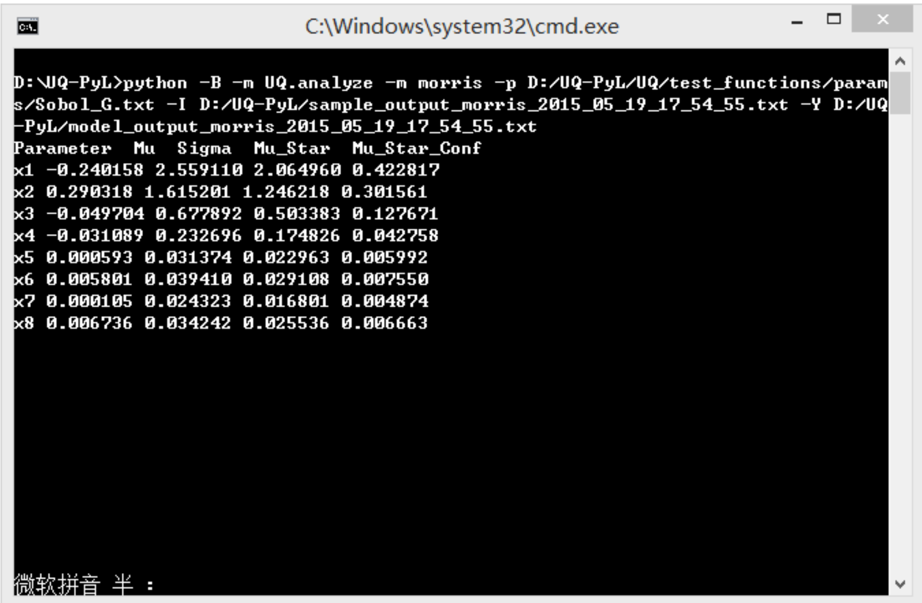
✧ Load input/output file you just generated: 1) Click "Choose Input File" button to load sample file, for example "UQ-PyL/sample_output_morris_2015_05_19_17_54_55.txt"; 2) Click "Choose Output File" button to load model output file, for example "UQ-PyL/model_output_morris_2015_05_19_17_54_55.txt".

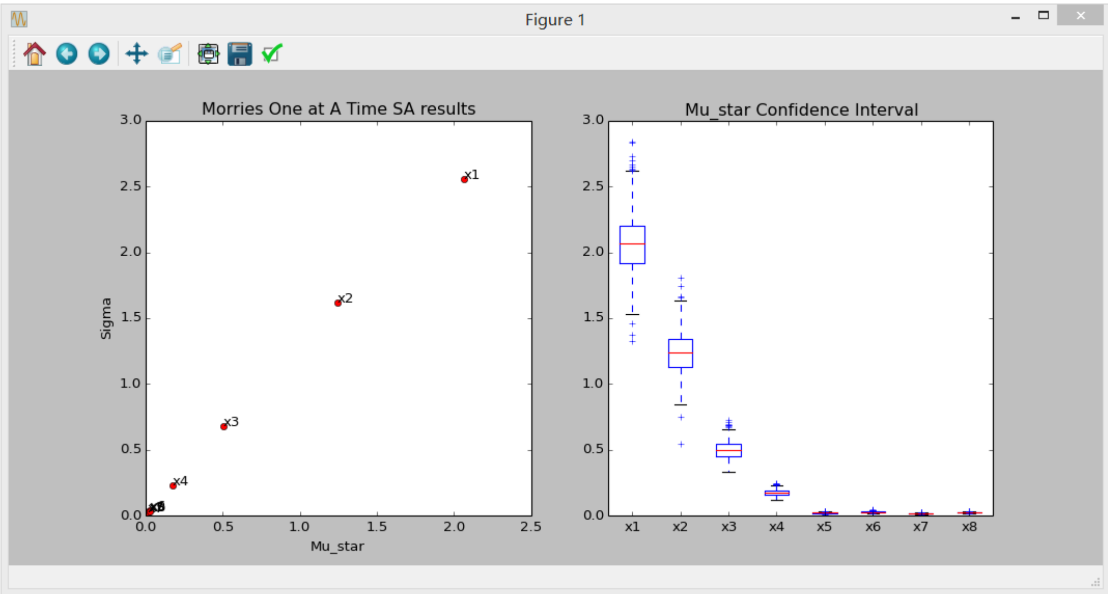


Step 3: Choose sensitivity analysis method and show results

- ✧ Choose sensitivity analysis method, like “Morris”;
- ✧ Click “Show Results” button to show sensitivity analysis results.

UQ-PyL gives the tabular and graphic results:





This step can also implemented using python script:

Python script file (Sobol_G_SA.py)

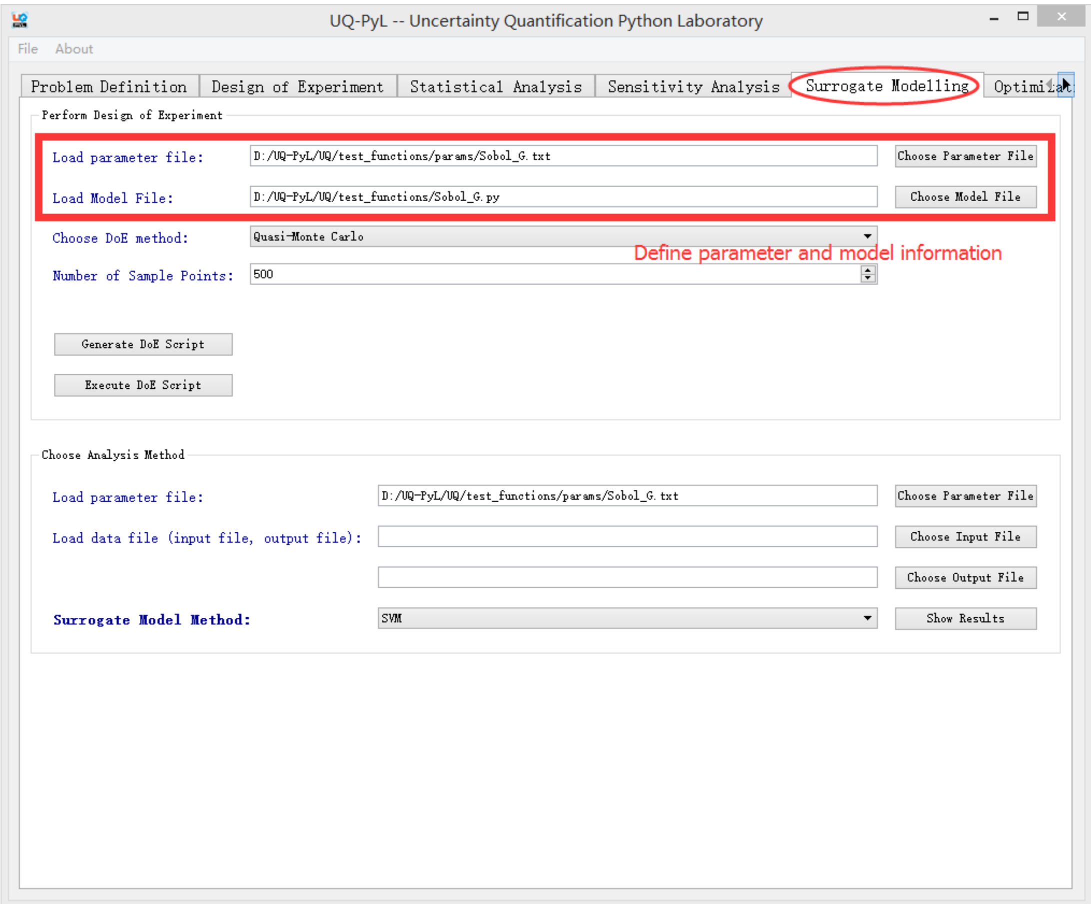
```
# Optional - turn off bytecode (.pyc files)
import sys
sys.dont_write_bytecode = True

from UQ.DoE import morris_oat
from UQ.analyze import *
from UQ.test_functions import Sobol_G
from UQ.util import scale_samples_general, read_param_file
import numpy as np
import random as rd

# Set random seed (does not affect quasi-random Sobol sampling)
seed = 1
np.random.seed(seed)
rd.seed(seed)

# Read the parameter range file and generate samples
param_file = './UQ/test_functions/params/Sobol_G.txt'
pf = read_param_file(param_file)

# Generate samples (choose method here)
param_values = morris_oat.sample(50, pf['num_vars'], num_levels = 10,
grid_jump = 5)

# Samples are given in range [0, 1] by default. Rescale them to your
```

```
parameter bounds.
scale_samples_general(param_values, pf['bounds'])
np.savetxt('Input_Sobol\'.txt', param_values, delimiter=' ')

# Run the "model" and save the output in a text file
# This will happen offline for external models
Y = Sobol_G.predict(param_values)
np.savetxt("Output_Sobol\'.txt", Y, delimiter=' ')

# Perform the sensitivity analysis/uncertainty analysis using the model
output
# Specify which column of the output file to analyze (zero-indexed)
morris.analyze(param_file, 'Input_Sobol\'.txt', 'Output_Sobol\'.txt',
column = 0)
```

4.1.5 Surrogate Modeling

Next, we do surrogate modeling using UQ-PyL. There are three steps:

1) Define parameter and model information;
2) Do specific Design of Experiment or load Design of Experiment results;
3) Choose surrogate modeling method and show the results.

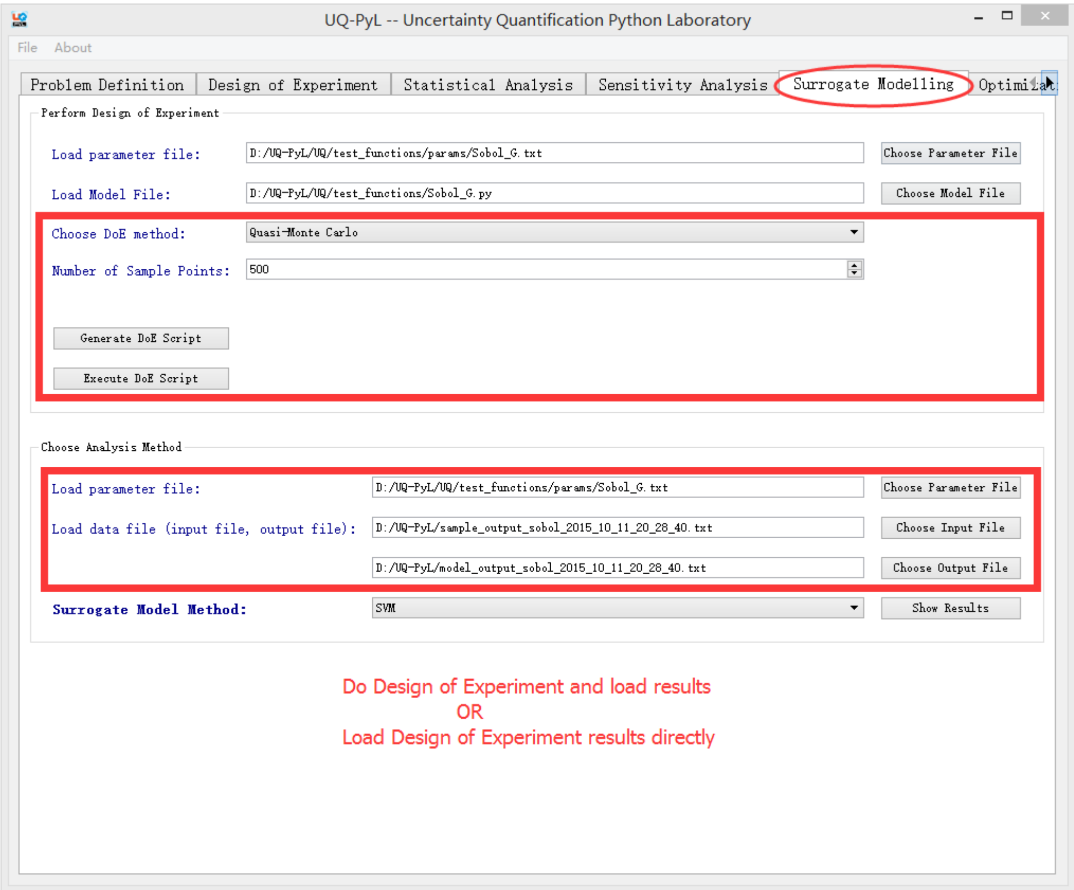


Step 1: Define parameter and model information

✧ Switch to “Surrogate Modeling” tab;

✧ Click “Choose Parameter File” button to choose “UQ-PyL/UQ/test_functions/params/Sobol_G.txt” file;

✧ Click “Choose Model File” button to choose “UQ-PyL/UQ/test_functions/Sobol_G.py” file.



Step 2: Do DoE for surrogate modeling method and load results.

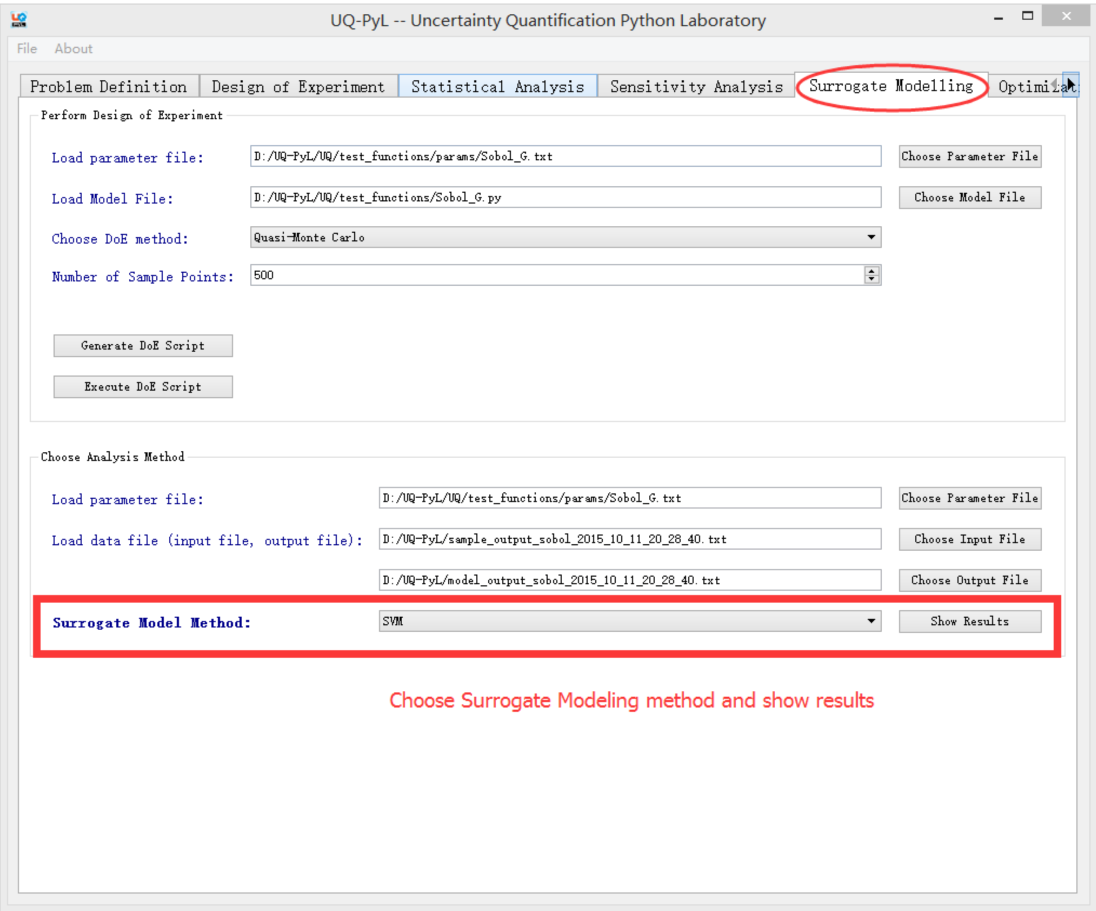
✧ Choose DoE method, for example “Quasi Monte Carlo”;

✧ Set “Number of Trajectories”, for example: 500;

✧ Click “Generate DoE Script” button to generate script;

✧ Click “Execute DoE Script” button to run script and acquire DoE result;

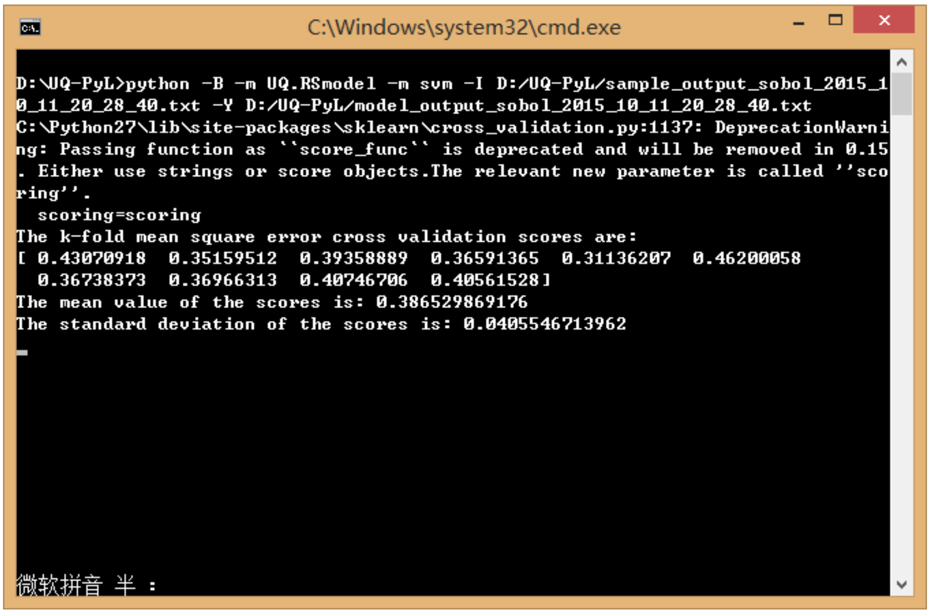
✧ Load input/output file you just generated: 1) Click “Choose Input File” button to load sample file, for example “UQ-PyL/sample_output_sobol_2015_10_11_17_54_55.txt”; 2) Click “Choose Output File” button to load model output file, for example “UQ-PyL/model_output_sobol_2015_10_11_17_54_55.txt”.

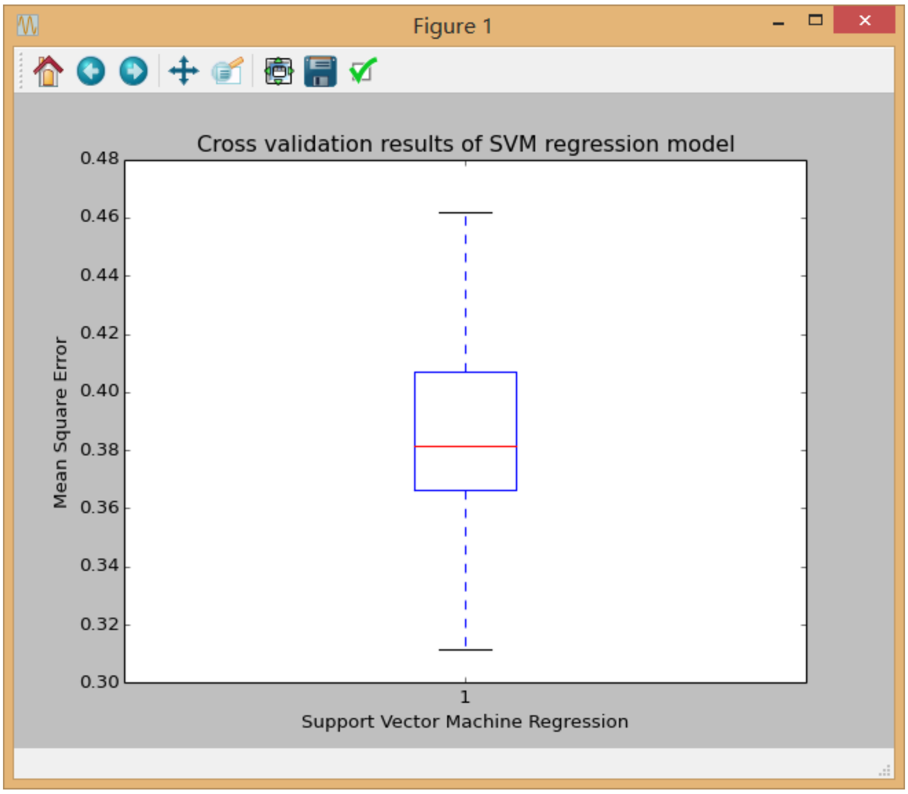


Step 3: Choose surrogate modeling method and show results

- ✧ Choose surrogate modeling method, like “SVM”;
- ✧ Click “Show Results” button to show sensitivity analysis results.

UQ-PyL gives the tabular and graphic results:





In this new version of UQ-PyL, the software also save surrogate model as a *.pickle file automatically. For this example is “SVRmodel.pickle” file.

This file can be opened by a Text Editor, please see the context of this file below:

SVRmodel.pickle


```
ccopy_reg
_reconstructor
p0
(csklearn.svm.classes
SVR
p1
c__builtin__
object
p2
Ntp3
Rp4
(dp5
S'_impl'
p6
S'epsilon_svr'
p7
sS'kernel'
p8
S'rbf'
p9
sS'verbose'
p10
I00
sS'probability'
p11
I00
sS'_label'
p12
cnumpy.core.multiarray
_reconstruct
p13
(cnumpy
ndarray
p14
(I0
tp15
S'b'
p16
tp17
Rp18
```


It saved the data structure of the surrogate model you built.

In section 4.3, we will introduce how to run simulations on surrogate models you built.

This step can also implemented using python script:

Python script file (Sobol_G_Surrogate.py)

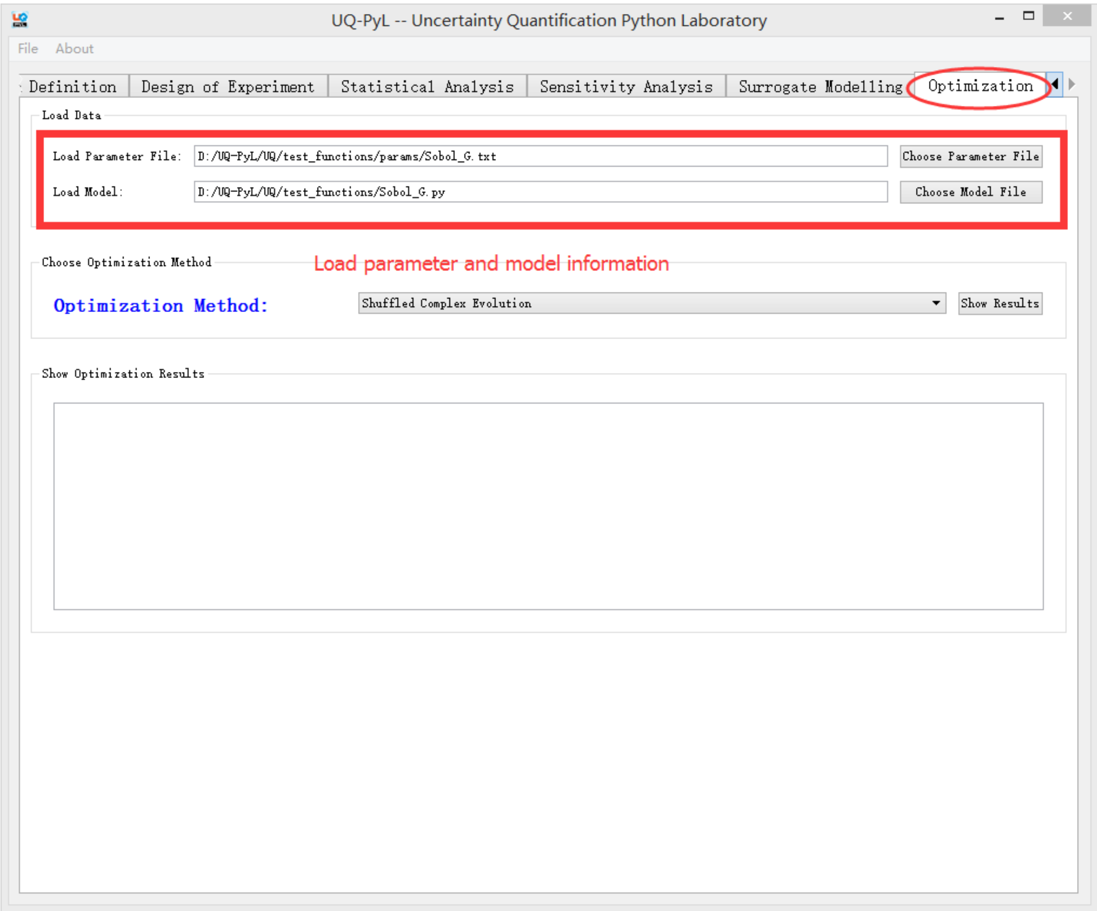
```python
# Optional - turn off bytecode (.pyc files)
import sys
sys.dont_write_bytecode = True

from UQ.DoE import sobol
from UQ.RSmodel import SVR
from UQ.test_functions import Sobol_G
from UQ.util import scale_samples_general, read_param_file, discrepancy
import numpy as np
import random as rd
```

```
# Set random seed (does not affect quasi-random Sobol sampling)
seed = 1
np.random.seed(seed)
rd.seed(seed)

# Read the parameter range file and generate samples
param_file = './UQ/test_functions/params/Sobol_G.txt'
pf = read_param_file(param_file)

# Generate samples (choose method here)
param_values = sobol.sample(500, pf['num_vars'])

# Samples are given in range [0, 1] by default. Rescale them to your
parameter bounds.
scale_samples_general(param_values, pf['bounds'])
np.savetxt('Input_Sobol\'.txt', param_values, delimiter=' ')

# Run the "model" and save the output in a text file
# This will happen offline for external models
Y = Sobol_G.predict(param_values)
np.savetxt("Output_Sobol\'.txt", Y, delimiter=' ')

# Perform regression analysis using the model output
# Specify which column of the output file to analyze (zero-indexed)
model = SVR.regression('Input_Sobol\'.txt', 'Output_Sobol\'.txt',
column = 0, cv = True)
```

4.1.6 Parameter Optimization

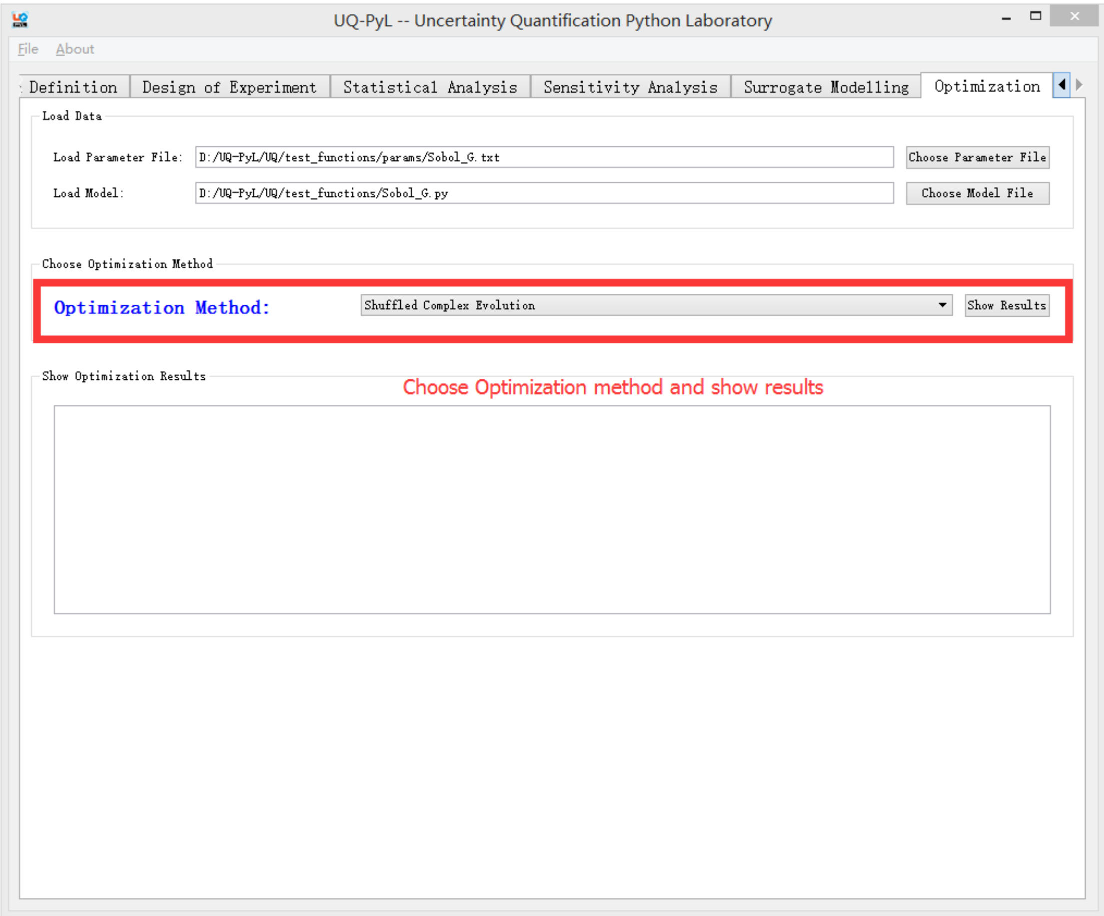
At last, we do parameter optimization using UQ-PyL. There are two steps:

1) Define parameter and model information;
2) Choose parameter optimization method and show the results.



Step 1: Define parameter and model information

- Switch to "Optimization" tab;
- Click "Choose Parameter File" button to choose "UQ-PyL/UQ/test_functions/params/Sobol_G.txt" file;
- Click "Choose Model File" button to choose "UQ-PyL/UQ/test_functions/Sobol_G.py" file.

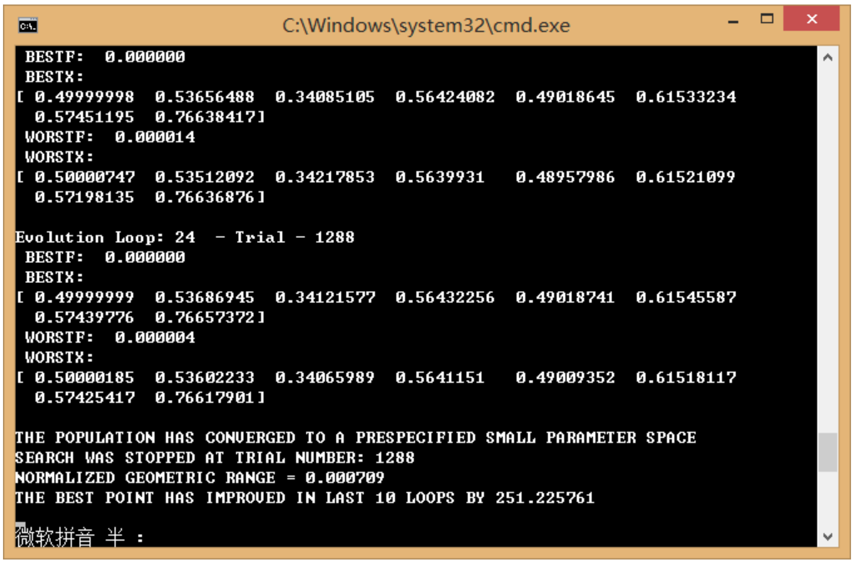


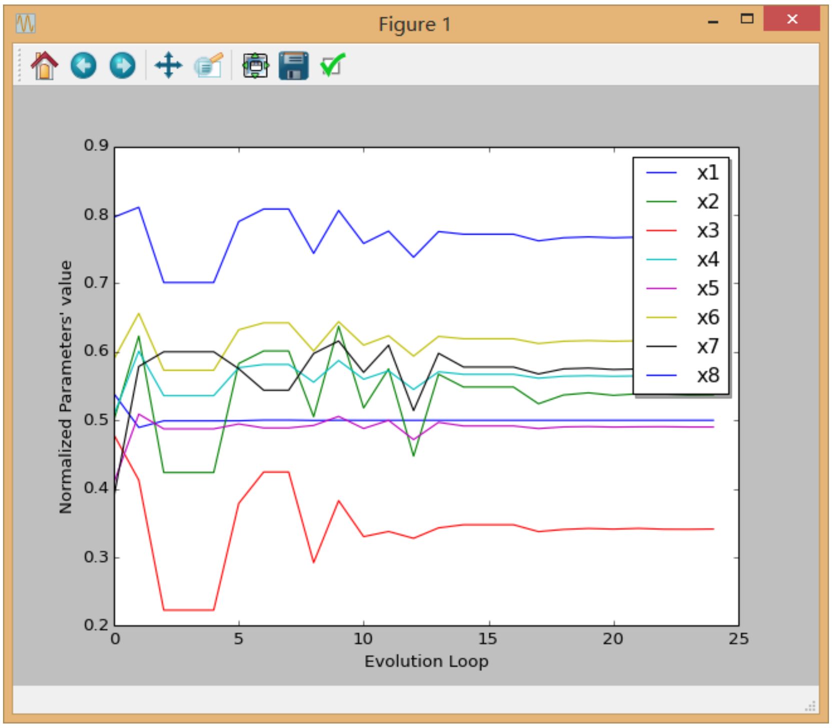
Step 2: Choose parameter optimization method and show results

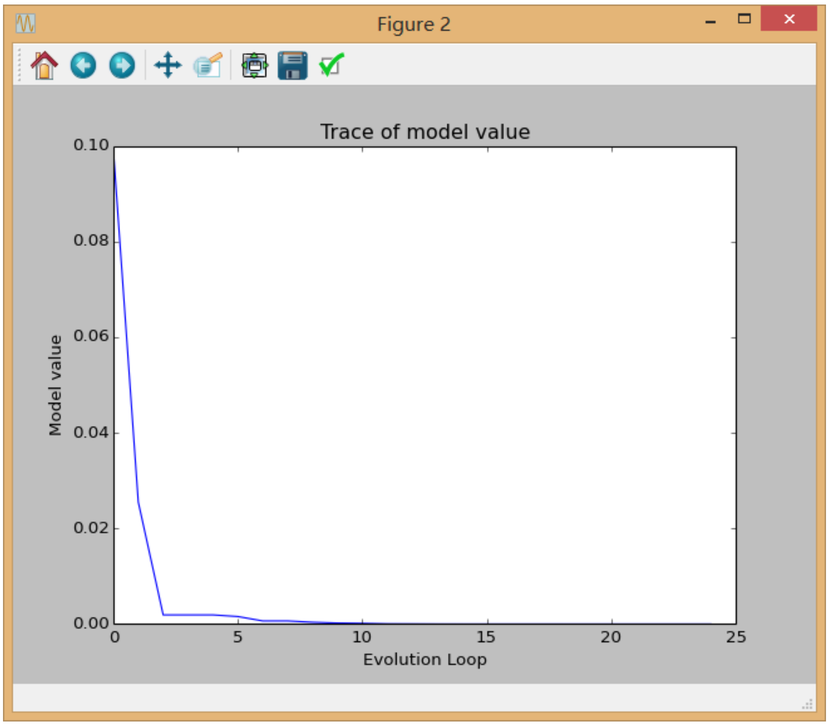
✧ Choose parameter optimization method, like "Shuffled Complex Evolution";

✧ Click "Show Results" button to show parameter optimization results.

UQ-PyL gives the tabular and graphic results:







This step can also implemented using python script:

Python script file (Sobol_G_Optimization.py)

```
# Optional - turn off bytecode (.pyc files)
import sys
sys.dont_write_bytecode = True
import shutil
```

```python
from UQ.optimization import SCE, ASMO, DDS, PSO
from UQ.util import scale_samples_general, read_param_file
import numpy as np
import random as rd

# Read the parameter range file
param_file = './UQ/test_functions/params/Sobol_G.txt'

bl=np.empty(0)
bu=np.empty(0)
pf = read_param_file(param_file)
for i, b in enumerate(pf['bounds']):
    bl = np.append(bl, b[0])
    bu = np.append(bu, b[1])

dir = './UQ/test_functions/'
shutil.copy(dir+'Sobol_G.py', dir+'functn.py')

# Run SCE-UA optimization algorithm
SCE.sceua(bl, bu, pf, ngs=2)
```

4.2 SAC-SMA model

4.2.1 Problem Definition

The SAC-SMA is a rainfall-runoff model which has a highly non-linear, non-monotonic input parameter-model output relationship. There are sixteen parameters in the SAC-SMA model. Thirteen of them are considered tunable, and the other three parameters are fixed at pre-specified values according to Brazil (1988). Table 1 describes those parameters and their ranges.

No.	Parameter	Description	Range
1	UZTWM	Upper zone tension water maximum storage (mm)	[10.0, 300.0]
2	UZFWM	Upper zone free water maximum storage (mm)	[5.0, 150.0]
3	UZK	Upper zone free water lateral drainage rate (day^{-1})	[0.10, 0.75]
4	PCTIM	Impervious fraction of the watershed area (decimal fraction)	[0.0, 0.10]
5	ADIMP	Additional impervious area (decimal fraction)	[0.0, 0.20]
6	ZPERC	Maximum percolation rate (dimensionless)	[5.0, 350.0]
7	REXP	Exponent of the percolation equation (dimensionless)	[1.0, 5.0]
8	LZTWM	Lower zone tension water maximum storage (mm)	[10.0, 500.0]

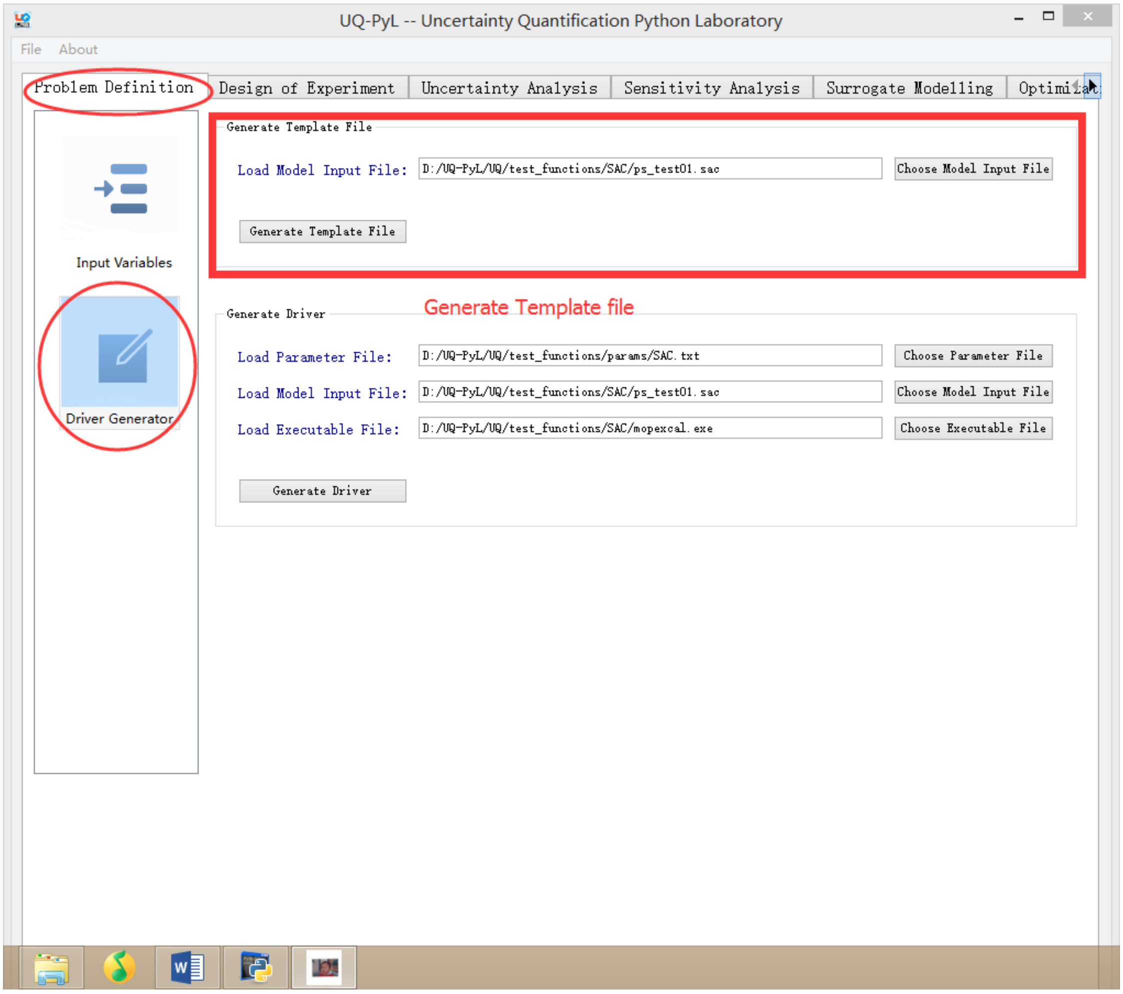
9	LZFSM	Lower zone supplemental free water maximum storage (mm)	[5.0, 400.0]
10	LZFPM	Lower zone primary free water maximum storage (mm)	[10.0, 1000.0]
11	LZSK	Lower zone supplemental free water lateral drainage rate (day^{-1})	[0.01, 0.35]
12	LZPK	Lower zone primary free water lateral drainage rate (day^{-1})	[0.001, 0.05]
13	PFREE	Fraction of water percolating from upper zone directly to lower zone free water (decimal fraction)	[0.0, 0.9]
14	RIVA	Riverside vegetation area (decimal fraction)	0.30
15	SIDE	Ration of deep recharge to channel base flow (dimensionless)	0.0
16	RSERV	Fraction of lower zone free water not transferrable to lower zone tension water (decimal fraction)	0.0

Table 6. Parameters of SAC-SMA model

So we generate the parameter file (UQ-PyL/UQ/test_functions/params/SAC.txt) as:

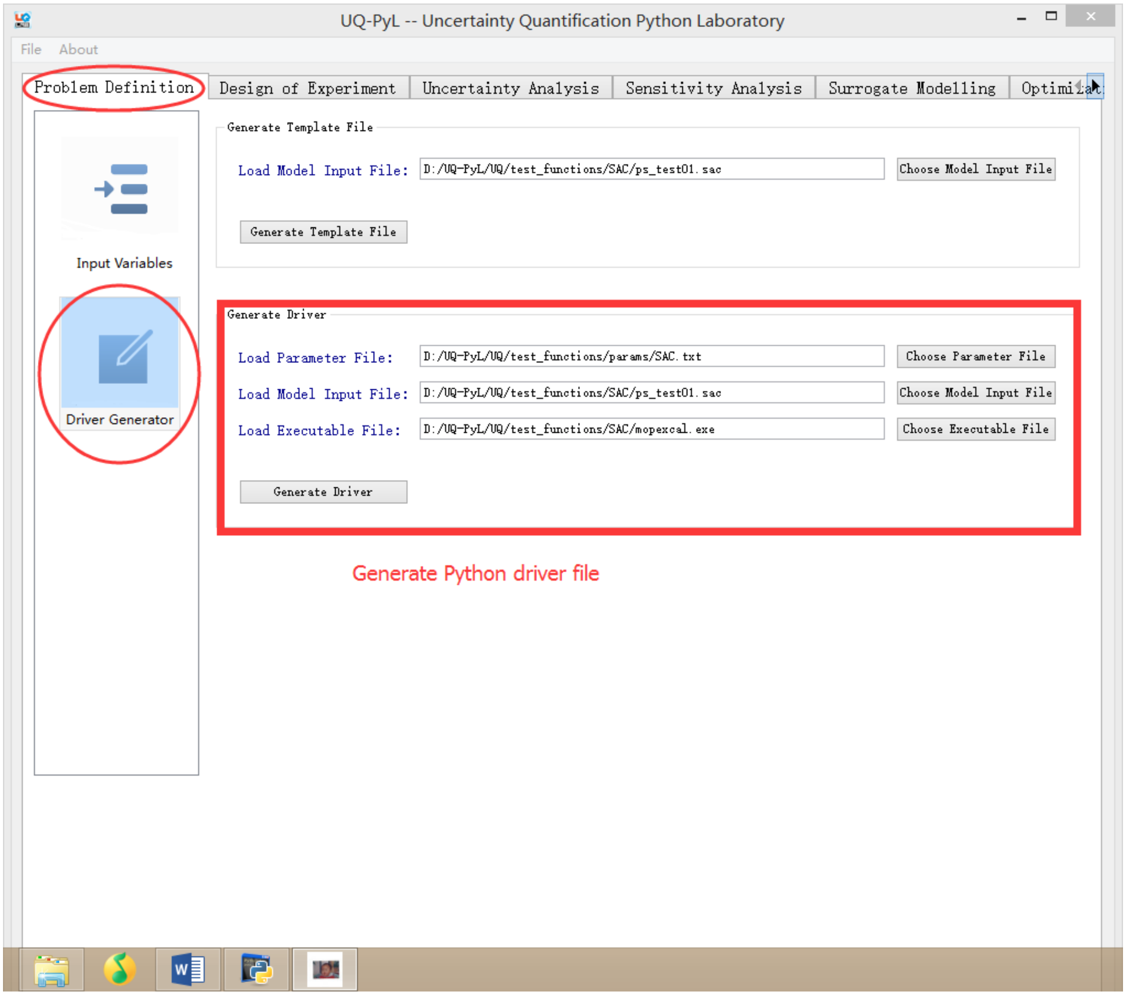
```
UZTWM 10 300
UZFWM 5 150
UZK 0.1 0.75
PCTIM 0 0.1
ADIMP 0 0.2
ZPERC 5 350
REXP 1 5
LZTWM 10 500
LZFSM 5 400
LZFPM 10 1000
LZSK 0.01 0.35
LZPK 0.001 0.05
PFREE 0 0.8
```

SAC-SMA model is an executable file on Windows or Linux or MacOS system. In order to using UQ-PyL, we need to generate a python driver to couple SAC-SMA model and UQ-PyL platform. The driver file can be generated automatically by UQ-PyL's GUI.



Step 1: Generate template file

- ✧ Choose "Problem Definition" tab, click on "Driver Generator" widget;
- ✧ Click "Choose Model Input File" to load model configuration file, for SAC model is "UQ-PyL/UQ/test_functions/SAC/ps_test01.sac";
- ✧ Click "Generate Template File" to generate model configuration template file, this file will be used in model driver file.



Step 2: Generate driver file

✧ Click "Choose Parameter File" to load model parameter file, for SAC model is "UQ-PyL/UQ/test_functions/params/SAC.txt";
✧ Click "Choose Model Input File" to load model configuration file, for SAC model is "UQ-PyL/UQ/test_functions/SAC/ps_test01.sac";
✧ Click "Choose Executable File" to load model executable file, for SAC model is "UQ-PyL/UQ/test_functions/SAC/mopexcal.exe";
✧ Click "Generate Driver" button to acquire model driver file.

The driver file (UQ-PyL/UQ/test_functions/SAC.py) shows below:

```
import os
import math
import string
import numpy as np
from ..util import read_param_file

########################################################
# USER SPECIFIC SECTION
#=======================================================
controlFileName = "D:/UQ-PyL/UQ/test_functions/params/SAC.txt"
```

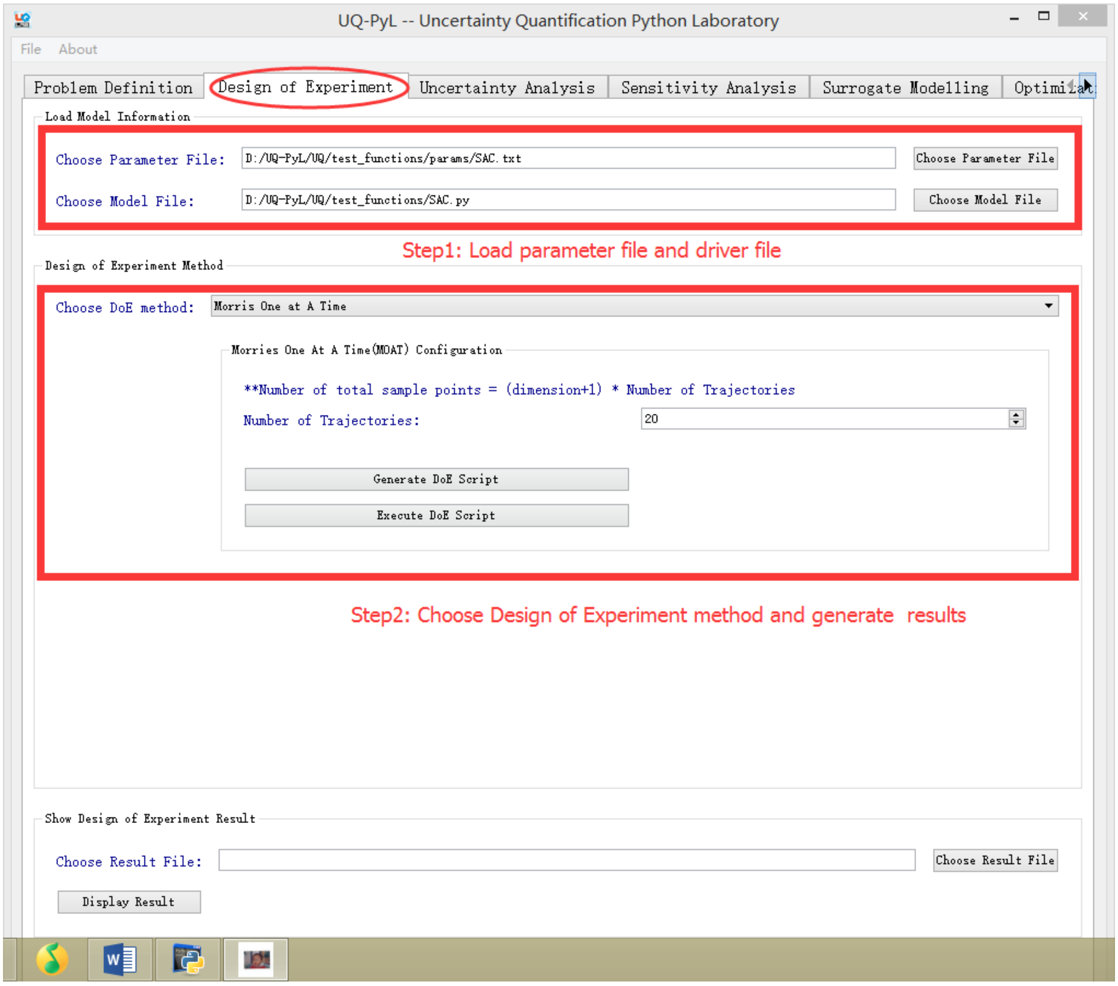
```
appInputFiles = "ps_test01.sac"
appInputTmplts = appInputFiles + ".Tmplt"

#######################################################
# FUNCTION: GENERATE MODEL INPUT FILE
#======================================================
def
genAppInputFile(inputData,appTmpltFile,appInputFile,nInputs,inputName
s):
    infile = open(appTmpltFile, "r")
    outfile = open(appInputFile, "w")
    while 1:
        lineIn  = infile.readline()
        if lineIn == "":
            break
        lineLen = len(lineIn)
        newLine = lineIn
        if nInputs > 0:
            for fInd in range(nInputs):
                strLen = len(inputNames[fInd])
                sInd = string.find(newLine, inputNames[fInd])
                if sInd >= 0:
                    sdata = '%7.3f' % inputData[fInd]
                    strdata = str(sdata)
                    next = sInd + strLen
                    lineTemp = newLine[0:sInd] + strdata +  " " +
newLine[next:lineLen+1]
                    newLine = lineTemp
                    lineLen = len(newLine)
        outfile.write(newLine)
    infile.close()
    outfile.close()
    return

#######################################################
# FUNCTION: RUN MODEL
#======================================================
def runApplication():
    sysComm = "mopexcal.exe"
    os.system(sysComm)
    return

#######################################################
# FUNCTION: CALCULATE DESIRE OUTPUT
```

```
#======================================================
def getOutput():
    Qe = []
    Qo = []
    functn = 0.0
    ignore  = 92
    I = 0
    outfile = open("ps_test01.sac.day", "r")
    for jj in range(ignore):
        lineIn  = outfile.readline()

    while 1:
        lineIn  = outfile.readline()
        if lineIn == "":
            break
        nCols = string.split(lineIn)
        Qe.append(eval(nCols[4]))
        Qo.append(eval(nCols[5]))
        functn = functn + (Qe[I] - Qo[I]) * (Qe[I] - Qo[I])
        I=I+1
    outfile.close()

    functn = functn/I
    functn = math.sqrt(functn)
    return functn

#######################################################
# MAIN PROGRAM
#======================================================
def predict(values):
    pf = read_param_file(controlFileName)
    for n in range(pf['num_vars']):
        pf['names'][n] = 'UQ_' + pf['names'][n]

    Y = np.empty([values.shape[0]])
    os.chdir('D:/UQ-PyL/UQ/test_functions/SAC')

    for i, row in enumerate(values):
        inputData = values[i]

genAppInputFile(inputData,appInputTmplts,appInputFiles,pf['num_vars']
,pf['names'])
        runApplication()
        Y[i] = getOutput()
```

```
        print "Job ID " + str(i+1)
    return Y
```

4.2.2 Design of Experiment

We do Design of Experiment for SAC-SMA model:



Step 1: Define parameter and model information

- ✧ Choose “Design of Experiment” tab;
- ✧ Load parameter file “UQ-PyL/UQ/test_functions/params/SAC.txt” and model file “UQ-PyL/UQ/test_functions/SAC.py” (for SAC model, it’s the model driver file generated before).

Step 2: Choose DoE method and run the results

- ✧ Choose DoE method “Morris One at A Time” and set “Number of Trajectories” = 20;
- ✧ Click “Generate DoE Script” button and “Execute DoE Script” button to acquire DoE results.

UQ-PyL gives the tabular and graphic results:

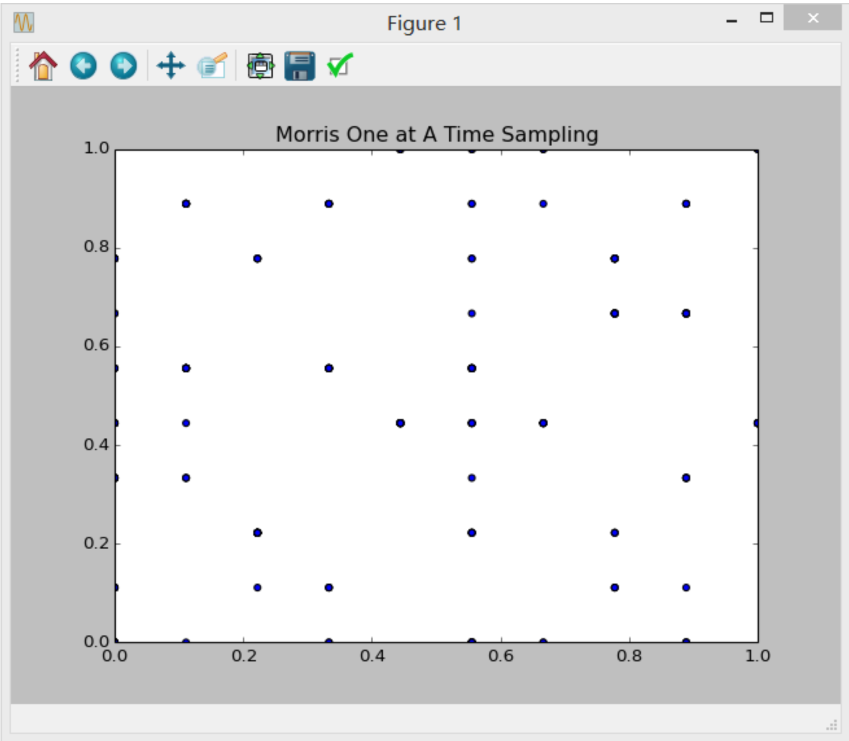
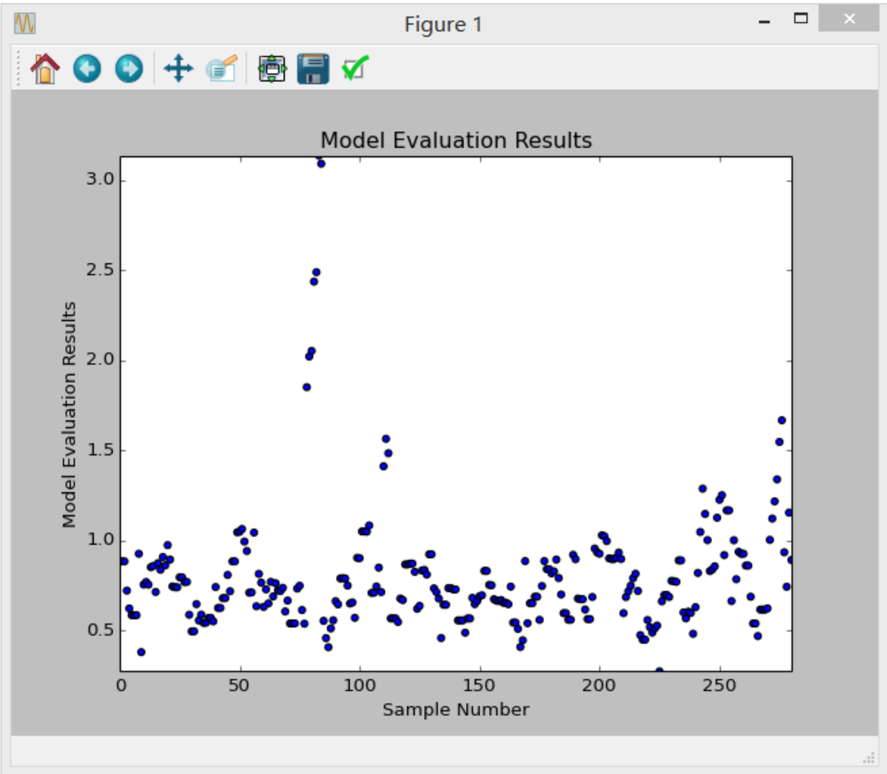


Figure 1
Morris One at A Time Sampling
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0


C:\Python27\python.exe
Job ID 6
Job ID 7
Job ID 8
Job ID 9
Job ID 10
Job ID 11
Job ID 12
Job ID 13
Job ID 14
Job ID 15
Job ID 16
Job ID 17
Job ID 18
Job ID 19
Job ID 20
Job ID 21
Job ID 22
Job ID 23
Job ID 24
Job ID 25
Job ID 26
Job ID 27
Job ID 28
微软拼音 半 ：



This step can also implemented using python script:

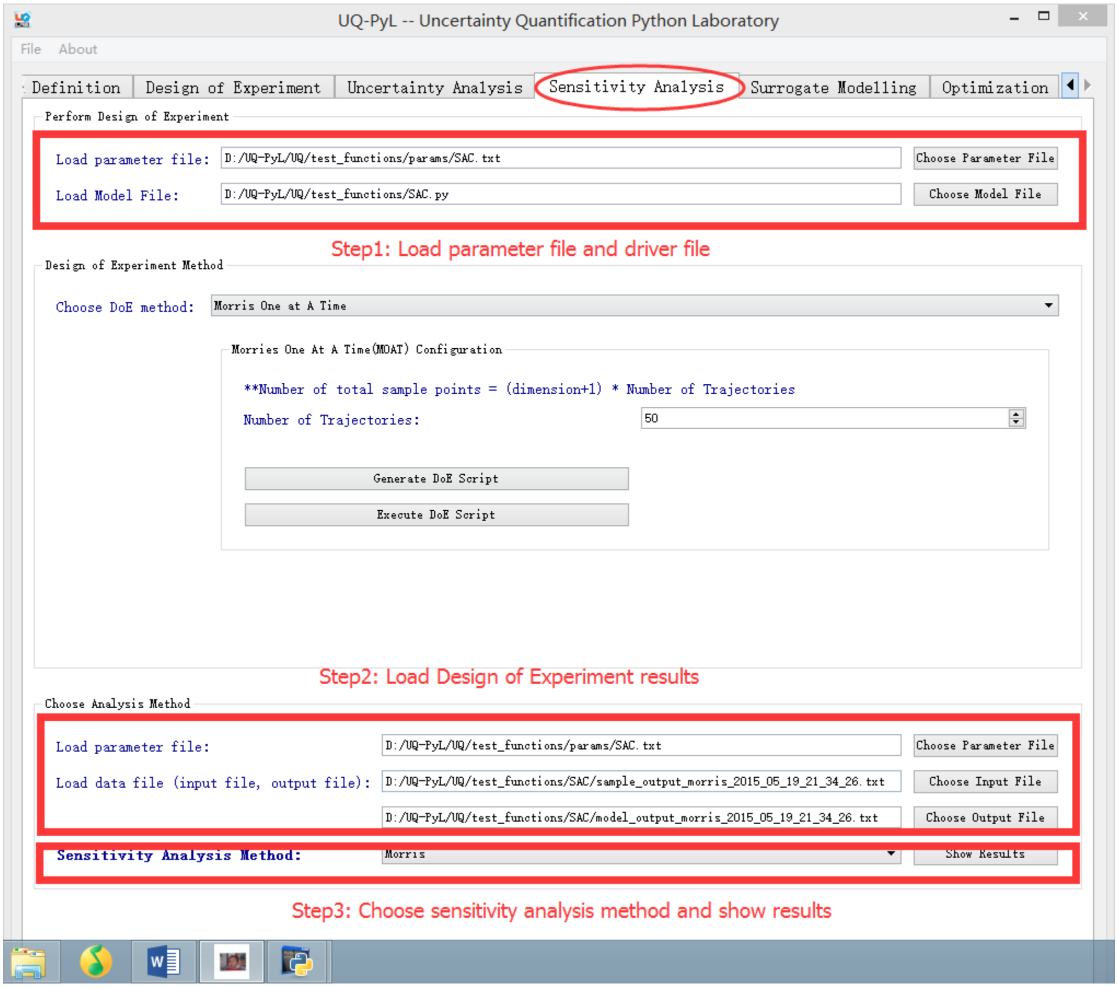
Python script file (SAC_DoE.py)

```
# Optional - turn off bytecode (.pyc files)
import sys
sys.dont_write_bytecode = True

from UQ.DoE import morris_oat
from UQ.test_functions import SAC
from UQ.util import scale_samples_general, read_param_file, discrepancy
import numpy as np
import random as rd

# Set random seed (does not affect quasi-random Sobol sampling)
seed = 1
np.random.seed(seed)
rd.seed(seed)

# Read the parameter range file and generate samples
param_file = './UQ/test_functions/params/SAC.txt'
pf = read_param_file(param_file)

# Generate samples (choose method here)
param_values = morris_oat.sample(20, pf['num_vars'], num_levels = 10,
```

```
grid_jump = 5)

# Samples are given in range [0, 1] by default. Rescale them to your
parameter bounds.
scale_samples_general(param_values, pf['bounds'])
np.savetxt('Input_Sobol\'.txt', param_values, delimiter=' ')

# Run the "model" and save the output in a text file
# This will happen offline for external models
Y = SAC.predict(param_values)
np.savetxt("Output_Sobol\'.txt", Y, delimiter=' ')
```

4.2.3 Sensitivity Analysis

Then, we do sensitivity analysis for 13 parameters of SAC-SMA model:



Step 1: Define parameter and model information

- ✧ Choose "Sensitivity Analysis" tab;
- ✧ Load parameter file "UQ-PyL/UQ/test_functions/params/SAC.txt" and model file (driver file) "UQ-PyL/UQ/test_functions/SAC.py".

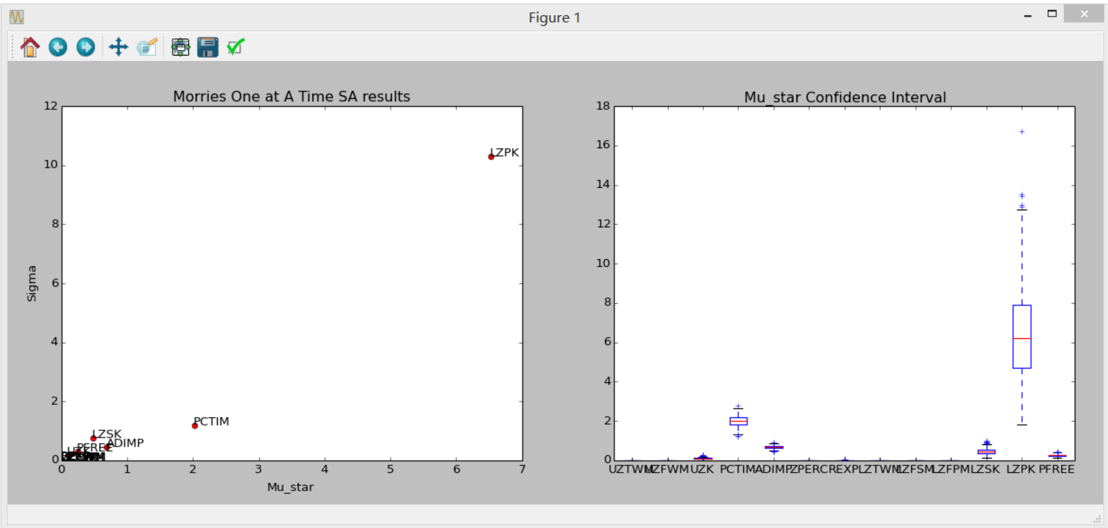
Step 2: Load DoE results

✧ Load DoE results, sample input file "UQ-PyL/UQ/test_functions/SAC/sample_output_morris_2015_05_19_21_34_26.txt" and model output file "UQ-PyL/UQ/test_functions/SAC/model_output_morris_2015_05_19_21_34_26.txt".

Step 3: Choose sensitivity analysis method and show results

✧ Choose sensitivity analysis method "Morris" and click "Show Results" button to acquire sensitivity analysis results.

UQ-PyL gives the tabular and graphic results:



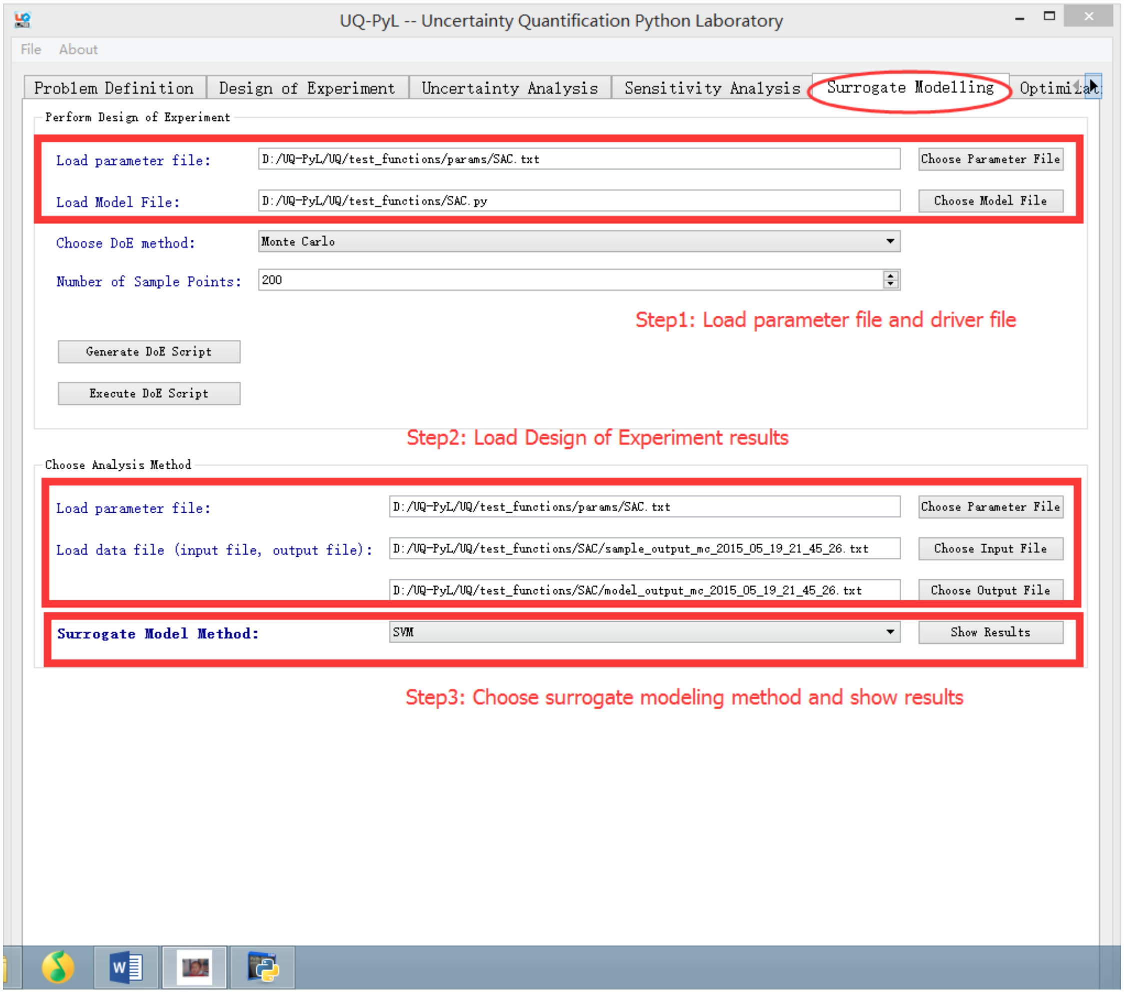
This step can also implemented using python script:

Python script file (SAC_SA.py)

```
# Optional - turn off bytecode (.pyc files)
import sys
sys.dont_write_bytecode = True

from UQ.DoE import morris_oat
from UQ.analyze import *
from UQ.test_functions import SAC
from UQ.util import scale_samples_general, read_param_file
import numpy as np
import random as rd

# Set random seed (does not affect quasi-random Sobol sampling)
seed = 1
np.random.seed(seed)
```

```
rd.seed(seed)

# Read the parameter range file and generate samples
param_file = './UQ/test_functions/params/SAC.txt'
pf = read_param_file(param_file)

# Generate samples (choose method here)
param_values = morris_oat.sample(20, pf['num_vars'], num_levels = 10,
grid_jump = 5)

# Samples are given in range [0, 1] by default. Rescale them to your
parameter bounds.
scale_samples_general(param_values, pf['bounds'])
np.savetxt('Input_SAC.txt', param_values, delimiter=' ')

# Run the "model" and save the output in a text file
# This will happen offline for external models
Y = SAC.predict(param_values)
np.savetxt("Output_SAC.txt", Y, delimiter=' ')

# Perform the sensitivity analysis/uncertainty analysis using the model
output
# Specify which column of the output file to analyze (zero-indexed)
morris.analyze(param_file, 'Input_SAC.txt', 'Output_SAC.txt', column =
0)
```

4.2.4 Surrogate Modeling



Step 1: Define parameter and model information

- ✧ Choose “Surrogate Modeling” tab;
- ✧ Load parameter file “UQ-PyL/UQ/test_functions/params/SAC.txt” and model file (driver file) “UQ-PyL/UQ/test_functions/SAC.py”.

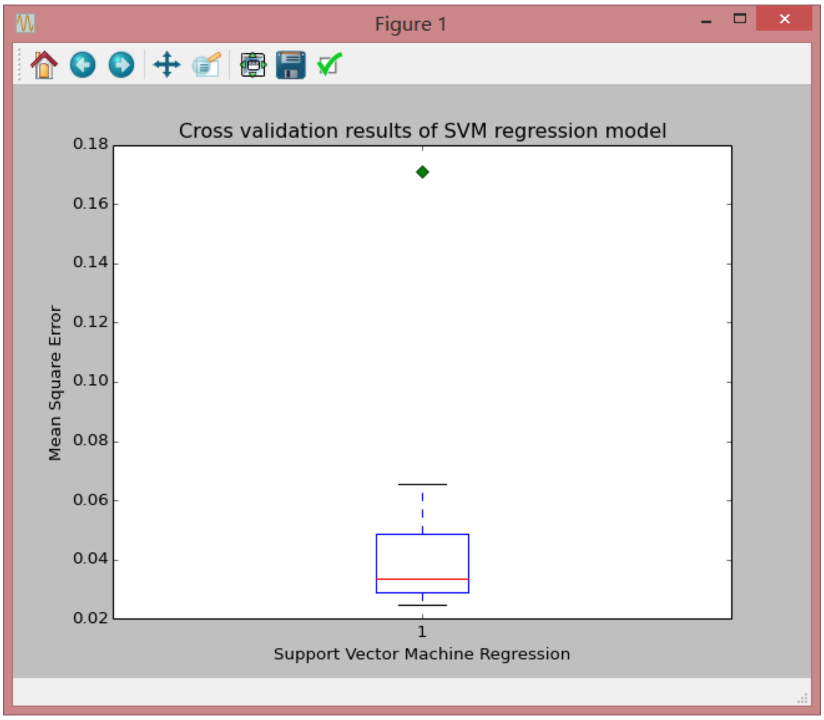
Step 2: Load DoE results for surrogate modeling

- ✧ Choose DoE results, sample input file “UQ-PyL/UQ/test_functions/SAC/sample_output_mc_2015_05_19_21_45_26.txt” and model output file “UQ-PyL/UQ/test_functions/SAC/model_output_mc_2015_05_19_21_45_26.txt”.

Step 3: Choose surrogate modeling method and show results

- ✧ Choose surrogate modeling method “SVM”;
- ✧ Click “Show Results” button to acquire surrogate modeling results.

UQ-PyL gives the tabular and graphic results:



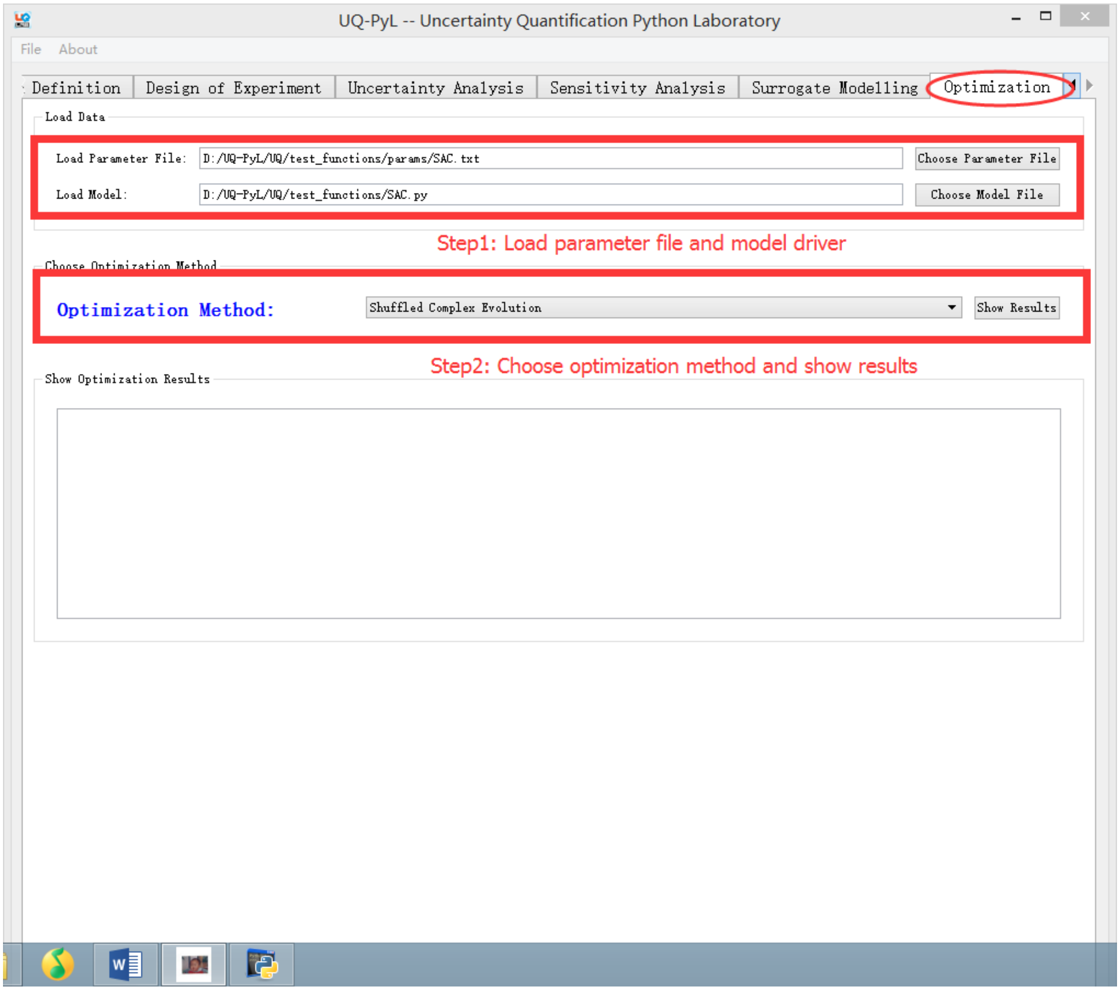
This step can also implemented using python script:

Python script file (SAC_Surrogate.py)

```
# Optional - turn off bytecode (.pyc files)
import sys
sys.dont_write_bytecode = True

from UQ.DoE import monte_carlo
from UQ.test_functions import SAC
from UQ.util import scale_samples_general, read_param_file, discrepancy
import numpy as np
import random as rd

# Set random seed (does not affect quasi-random Sobol sampling)
seed = 1
np.random.seed(seed)
rd.seed(seed)

# Read the parameter range file and generate samples
param_file = './UQ/test_functions/params/SAC.txt'
pf = read_param_file(param_file)

# Generate samples (choose method here)
param_values = monte_carlo.sample(500, pf['num_vars'])
```

```
# Samples are given in range [0, 1] by default. Rescale them to your
parameter bounds.
scale_samples_general(param_values, pf['bounds'])
np.savetxt('Input_SAC.txt', param_values, delimiter=' ')

# Run the "model" and save the output in a text file
# This will happen offline for external models
Y = SAC.predict(param_values)
np.savetxt("Output_SAC.txt", Y, delimiter=' ')

# Perform regression analysis using the model output
# Specify which column of the output file to analyze (zero-indexed)
model = SVR.regression('Input_SAC', 'Output_SAC', column = 0, cv = True)
```

4.2.5 Parameter Optimization



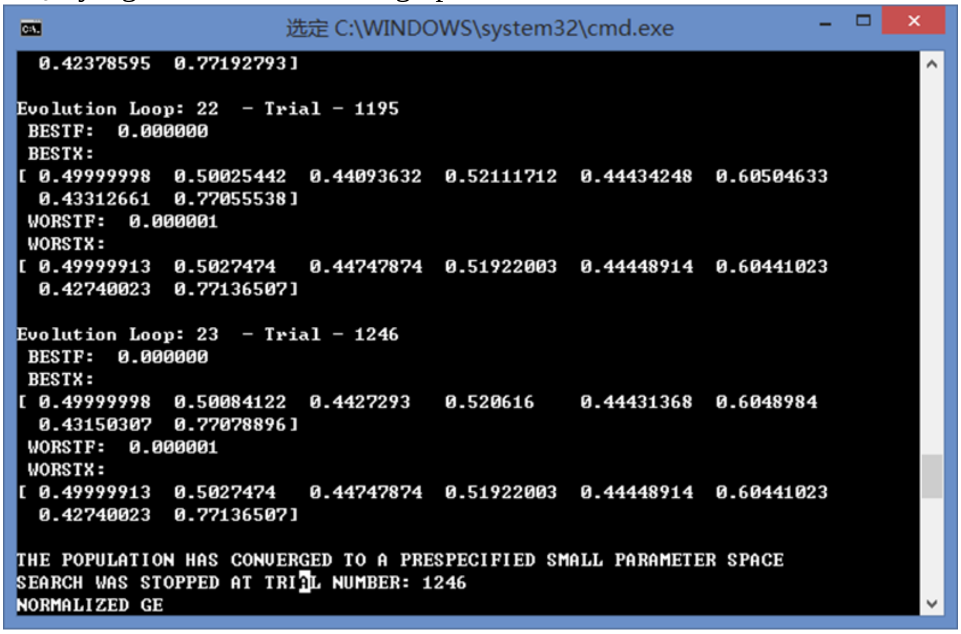
Step 1: Define parameter and model information

- ✧ Choose “Optimization” tab;
- ✧ Load parameter file “UQ-PyL/UQ/test_functions/params/SAC.txt” and model file (driver file) “UQ-PyL/UQ/test_functions/SAC.py”.

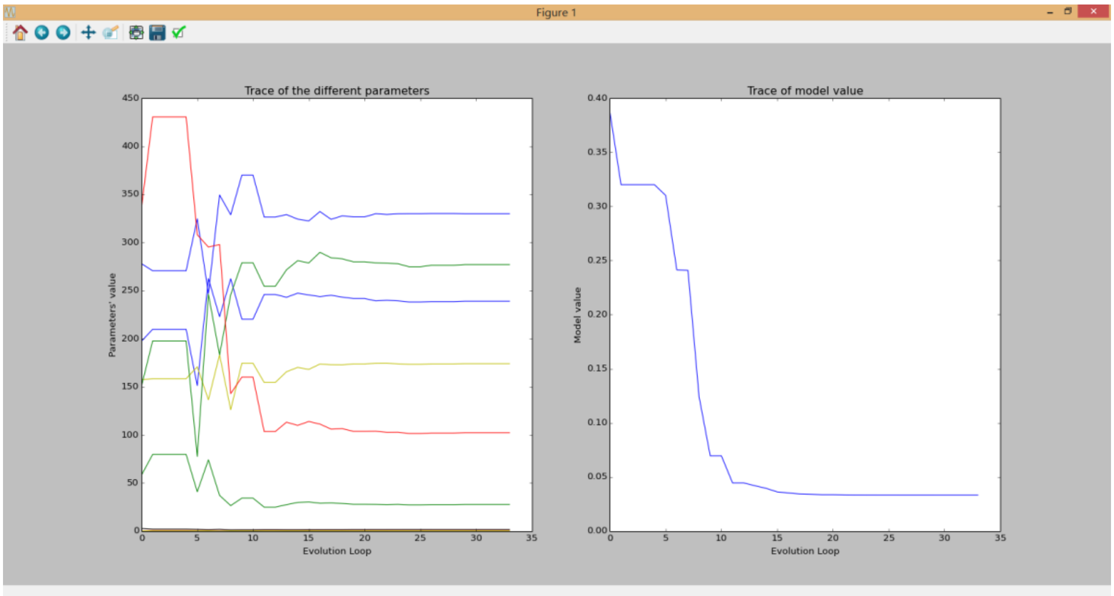
Step 2: Choose optimization method and show results

✧ Choose optimization method “Shuffled Complex Evolution” and click “Show Results” button to acquire optimization results.

UQ-PyL gives the tabular and graphic results:



```
选定 C:\WINDOWS\system32\cmd.exe
  0.42378595  0.77192793]

Evolution Loop: 22  - Trial - 1195
 BESTF:  0.000000
 BESTX:
[ 0.49999998  0.50025442  0.44093632  0.52111712  0.44434248  0.60504633
  0.43312661  0.77055538]
 WORSTF:  0.000001
 WORSTX:
[ 0.49999913  0.5027474   0.44747874  0.51922003  0.44448914  0.60441023
  0.42740023  0.77136507]

Evolution Loop: 23  - Trial - 1246
 BESTF:  0.000000
 BESTX:
[ 0.49999998  0.50084122  0.4427293   0.520616    0.44431368  0.6048984
  0.43150307  0.77078896]
 WORSTF:  0.000001
 WORSTX:
[ 0.49999913  0.5027474   0.44747874  0.51922003  0.44448914  0.60441023
  0.42740023  0.77136507]

THE POPULATION HAS CONVERGED TO A PRESPECIFIED SMALL PARAMETER SPACE
SEARCH WAS STOPPED AT TRIAL NUMBER: 1246
NORMALIZED GE
```



This step can also implemented using python script:

Python script file (SAC_Optimization.py)

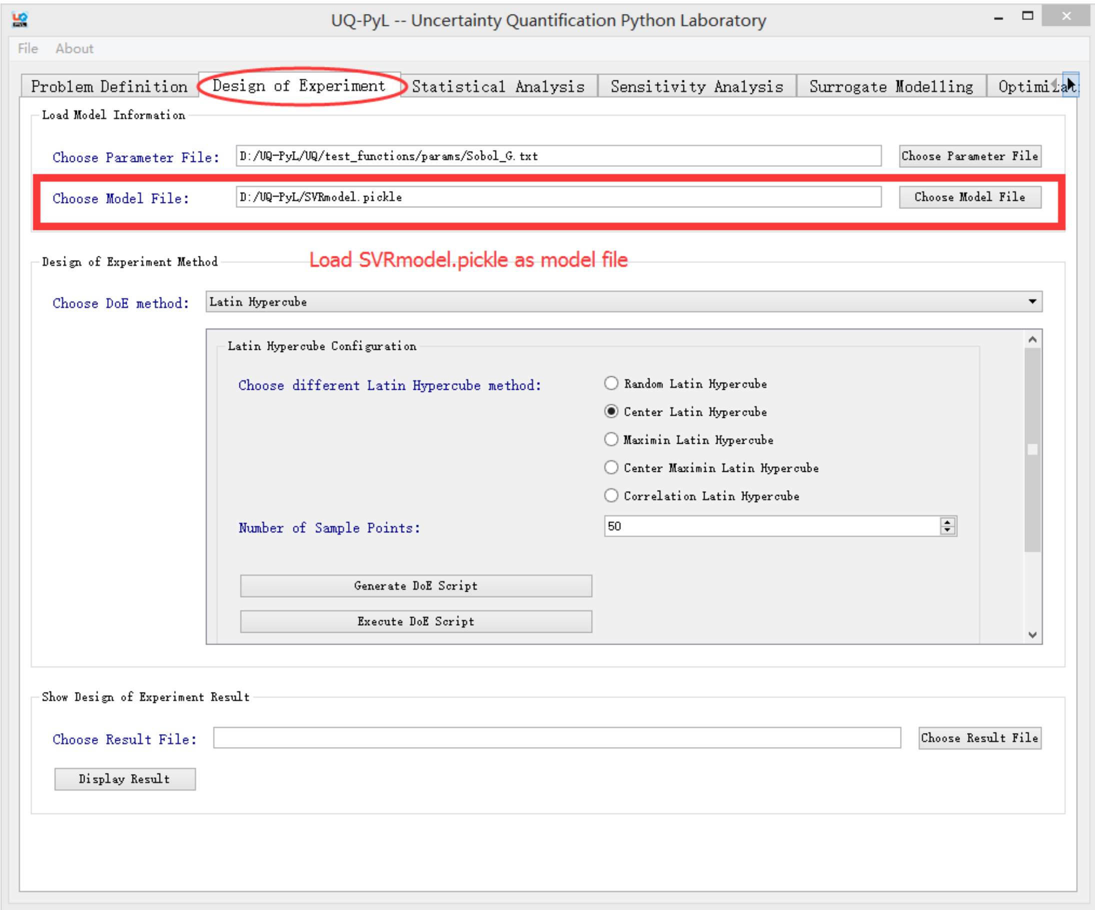
```
# Optional - turn off bytecode (.pyc files)
import sys
sys.dont_write_bytecode = True
import shutil
```

```
from UQ.optimization import SCE
from UQ.util import scale_samples_general, read_param_file, discrepancy
import numpy as np
import random as rd

# Read the parameter range file
param_file = './UQ/test_functions/params/SAC.txt'

bl=np.empty(0)
bu=np.empty(0)
pf = read_param_file(param_file)
for i, b in enumerate(pf['bounds']):
    bl = np.append(bl, b[0])
    bu = np.append(bu, b[1])

dir = './UQ/test_functions/'
shutil.copy(dir+'SAC.py', dir+'functn.py')

# Run SCE-UA optimization algorithm
SCE.sceua(bl, bu, ngs=2)
```

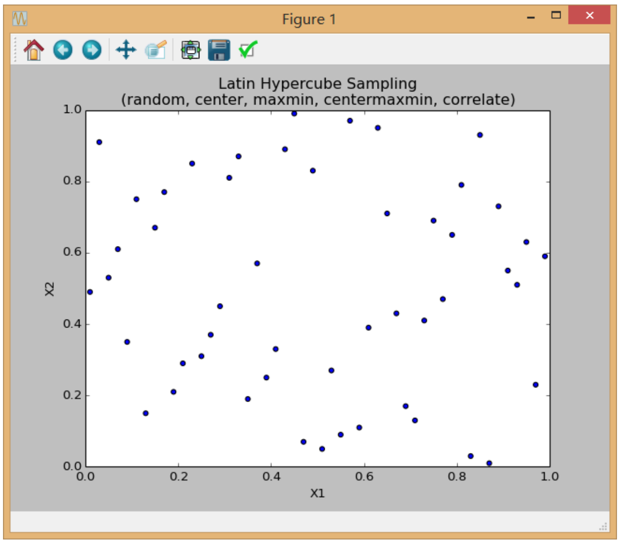
4.3 Run simulation on surrogate model

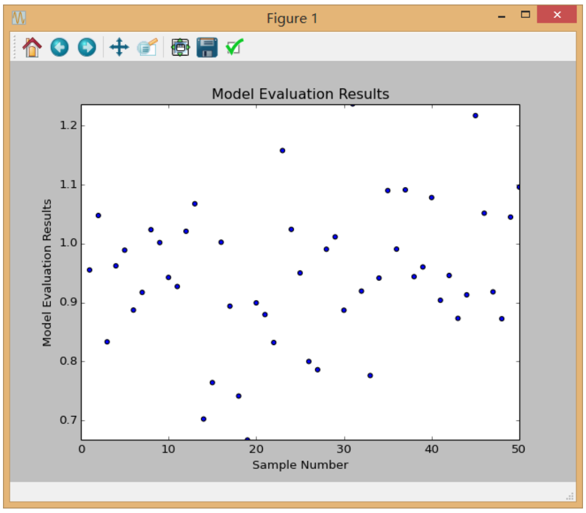
In Surrogate Modeling part, we generate a surrogate model from data sets of original model and save the surrogate model in a *.pickle file. Then we can run simulation on the surrogate model we saved.

For Design of Experiment part, we choose the model file as *.pickle file, then it can run DoE on the surrogate model you created. Let's take Sobol' G function as an example. In section 4.1.5 we have created a surrogate model and saved it as "SVRmodel.pickle" file. In Design of Experiment tab, we load "UQ-PyL/ SVRmodel.pickle" file as model file, all the others as same as section 4.1.2:



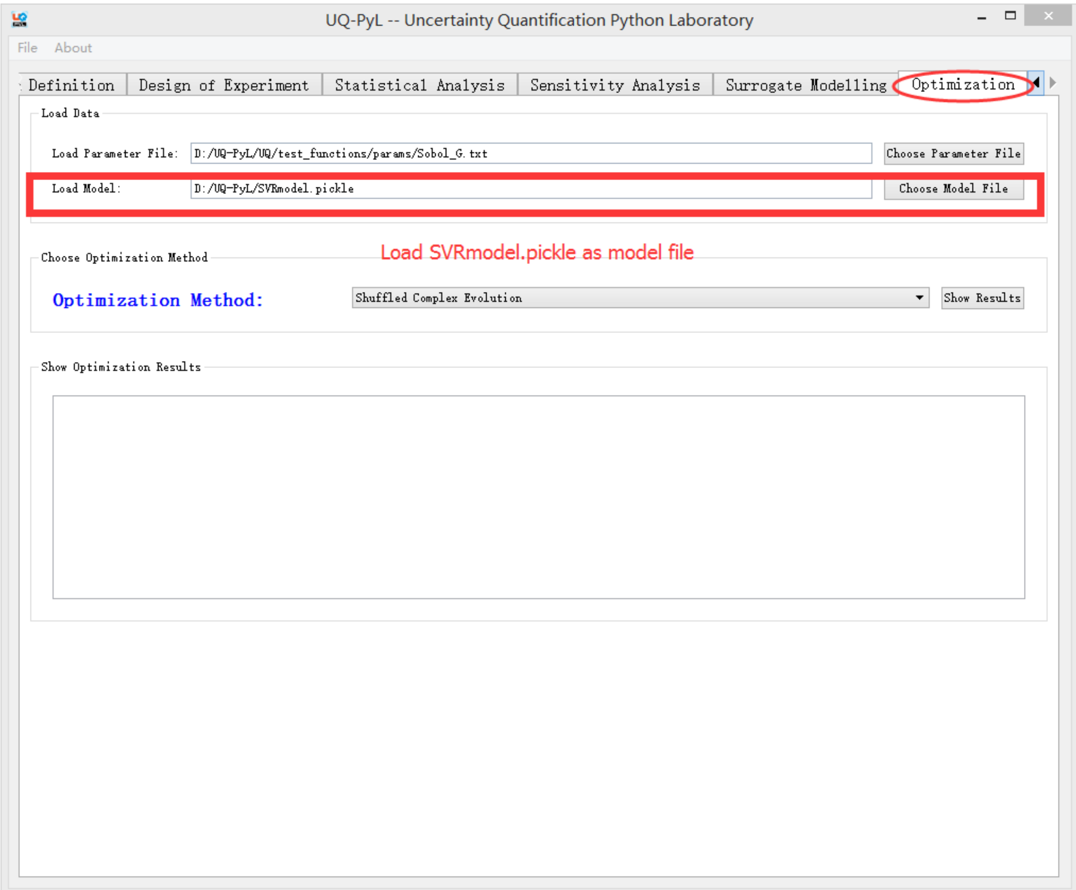
Then we do DoE analysis, it can obtain tabular and graphic results:



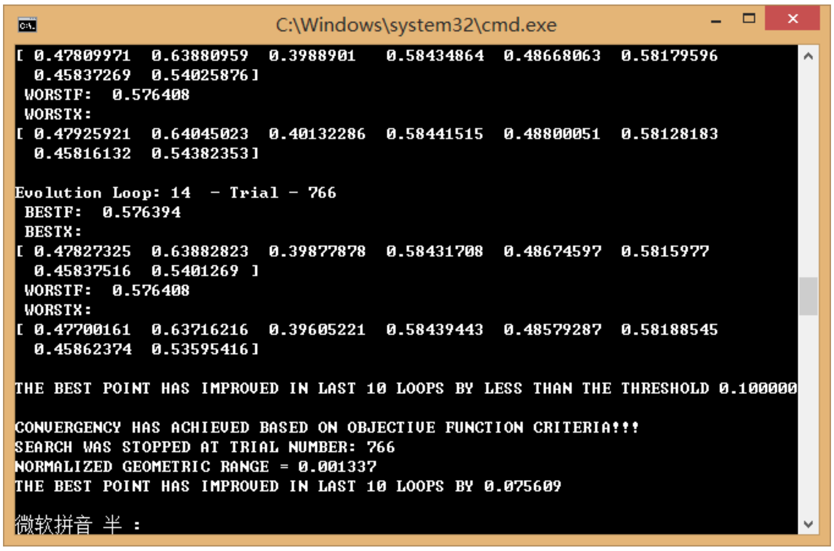


The result is different from run the same algorithm on the original Sobol' G function model.

For Parameter Optimization part, we also choose the model file as *.pickle file, then it can run global optimization algorithm on the surrogate model.



Then we do SCE parameter optimization algorithm, it can obtain tabular and graphic results:


C:\Windows\system32\cmd.exe
[0.47809971 0.63880959 0.3988901 0.58434864 0.48668063 0.58179596
0.45837269 0.54025876]
WORSTF: 0.576408
WORSTX:
[0.47925921 0.64045023 0.40132286 0.58441515 0.48800051 0.58128183
0.45816132 0.54382353]
Evolution Loop: 14 - Trial - 766
BESTF: 0.576394
BESTX:
[0.47827325 0.63882823 0.39877878 0.58431708 0.48674597 0.5815977
0.45837516 0.5401269]
WORSTF: 0.576408
WORSTX:
[0.47700161 0.63716216 0.39605221 0.58439443 0.48579287 0.58188545
0.45862374 0.53595416]
THE BEST POINT HAS IMPROVED IN LAST 10 LOOPS BY LESS THAN THE THRESHOLD 0.100000
CONVERGENCY HAS ACHIEVED BASED ON OBJECTIVE FUNCTION CRITERIA!!!
SEARCH WAS STOPPED AT TRIAL NUMBER: 766
NORMALIZED GEOMETRIC RANGE = 0.001337
THE BEST POINT HAS IMPROVED IN LAST 10 LOOPS BY 0.075609
微软拼音 半 :

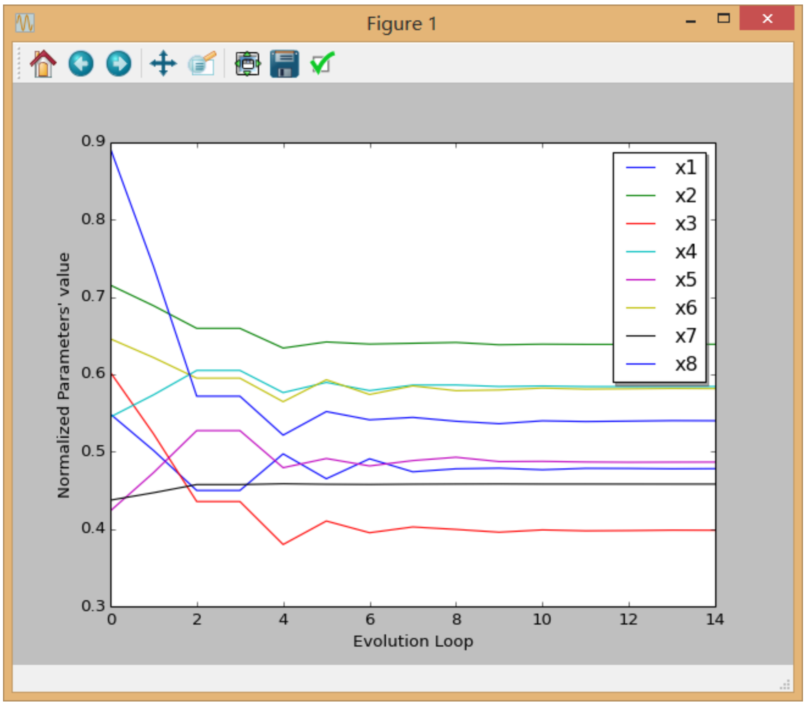
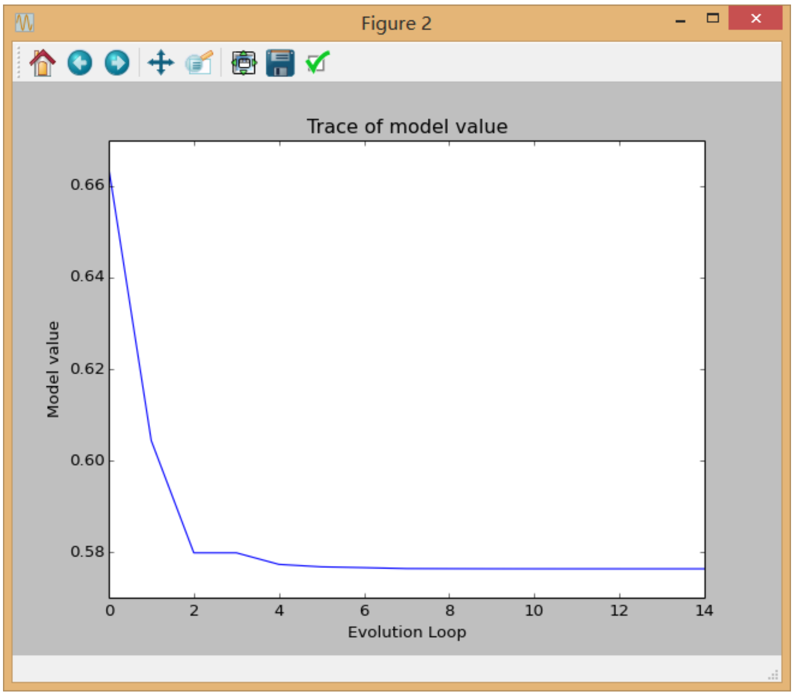


Figure 1
Normalized Parameters' value
Evolution Loop
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0
2
4
6
8
10
12
14
x1
x2
x3
x4
x5
x6
x7
x8



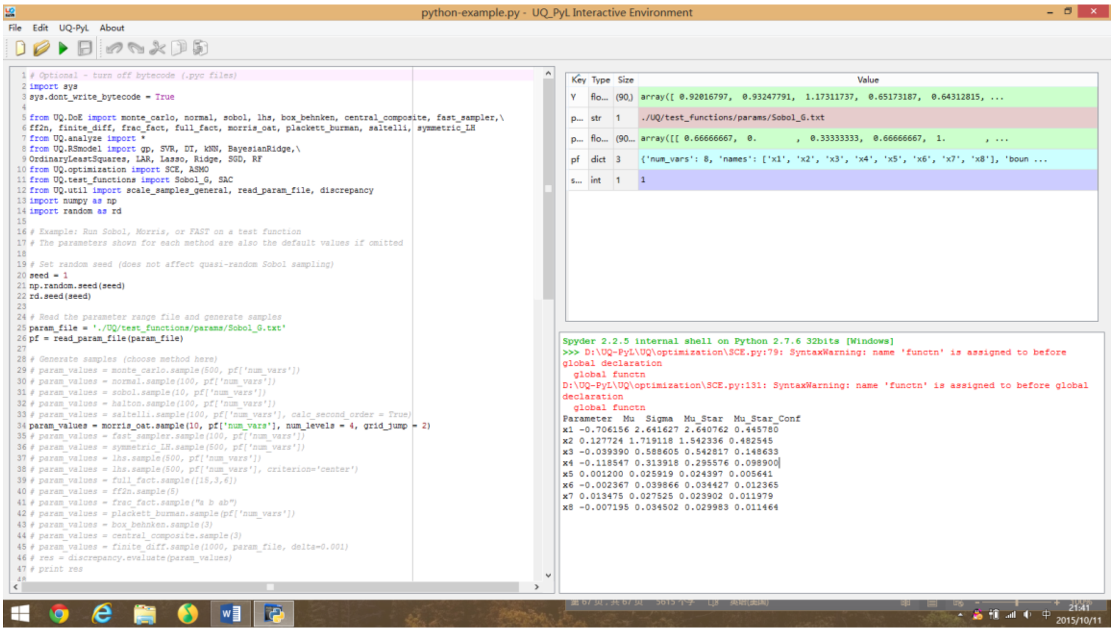
Also, the result is different from run the same algorithm on the original Sobol' G function model.

4.4 Use Interactive UQ-PyL Software

4.4.1 How to run interactive UQ-PyL Software

In version 1.1, we have an interactive version of UQ-PyL software. Double click the "UQ-PyL Interactive" icon 

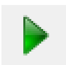
you can enter the software. Also, you can run ".\UQ-PyL\main_interactive.pyw" file to enter into the interactive version of UQ-PyL software. Below is the main page of the software:

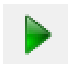


Interactive version of UQ-PyL software

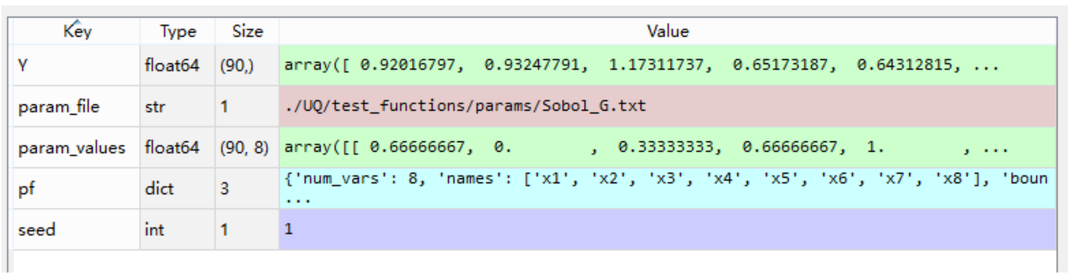
The interface is very similar to MATLAB GUI, we use Spyder package (http://pythonhosted.org/spyder/) to achieve this function. The left part of the interface is a code editor, you can type your python code here. After run the python code, you can see internal variable values in the upper right of the interface and output results in the lower right part.

4.4.2 How to use interactive UQ-PyL Software

Method One: You can write your own python code in the editor part then click "Run" button  to run the python script. Variable values and output values will be display on the upper right part and lower right part of the interface.

Method Two: Also you can click "Open" button  to load a exist python script file, for example ".\UQ-PyL\python-example.py", then click "Run" button  to run the python script.

You can see the variable values below:



Key	Type	Size	Value
Y	float64	(90,)	array([0.92016797, 0.93247791, 1.17311737, 0.65173187, 0.64312815, ...
param_file	str	1	./UQ/test_functions/params/Sobol_G.txt
param_values	float64	(90, 8)	array([[0.66666667, 0. , 0.33333333, 0.66666667, 1. , ...
pf	dict	3	{'num_vars': 8, 'names': ['x1', 'x2', 'x3', 'x4', 'x5', 'x6', 'x7', 'x8'], 'boun ...
seed	int	1	1

And tabular and graphic outputs:

Parameter	Mu	Sigma	Mu_Star	Mu_Star_Conf
x1	-0.706156	2.641627	2.640762	0.445780
x2	0.127724	1.719118	1.542336	0.482545
x3	-0.039390	0.588605	0.542817	0.148633
x4	-0.118547	0.313918	0.295576	0.098900
x5	0.001200	0.025919	0.024397	0.005641
x6	-0.002367	0.039866	0.034427	0.012365
x7	0.013475	0.027525	0.023902	0.011979
x8	-0.007195	0.034502	0.029983	0.011464