introducing

easyGSA

available on GitHub MENDELEY DATA MATLAB® File Exchange

Efficient global sensitivity analysis using mechanistic or machine learning models

+ Highly increased computational efficiency
+ Reliably rank important parameters
+ Quickly identify key design parameters in a design space
+ Tap into the power of machine learning libraries

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Outline

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Introducing syntax and features

Benchmark problems

1. Ishigami function
2. gSobol function
3. Cantilever Beam functions

Engineering applications

1. Wastewater treatment plant design space exploration

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What it can do for you

easyGSA at a glance

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> Easy-to-work syntax to perform GSA using Sobol method and SRC method.

> Sampling schemes: Sobol sequences, Latin hypercube sampling (LHS).

> Automatic hyperparameter optimization for Gaussian process models

> Gridsearch optimization algorithm for finding best neural networks configuration

> Allowing user provided data to fit surrogates and perform Sobol GSA.

> Automatic data cleaning.

> Efficient use of available parallelization architecture.

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How to use

easyGSA: basic syntax

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```
[Si,STi] = easyGSA(f,N,InputSpace{:})
```

First order indices

Total order indices

Handle of the model s.t. GSA

Size of the sampling matrices used by Sobol GSA

A cell array of input parameter names, lower/upper bounds or means/sigmas.

```
InputSpace = {'ParNames',pars,...
              'LowerBounds',lbs,...
              'UpperBounds',ubs};
```

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```
[Si,STi,results] = easyGSA(f,N,InputSpace{:},...
                           'SamplingMethod','LHS',...
                           'Estimator','Saltelli',...
                           'UseSurrogate','GPR',...
                           'UseParallel',true,...
                           'Verbose',false)
```

Use Latin hypercube sampling to sample the input space

Use 'Saltelli' estimator for Sobol indices calculation

Use Gaussian process models as a surrogate

Activate parallel computing

Suppress command line messages

More detailed results of the analysis containing all the models and simulation results.

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How to use

easyGSA: Input arguments overview

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Required argument

Optional argument

Available options

Default setting in bold

Argument	Options
‘Model’	@ishigami @mymodel.m
‘N’	**2e3** ..
‘InputSpace’	‘LowerBounds’ ‘UpperBounds’
‘SamplingMethod’	**‘Sobol’** ‘LHS’
‘Estimator’	**‘Jansen’** ‘Saltelli’
‘UseSurrogate’	‘GPR’ ‘ANN’
‘Method’	**Sobol** SRC
‘UserData’	Data.X Data.Y
‘UseParallel’	true **false**
‘Verbose’	**true** false

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Ishigami function

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Easy syntax to perform GSA using Sobol method

```
%% Test on Ishigami function: Analytical sensitivities are known
f = @(x) sin(x(:,1)) + 7.*sin(x(:,2)).^2 + 0.1.*x(:,3).^4.*sin(x(:,1));
N = 1e3; % Number of MC samples

% define input parameter space
pars = strseq('x',1:3); % input parameter names
lbs  = -pi.*ones(1,3);  % lower bounds of input parameters
ubs  =  pi.*ones(1,3);  % upper bounds of input parameters
InputSpace = {'ParNames',pars,'LowerBounds',lbs,'UpperBounds',ubs};

% call easyGSA to perform Sobol sensitivity analysis with MC approach
[Si,STi] = easyGSA(f,N,InputSpace{:})
```

$$f(x) = \sin(x_1) + a\sin^2(x_2) + bx_3^4\sin(x_1)$$

$$x_i \sim U(-\pi,\pi), \text{ for all } i = 1,2,3$$

Model implementation from https://www.sfu.ca/~ssurjano/ishigami.html

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Easy syntax to perform GSA using Sobol method

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InputSpace = {'ParNames',pars,'LowerBounds',lbs,'UpperBounds',ubs};

% call easyGSA to perform Sobol sensitivity analysis with MC approach
[Si,STi] = easyGSA(f,N,InputSpace{:})
```

Change sampling method and MC estimator

```
[Si,STi] = easyGSA(f,N,InputSpace{:}, ...
                 'SamplingMethod','LHS',... % also: 'Sobol'
                 'Estimator','Jansen')      % also: 'Saltelli'
```

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Use a Gaussian Process regression model to do the GSA

```
% use a GPR model instead
[gprSi, gprSTi] = easyGSA(f,N,parameters{:}, ...
                          'UseSurrogate','GPR')
```

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Use a Gaussian Process regression model to do the GSA

```
% use a GPR model instead
[gprSi, gprSTi] = easyGSA(f,N,parameters{:}, ...
                          'UseSurrogate','GPR')
```

Use an artificial neural network model to do the GSA

```
% use an ANN model instead
[annSi, annSTi] = easyGSA(f,N,parameters{:}, ...
                          'UseSurrogate','ANN')
```

Benchmark problems

Ishigami function

Use a Gaussian Process regression model to do the GSA

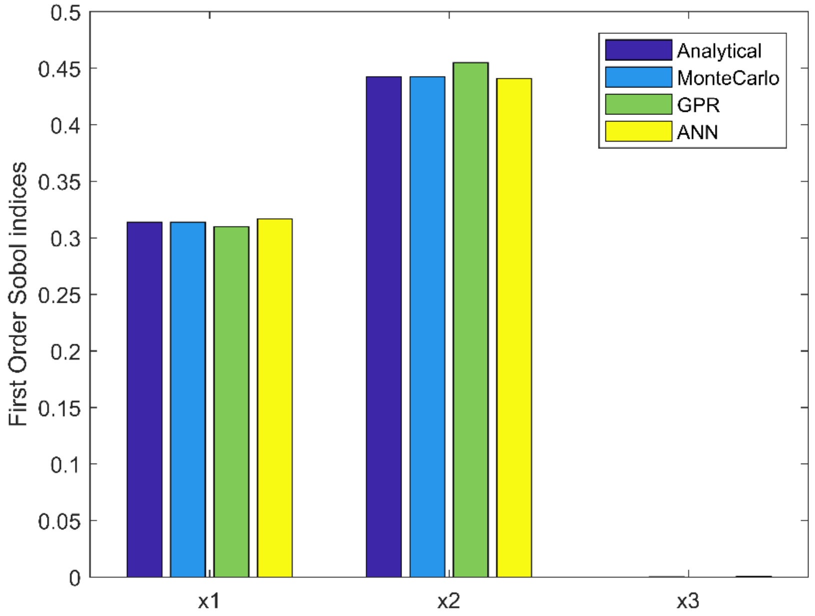
```
% use a GPR model instead
[gprSi, gprSTi] = easyGSA(f,N,parameters{:}, ...
                         'UseSurrogate','GPR')
```

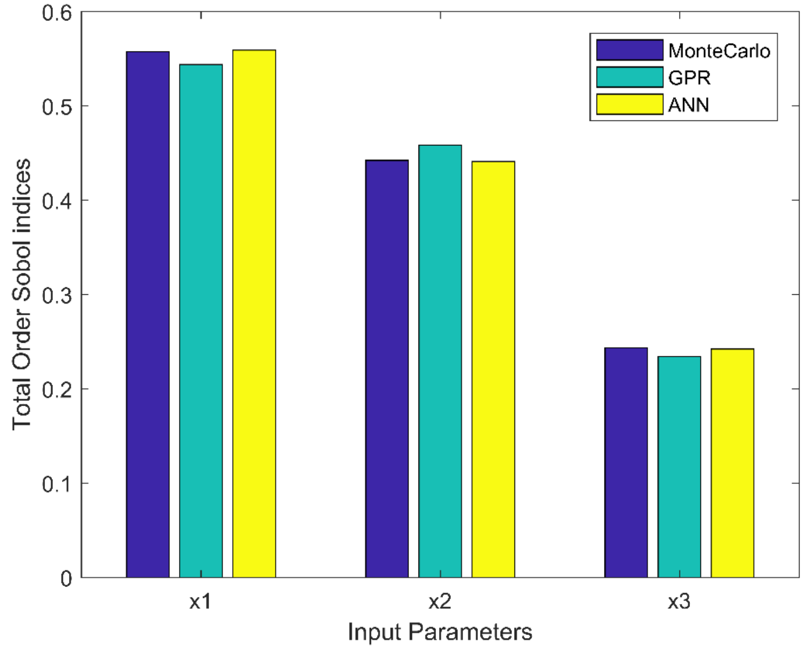
Use an artificial neural network model to do the GSA

```
% use an ANN model instead
[annSi, annSTi] = easyGSA(f,N,parameters{:}, ...
                         'UseSurrogate','ANN')
```

Use parallel computing to speed up

```
% use an ANN model instead
[annSi, annSTi] = easyGSA(f,N,parameters{:}, ...
                         'UseSurrogate','ANN', ...
                         'UseParallel','true')
```





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g-function of Sobol

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The model

$$f(x)=\prod_{i=1}^{d}\frac{|4x_i-2|+a_i}{1+a_i},\ \text{where}$$

$$a_i=\frac{i-2}{2},\ \text{for all } i=1,\dots,d$$

$$x_i\sim U(0,1),\ \text{for all } i=1,\dots,d$$

Model implementation from https://www.sfu.ca/~ssurjano/gfunc.html

Analytical Si indices can be found below.

Marrel, A., Iooss, B., Laurent, B., Roustant, O., 2009. Calculations of Sobol indices for the Gaussian process metamodel. Reliab. Eng. Syst. Saf. 94, 742–751. https://doi.org/10.1016/j.ress.2008.07.008

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g-function of Sobol

```
f = @(x) gSobol(x);
N = 1e6; % Number of MC samples

pars = strseq('x',1:5); % input parameter names
lbs  = zeros(1,5);      % lower bounds of input parameters
ubs  = ones(1,5);       % upper bounds of input parameters
parameters = {'ParNames',pars,'LowerBounds',lbs,'UpperBounds',ubs};

% Monte Carlo indices from the original model
[mcSi,mcSTi] = easyGSA(f,N,parameters{:});

% GPR indices
[gprSi, gprSTi] = easyGSA(f,N,parameters{:},'UseSurrogate','GPR')

% ANN indices
[annSi, annSTi] = easyGSA(f,N,parameters{:},'UseSurrogate','ANN')
```

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```
f = @(x) gSobol(x);
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pars = strseq('x',1:5); % input parameter names
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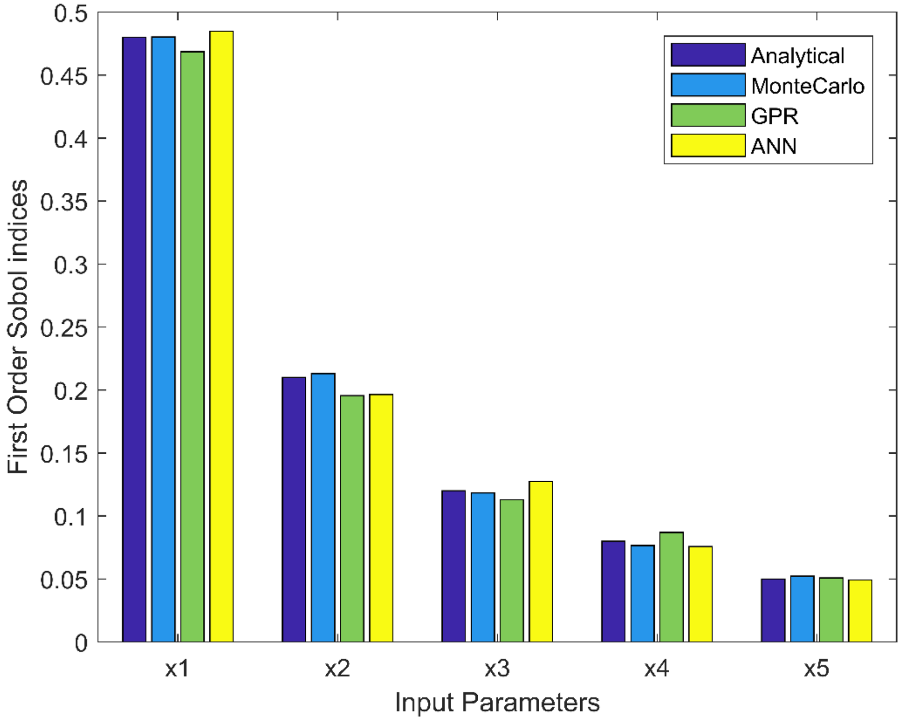
% Monte Carlo indices from the original model
[mcSi,mcSTi] = easyGSA(f,N,parameters{:});

% GPR indices
[gprSi, gprSTi] = easyGSA(f,N,parameters{:},'UseSurrogate','GPR')

% ANN indices
[annSi, annSTi] = easyGSA(f,N,parameters{:},'UseSurrogate','ANN')
```



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Benchmark problems

The Cantilever Beam functions

Multiple outputs

$$D(x) = \frac{4L^3}{E\omega t}\sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{\omega^2}\right)^2}$$

$$S(x) = \frac{600Y}{\omega t^2} + \frac{600X}{\omega t^2}$$

The Cantilever Beam functions, used for uncertainty quantification, model a simple uniform cantilever beam with horizontal and vertical loads. The beam length L and displacement tolerance D0 at the free end of the beam are problem constants, with values L = 100 inches, and D0 = 2.2535 inches. The parameters w and t are width and thickness of the cross-section.

The responses are displacement (D) and stress (S).

Normally distributed input space

R ~ N(μ=40000, σ=2000)	yield stress
E ~ N(μ=2.9E7, σ=1.45E6)	Young's modulus of beam material
X ~ N(μ=500, σ=100)	horizontal load
Y ~ N(μ=1000, σ=100)	vertical load

Model implementation from
https://www.sfu.ca/~ssurjano/canti.html

Related tutorial

demo_canti.m

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The Cantilever Beam functions

Normally distributed input space with defined μ and σ

```
f = @cantibeam; % handle to the cantibeam.m model file
N = 2e3; % Number of Monte Carlo samples

% Input Space definiton
pars   = {'R','E','X','Y'};      % input parameter names
means  = [4e4 2.9e7 5e2 1e3];    % mean values of input parameters
stds   = [2e3 1.45e6 1e2 1e2];   % std deviations of input parameters
InputSpace = {'ParNames',pars,'Means',means,'Sigmas',stds};

% call easyGSA tool to perform Sobol GSA with MC approach
[Si,STi,results] = easyGSA(f,N,InputSpace{:},'UseParallel',true)
```

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Normally distributed input space with defined μ and σ

```
f = @cantibeam; % handle to the cantibeam.m model file
N = 2e3; % Number of Monte Carlo samples

% Input Space definiton
pars   = {'R','E','X','Y'};      % input parameter names
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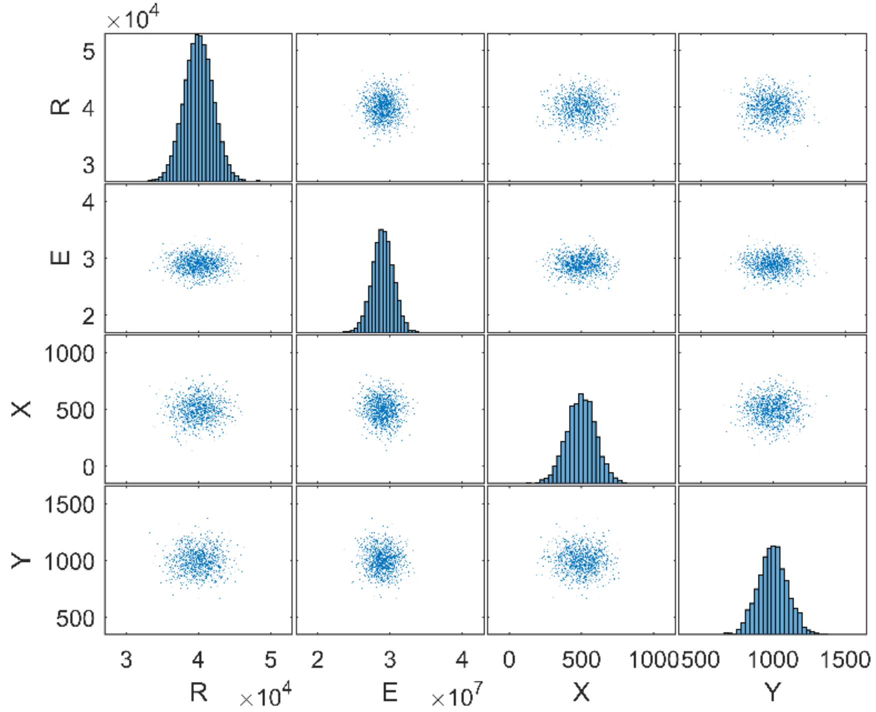
% call easyGSA tool to perform Sobol GSA with MC approach
[Si,STi,results] = easyGSA(f,N,InputSpace{:},'UseParallel',true)
```



Plot input sampling matrices

```
% visualize input sampling matrices
figure; [~,ax]=plotmatrix(results.A); np=numel(pars);
for i=1:np
    ylabel(ax(i,1),pars(i)); xlabel(ax(np,i),pars(i));
end
```

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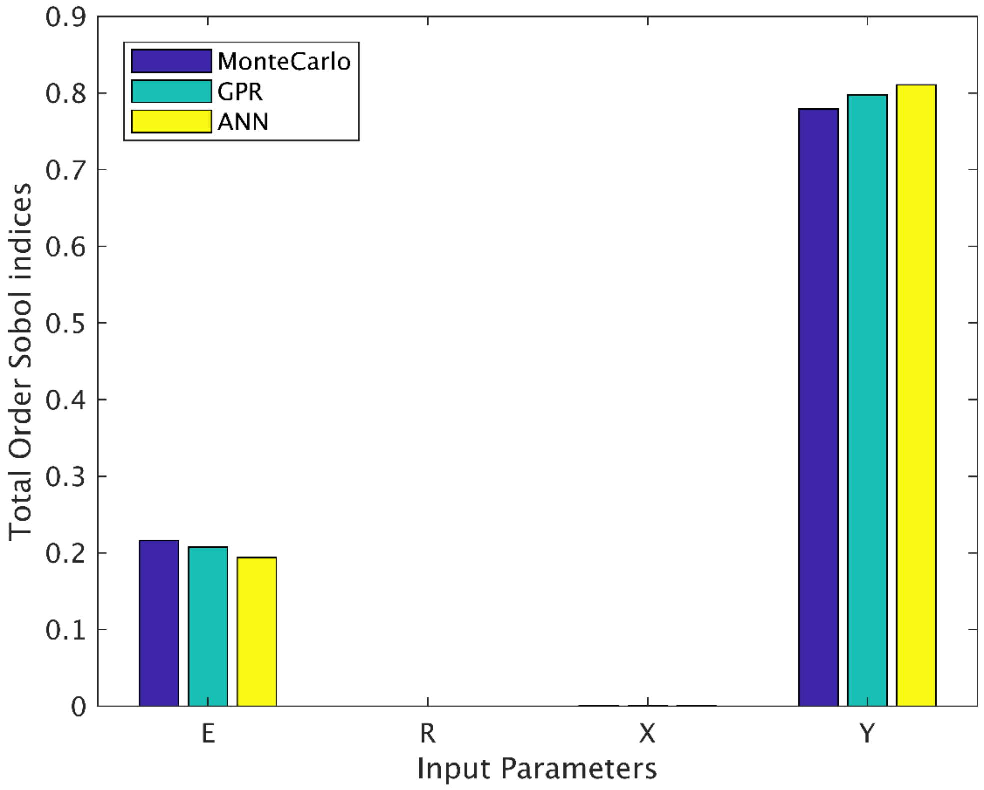

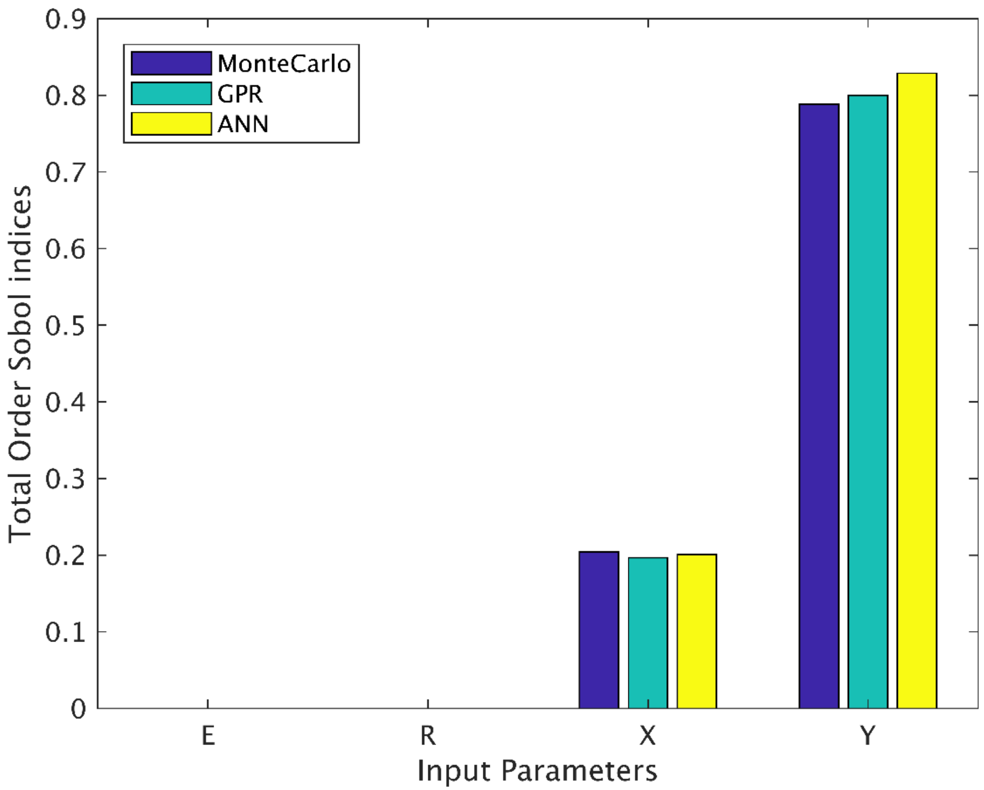

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Using your own data

User data support

Use your own Monte Carlo Simulation data to quickly fit GPR and ANN models and perform the GSA

```
% Inputting your own dataset to perform GPR and ANN-based GSA

% Step 1: Load your own data, eg. simulation results, etc.
[X,Y] = chemical_dataset; X=X'; Y=Y'; % a standard MATLAB dataset

% Step 2: Put your data into a struct. Only X and Y fields are expected.
Data.X = X; % inputs
Data.Y = Y; % outputs

% Step 3: pass your data into easyGSA
[Si,STi,results] = easyGSA('UserData',Data) % uses GPR models by default.

% Step 4: Fit ANN models and perform a Sobol GSA
[Si,STi,results] = easyGSA('UserData',Data,...
                           'UseSurrogate','ANN')
```

Related tutorial

demo_UserData.m

Simulation model integration

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```
function y= mySimModel(x)
    %% How to plug your Simulink model to easyGSA

    % load your system and itinial conditions.
    sys = 'bsm2_ol';
    load_system(sys);
    init_bsm2;

    % pass your input variables x to corresponding values
    Qinf = x(1);
    Qw = x(2);
    ...

    % simulate your system inside a function
    myOptions = simset('SrcWorkspace','current','DstWorkspace','current');
    sim(sys,[], myOptions);

    % process your simulation results and return an output y (for ex:KPI)
    perf_plant_bsm2;
    y = [];
end
```

Engineering Application

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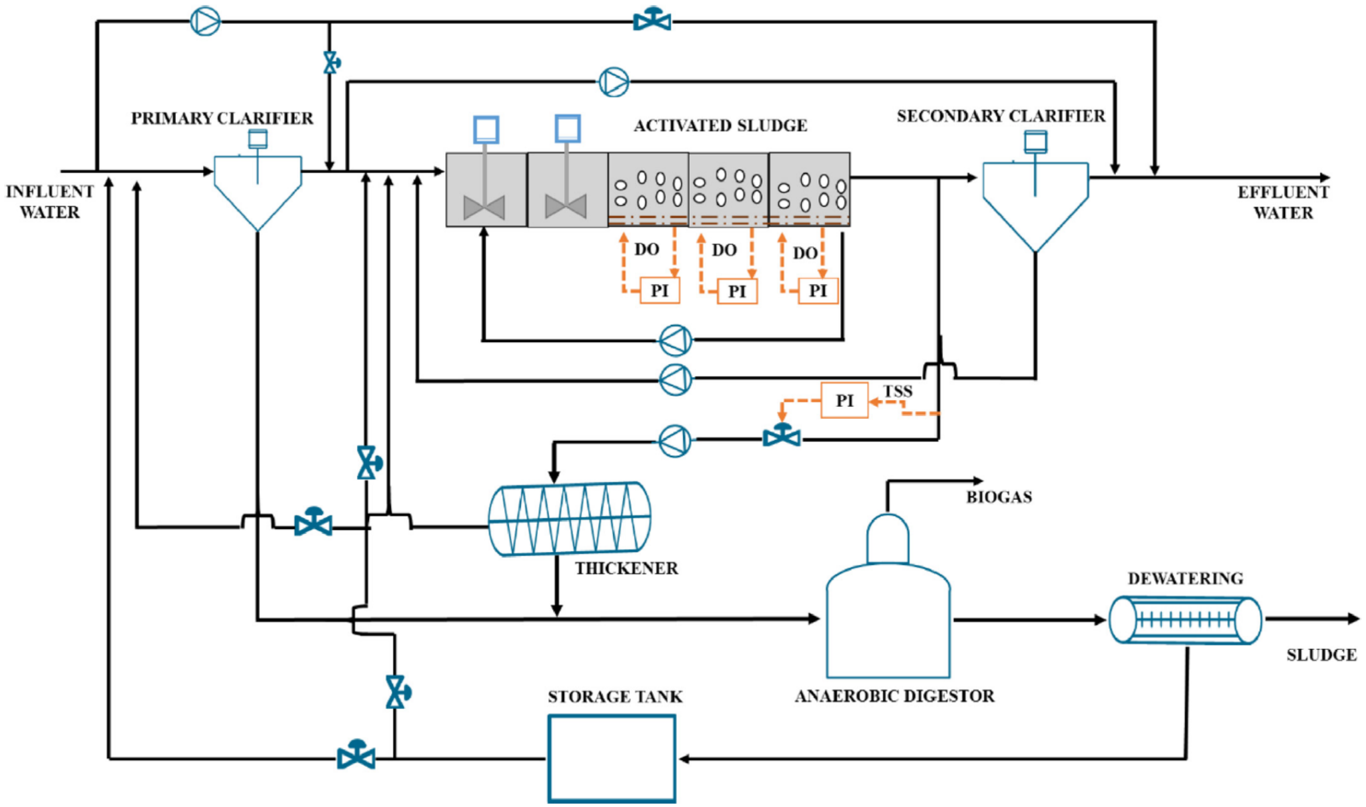
Find the design decisions that are most influencing the key plant performance indicators (KPIs).



Benefits of surrogate-based methodology becomes the most evident when you have expensive-to-evaluate simulation models.

e.g. Benchmark Simulation Model 2

Engineering Application

Wastewater treatment plant application

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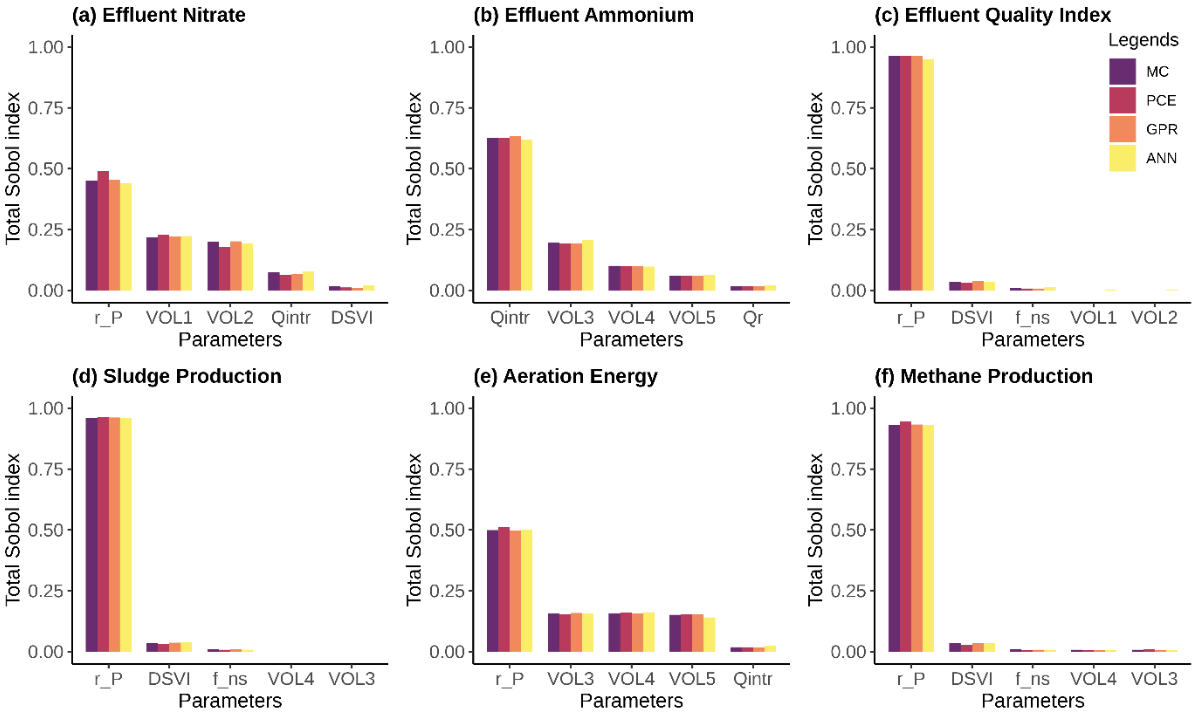
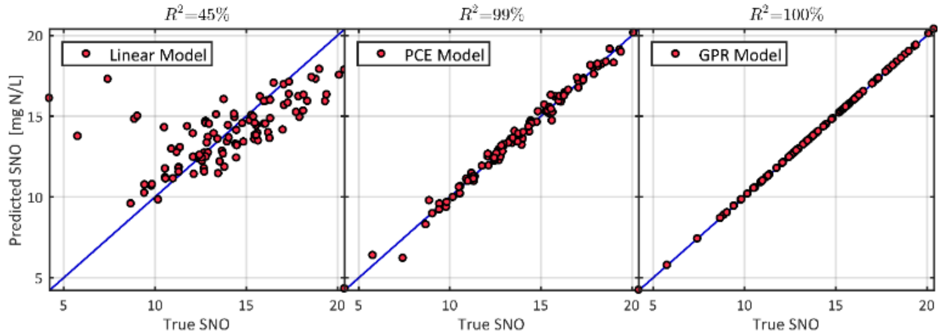
Refine engineering design spaces with Global sensitivity analysis





Al et al., 2019. *Comput Chem Eng* 127


Computers and Chemical Engineering 127 (2019) 233–246

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journal homepage: www.elsevier.com/locate/compchemeng

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Meta-modeling based efficient global sensitivity analysis for wastewater treatment plants – An application to the BSM2 model

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Computational gain

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How much is the computational gain?

Comparison of computational costs of different approaches for global sensitivity analysis.

Approach	# of plant-wide simulations used				Total computational cost
	Scenario 1 ($d = 7$)	Scenario 2 ($d = 20$)	Scenario 3 ($d = 10$)	Scenario 4 ($d = 37$)	
SRC with MCS	1000	1000	1000	1000	$4000 \times t_{BSM2}$
Sobol indices with MCS using BSM2	18,000	44,000	24,000	78,000	$164000 \times t_{BSM2}$
Sobol indices with MCS using GPR	150	100	100	250	$600 \times t_{BSM2}$
Sobol indices with MCS using ANN	150	100	100	450	$800 \times t_{BSM2}$
Sobol indices with PCE	250	150	100	250	$750 \times t_{BSM2}$

Al et al., 2019. *Comput Chem Eng* 127

On average, surrogates provide 200 times faster results.

For questions

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Gürkan Sin*
Associate professor
PROSYS Research Centre
Technical University of Denmark

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Horizon 2020

MARIE CURIE ACTIONS

MeD Life

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