L4_1 Morris Screening for sensitivity analysis
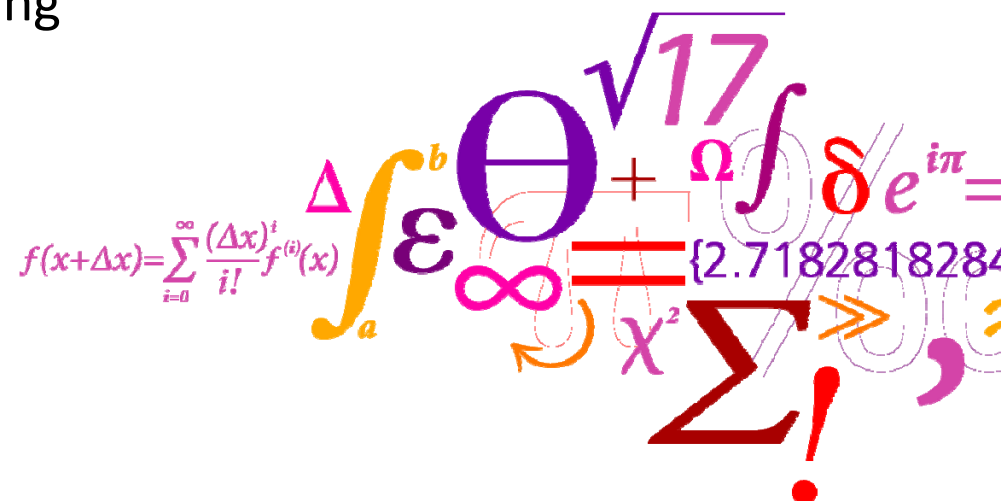
Gürkan Sin, Associate Professor
PROSYS- DTU Chemical Engineering

DTU Kemiteknik
Institut for Kemiteknik

Agenda

9:00-12:00	L4.1 Morris Screening
	Exercises
Lunch break	
1:00-4:00	Catch up with exercises
	Free time with instructors

Morris method for sensitivity analysis

Objective of this lecture

- At the end of the lecture, you should be able to:
  - Perform sensitivity analysis using Morris Screening on a simple model
  - Apply the method and Interpret the results on a slightly complex model

Outline

- On sensitivity analysis (recall)
- Morris method
    - Elementary effects (EE)
    - Morris sampling
- Case study: Morris method in batch fermentation models
- Example: Oxygen Uptake Rate (OUR)
- Exercise: Simple fermentation model

Sensitivity analysis – a definition

Sensitivity analysis "studies how variation (uncertainty) in the outputs of a model can be apportioned to different sources in the input of a model"

SA complimentary to uncertainty analysis: "quantifying uncertainty in the outputs of a model from uncertainty in its inputs "

Morris method for sensitivity analysis

Saltelli et al., 2008
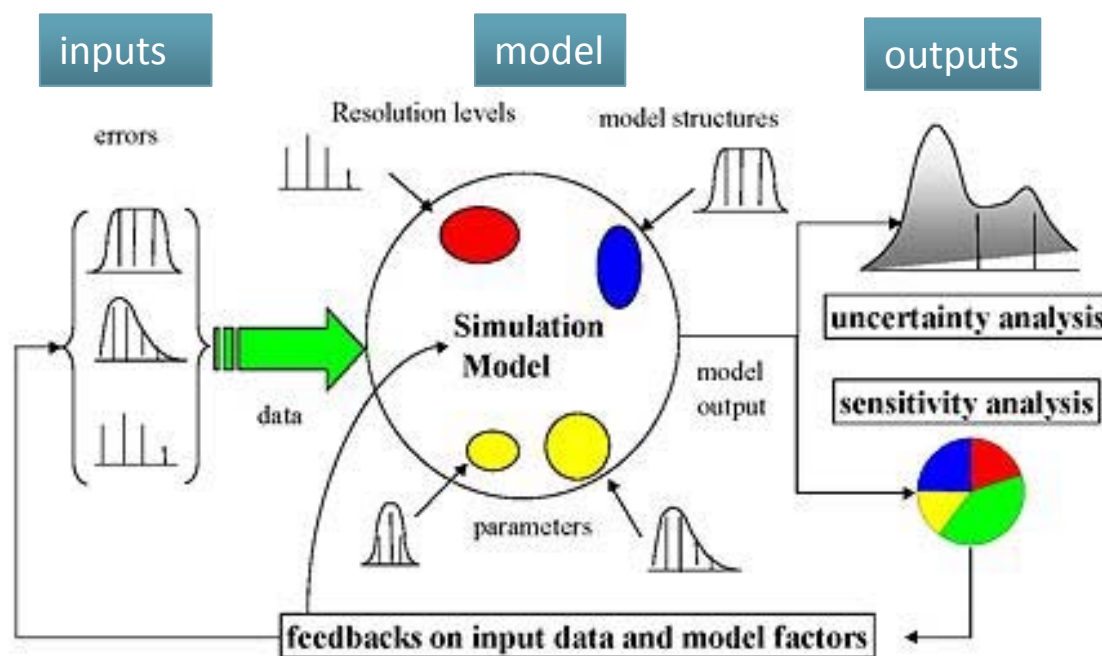
Sensitivity analysis – practices

SA may be used for a number of purposes:

1. Identify critical region in the input space of a model
2. Establish research priorities (by knowing to which inputs the model response is the most sensitive)
3. Debugging model coding errors (detecting a non-important parameter as important)
4. Simplify models / test hypothesis
5. ...

Sensitivity analysis – Putting Morris method in context

A number of methods available each with its own advantages/drawbacks

• Local methods

– Derivative based, One-factor-at-A-Time (OAT), …

– Local measure: small perturbation around base value

– Hence the analysis is locally bounding, not extrapolative!

• Global methods

– Regression, variance-based, …

– May be computationally demanding

Morris method (1991):

– Combines advantages of the two: Performs local sensitivity calculations in a global context (thanks to special sampling method)

Let us take a model of the form:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \boldsymbol{\theta}, \mathbf{u}, t); \quad \mathbf{x}(0) = \mathbf{x_0}$$

$$\mathbf{y} = \mathbf{g}(\mathbf{x}, \boldsymbol{\theta}, \mathbf{u}, t)$$

The elementary effect of the ith input factor, θ_i, in a point $\boldsymbol{\theta}^0$ (input space):

$$EE_i^0 = \frac{y\left(\theta_1^0, \theta_2^0, \theta_i^0 + \Delta, \ldots \theta_m^0\right) - y\left(\boldsymbol{\theta}^0\right)}{\Delta}$$

θ_2

$\left(\theta_1^0, \theta_2^0\right) \quad \left(\theta_1^0 + \Delta, \theta_2^0\right)$

θ_1
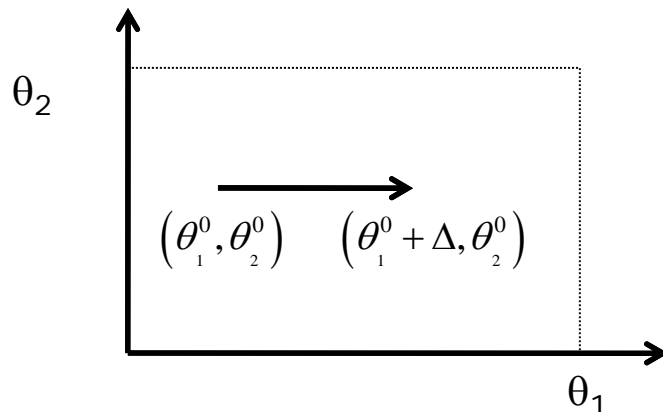
Note: it is hard to visualize m-dimensional input space.
Take a 2-D input space as an example!

Morris method (Morris, 1991)
Concept of elementary effects (EE)

Each input assumed to vary across p levels (discretized approach):

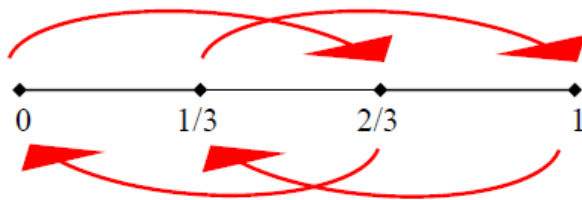For $\theta_i \sim U(0,1)$ & $p = 4$ → $p_1 = 0$, $p_2 = 1/3$, $p_3 = 2/3$ and $p_4 = 1$

Optimal choice of perturbation coefficient, Δ, depends on the levels:

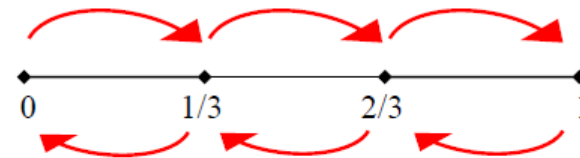$\Delta = p\,/\,2(p\text{-}1)$ (E.g. for $p = 4$, $\Delta = 2/3$)

Morris method (Morris, 1991) -am
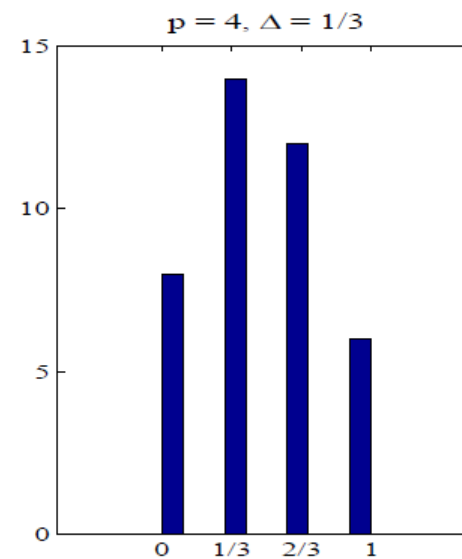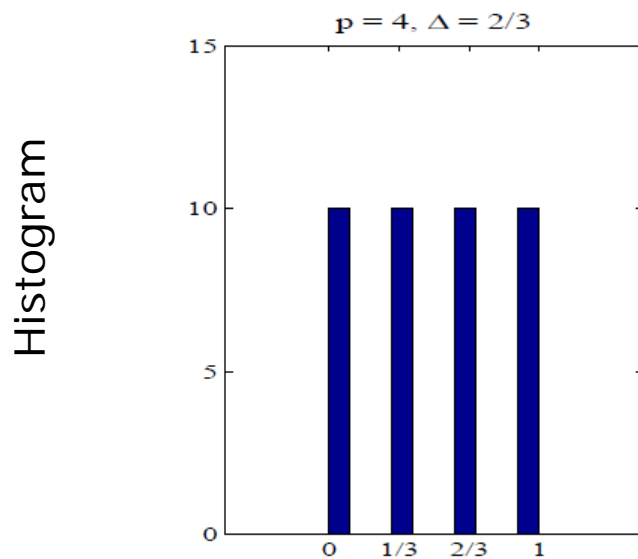# Concept of elementary effects (EE)

The choice of perturbation factor: Δ is optimal when $\Delta = p\,/\,2(p\text{-}1)$

Uniform sampling of input

Not-uniform sampling of input

Histogram

$p = 4, \Delta = 2/3$

$p = 4, \Delta = 1/3$

θ Morris method for sensitivity analysis θ

The Morris sampling

EEi is still a **local measure,** so**?**

Solution: take the average of several EEi !

Morris suggests calculations of EEi at randomly selected points in the input space (m-dimensional p-level grid) and to approximate the distribution of elementary effects, Fi.

To this end, Morris performs EEi calculations r times following an efficient randomized sampling scheme (see Morris Sampling, 1991).
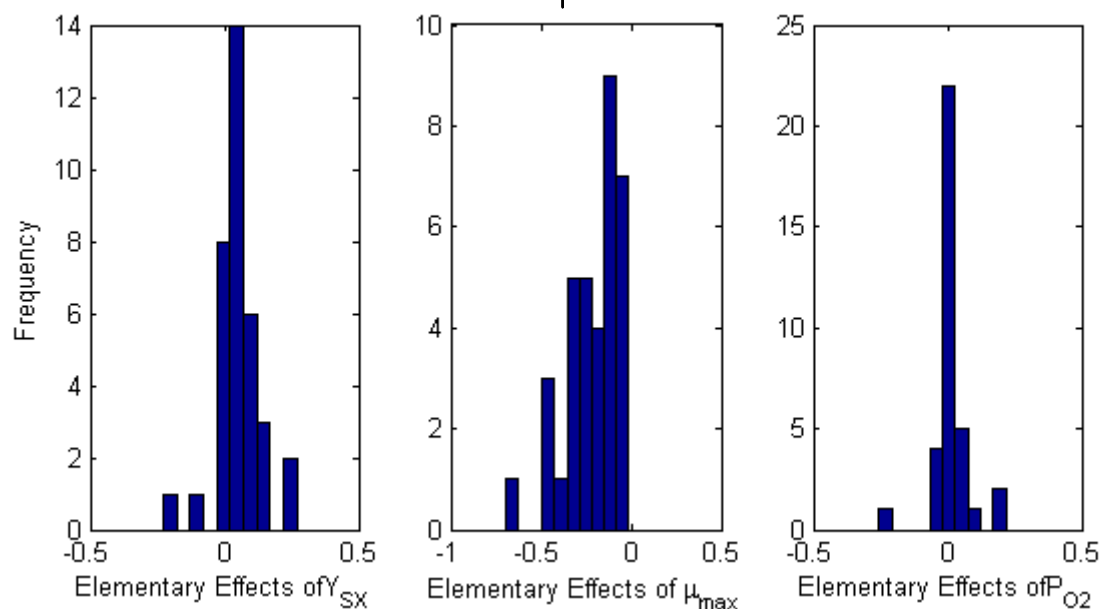
r is chosen in the range of 5-10.

$$EE_i^r = \frac{y\left(\theta_1^r, \theta_2^r, \theta_i^r + \Delta, \dots \theta_m^r\right) - y\left(\boldsymbol{\theta}^r\right)}{\Delta}$$

θ_2

$\boldsymbol{\theta}^1$

$\boldsymbol{\theta}^2$

$\boldsymbol{\theta}^{\cdots}$

$\boldsymbol{\theta}^r$

θ_1
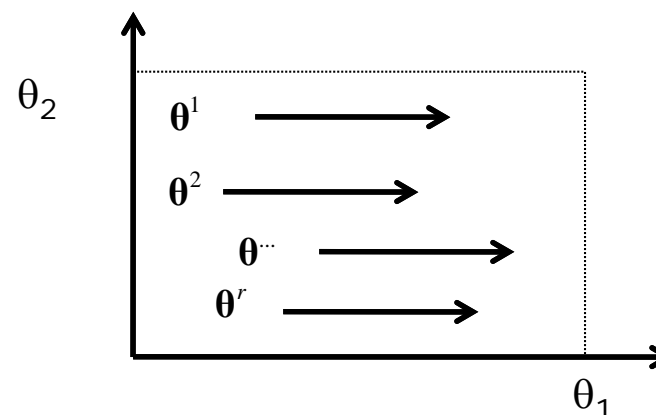
Interpretation of Morris method

The distribution of elementary effects of model inputs on the model outputs,

Fi: 35 random observation of EEi

Analyse & compare the mean and standard deviation of these distributions.
Higher mean and higher standard deviation of FEEi indicates strong sensitivity!

The Morris sampling

Low computational cost: *Morris requires only r*(k+1) model evaluations*

Example:

For k = 10 parameters, Fractional factorial design at 2 levels→ 2^{10} = 1024

Morris sampling = 10*(10+1) = 110

For k = 20 parameters, FF design at 2 levels → 2^{20} = 1048576

Morris sampling → 10*(20+1) = 210

Morris method for sensitivity analysis

Morris method – the extended

To enable comparison of the elementary effects on different model outputs, y_j, a relative measure of elementary effects is needed (where j >2)

A possible relative measure is obtained by sigma-scaling:

$$SEEij = EEij \frac{\sigma_{xi}}{\sigma_{yj}}$$

Case study: Application of Morris method to fermentation models

S. COELICOLOR CULTIVATION FOR ANTIBIOTIC PRODUCTION

Morris method: methodology

Morris sampling for EEi

Step 1. Specify range for each input parameter

Step 2. Morris Sampling

Step 3. Model evaluations of Morris samples

Step 4. Compute and plot elementary effects (EEi)

Step 5. Rank parameters according to μ_i & σ_i (Morris) or absolute μ_i* (Saltelli)

Morris method for sensitivity
analysis

Glucose, air, base

measurements:
Biomass,
glucose, NH_4^+

On-line
measurement:
CO_2, dissolved O_2,
temperature, pH,
Base addition, etc.

Many outputs (around 20)
Many parameters (around 60)

Model fits to measurements

Morris method for sensitivity analysis

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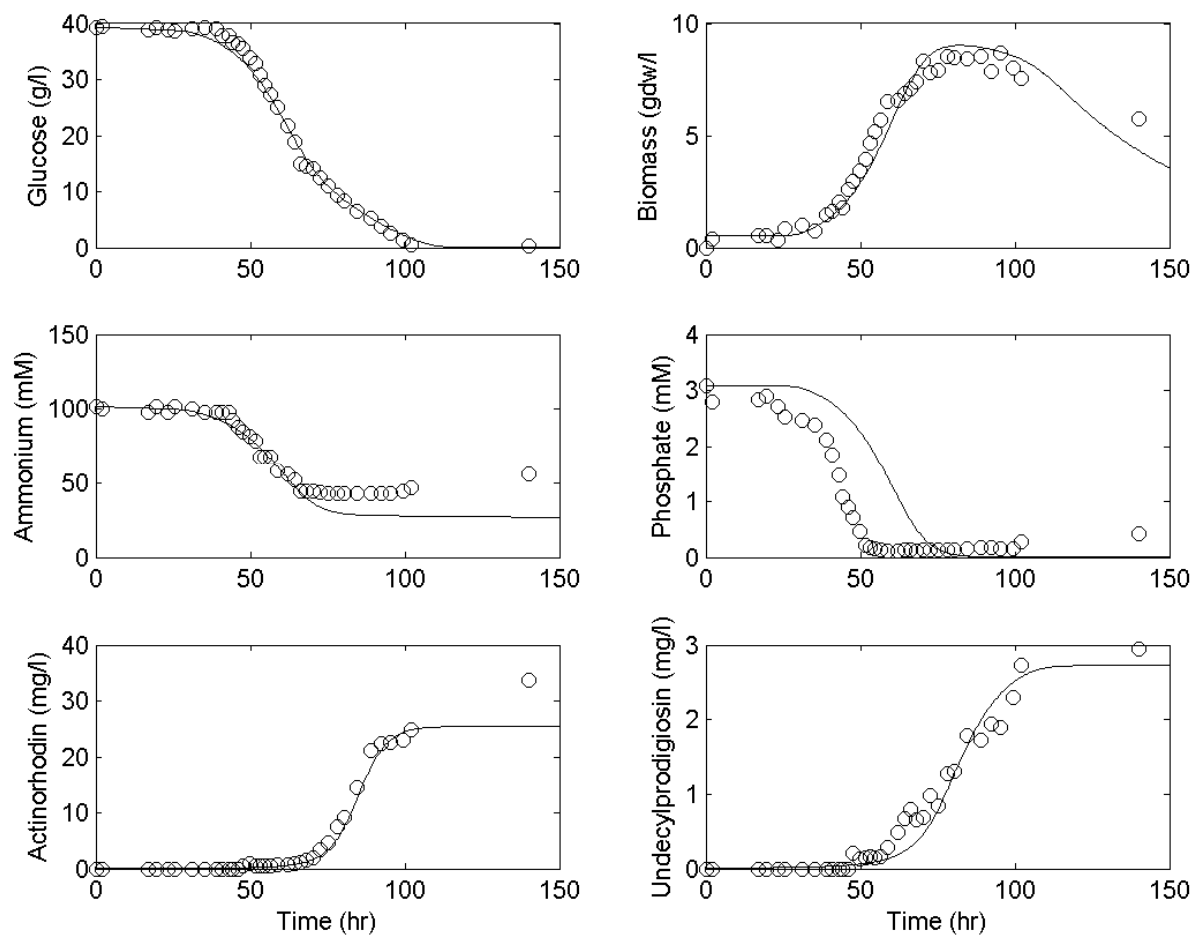
Morris method – sampling specifications

Morris method specifications:

$p = 4$, $\Delta = 2/3$, $r = 35$, k = 60 (# number of parameters)

Total model evaluations = $r*(k+1)$ = 2135

Improved Morris Sampling with $r = 35$
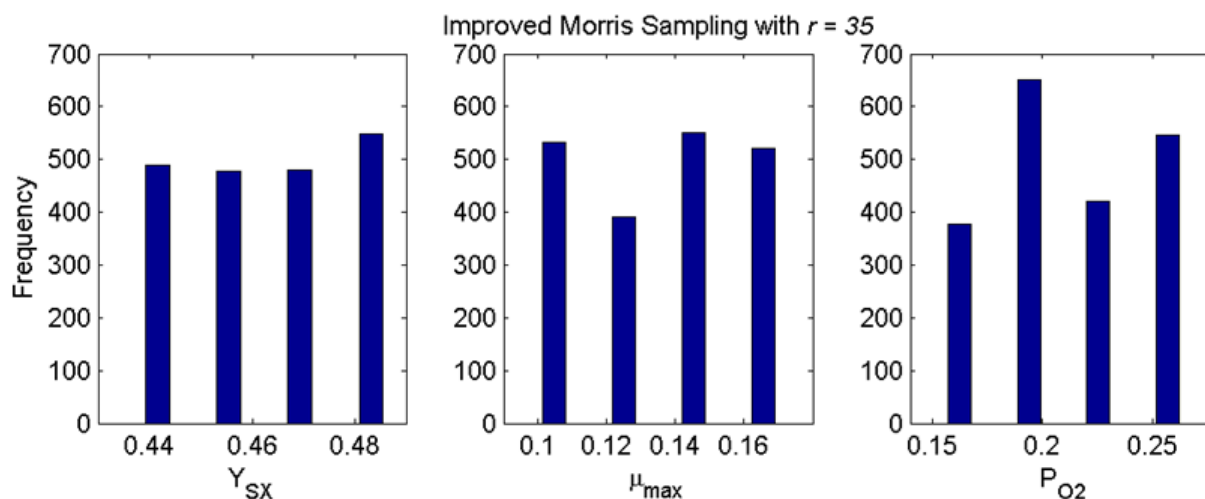
Morris sampling of 3 model parameters

Morris method for sensitivity analysis

The distribution of elementary effects of model inputs on the model outputs,

Fi: 35 random observation of EEi
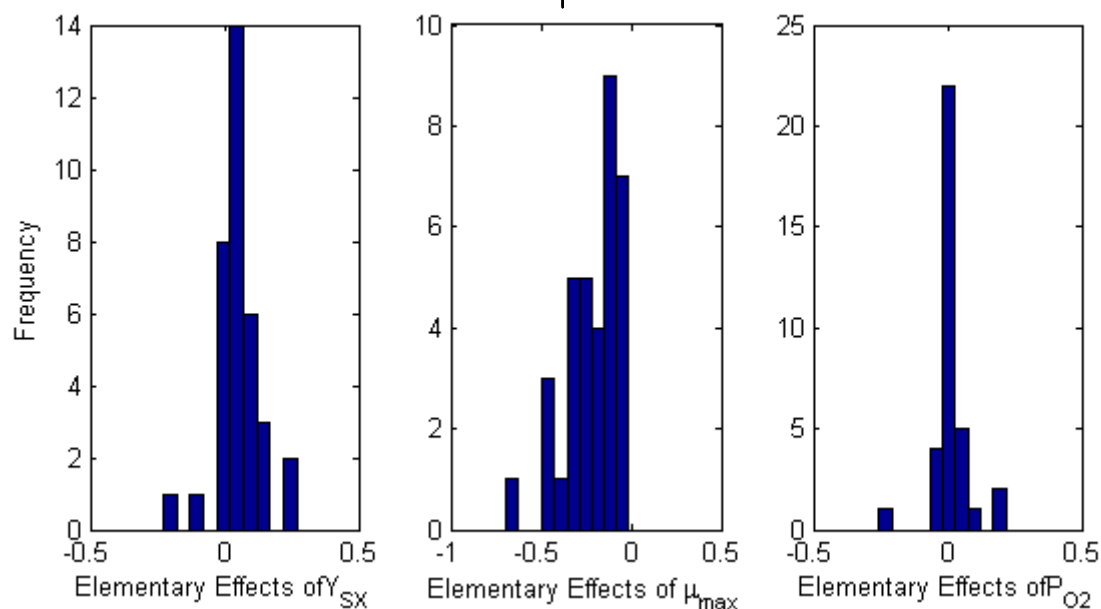
Model output:
glucose
model inputs:
Y_{SX}, μ^{max} and P_{O2}

Analyse & compare the mean and standard deviation of these distributions

Results – typical results of Morris method

Example: Glucose as model output versus a total of 56 input factors
Conclusion: 8 influential factors, the rest of the factors have insignificant contribution to the variation in glucose

$$SEMi = \pm std_i / \sqrt{r}$$

influential factors

Non-influential factors

influential factors

Standard deviation

Mean

Each point represents the effect of an input on respective outputs

Now one can zoom in and study in detail which input affects which output!

Comparison of extended Morris with Monte Carlo based regression method (SRC)

Table. Method comparison for screening influential factors: Model output glucose

Rank	Morris Method		Monte-Carlo based regression	
	Input symbol	μ^*	Input symbol	SRC*
1	i_{PX}	0.75	K_P	0.74
2	m_S	-0.30	μ_{max}	-0.65
3	K_P	0.30	i_{PX}	0.61
4	K_S	0.30	K_S	0.50
5	μ_{max}	-0.21	m_S	-0.47

Bottom line: Morris method agreed mostly (6/8) with the well established regression based method

Morris method for sensitivity analysis

Morris method for sensitivity analysis

EXAMPLE: AEROBIC GROWTH OF MICROORGANISMS

Morris method: methodology

Monte Carlo simulations + linear regression for sensitivity analysis

Step 1. Specify range for each input parameter

Step 2. Morris Sampling

Step 3. Model evaluations of Morris samples

Step 4. Compute and plot elementary effects (EEi)

Step 5. Rank parameters according to μi & σi (Morris) or absolute $\mu i*$ (Saltelli)
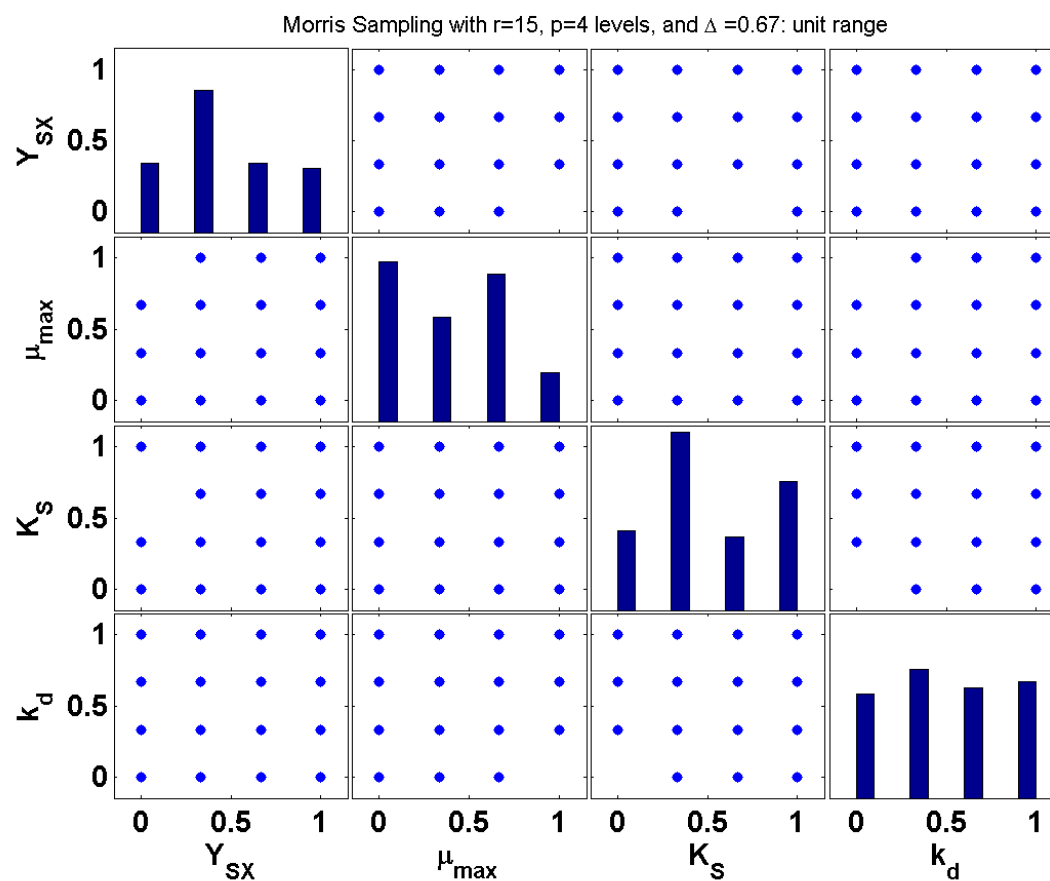
Matlab code (Morrissampling.m)

```matlab
ourinit
pmor=par(1:4); % get the reference parameter values /we assume we dont
have any data for PE. otherwise we dont use Monte Carlo
lp = {'Y_{SX}','\mu_{max}','K_S','k_d'};
inputunc=[0.05 0.10 0.25 0.25]; % expert input uncertainty indicates
degree of uncertainty [0: Low , 1: High]
k=length(pmor); % number of parameters
xl= pmor .* (ones(1,k)-inputunc);
xu= pmor .* (ones(1,k)+inputunc);
%% Morris sampling parameters
k = k ; % no of parameters or factors
p = 4 ; % number of levels {4,6,8}
dt = p/(2*(p-1)) ; % perturbation factor .
r = 15; % number of repetion for calculating the EEi, e.g. 4 - 15
%% Morris sampling will produce discrete uniform probabilities for each
%% factor.
X = morris(p,dt,k,r);
Xmean = mean(X) ;
```

Morris method for sensitivity
analysis

step 1 to 2: Morris sampling results

k=4 (parameters), p = 4 (levels), r = 15 (repetition), Δ=2/3, n= 75 (r*(k+1)

Morris Sampling with r=15, p=4 levels, and Δ =0.67: unit range
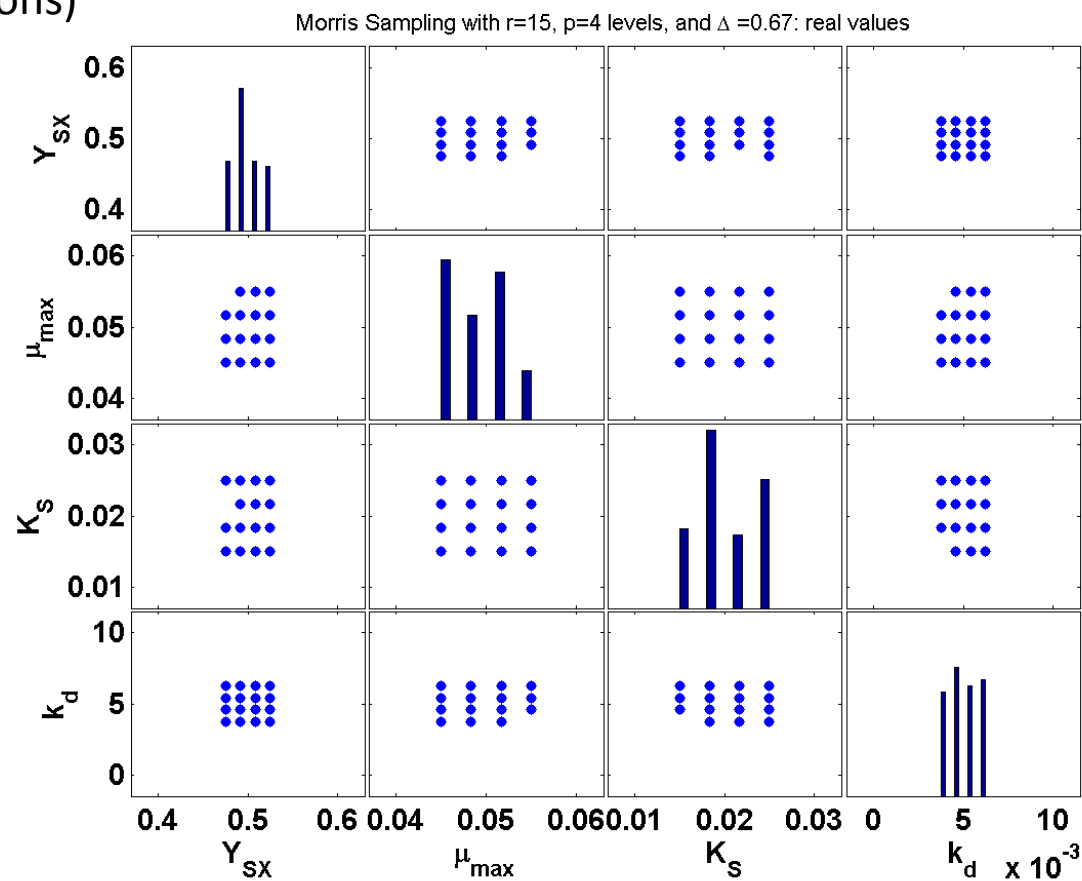
Morris method for sensitivity analysis

step 1 to 2: Morris sampling results

m=4 (parameters), p = 4 (levels), r = 15 (repetition), $\Delta=2/3$, n = 75 (15*4+1) (# simulations)

Morris Sampling with r=15, p=4 levels, and Δ =0.67: real values

Morris method for sensitivity analysis

step 3: Model evaluations of Morris samples (raw data)

Matlab code (morrissim.m)

```matlab
% load sampling matrix
load MorrisSampling_r15_p4
[n m] = size(Xval) ;
% specify time (in hr) % initialize:
time = [0:(1/50):0.5];
ourinit
% run Morris simulations
for i=1:n
% update the uncertain parameters
par(1:4)=Xval(i,:);
%% Solution of the model
options=odeset('RelTol',1e-7,'AbsTol',1e-8);
[t,y] = ode45(@ourmod,time,x0,options,par);
%% calculate oyxgen uptake rate (O-mmol/l-min)
y1(:,i) = y(:,1);
y2(:,i) = y(:,2);
y3(:,i) = y(:,3);
end
```

Total number of simulations, n = 75 (=15*(4+1))

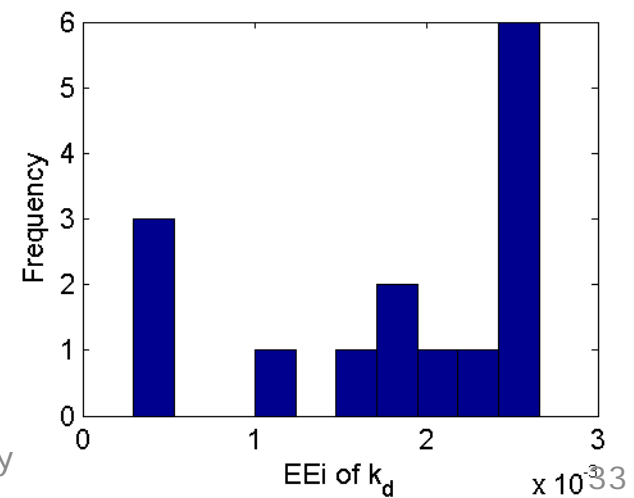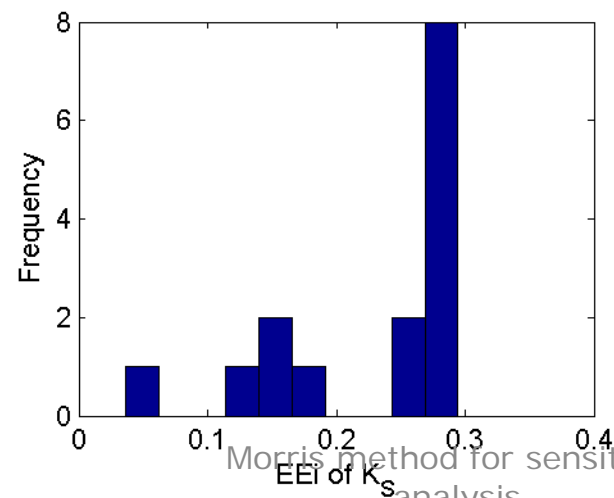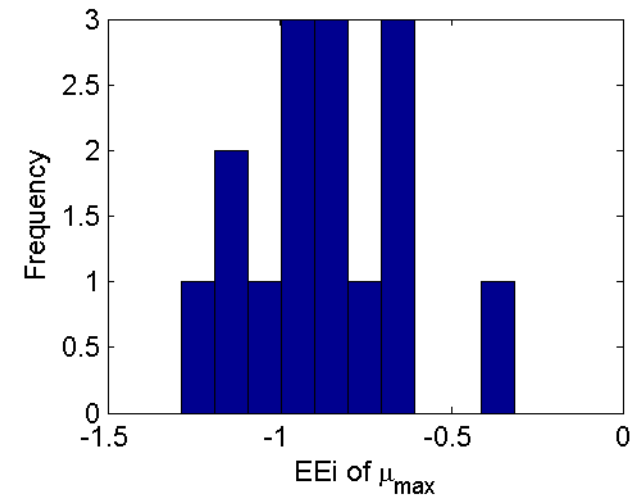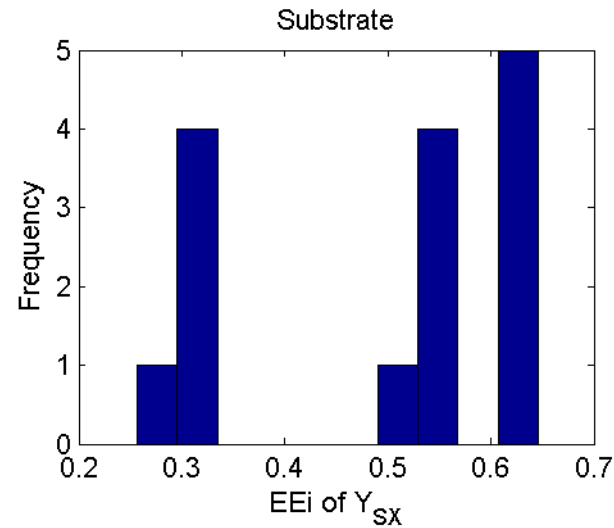Morris method for sensitivity analysis
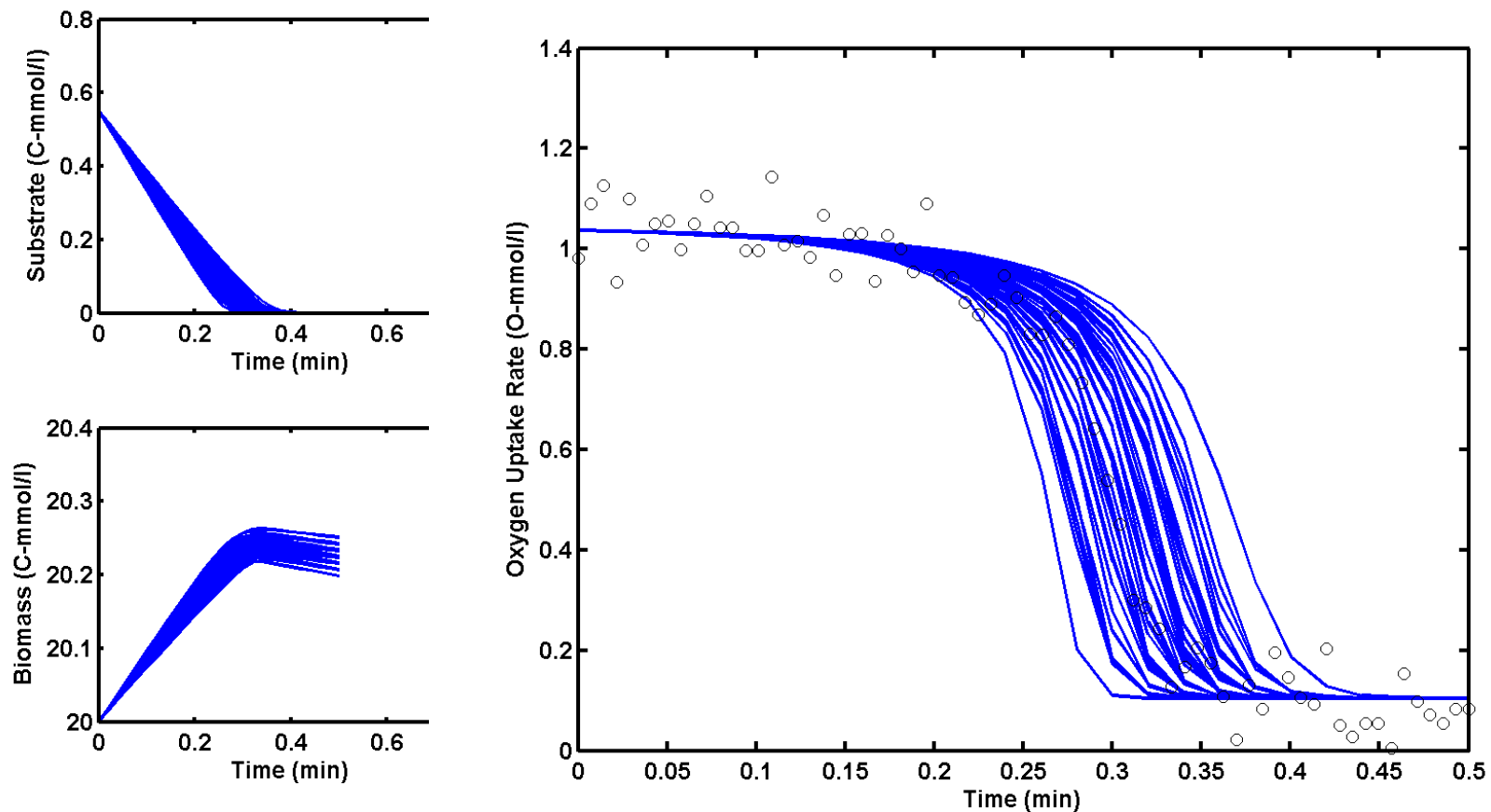
step 4: Compute elementary effects

Matlab code: computeEEi.m

```matlab
load MorrisSims_r15_p4.mat
%% this method requires scalar outputs, y:
% hence one needs to specify a meaningful property of time-series data: Let us
focus on time=0.3 hr
ii = find(time == 0.3) ;
y1s = y1(ii,:); y2s = y2(ii,:); y3s = y3(ii,:); ours = our(ii,:);
%% compile an model output matrix
Sim = [y1s' y2s' y3s' ours'];[n k] = size(X) ; n = n / (k+1);
[mm ll] = size(Sim) ;
%% below info needed for sigma-scaling of EEi
sig_y = std(Sim);
sig_x = std(Xval);
 %% compute the corresponding Eei
for i=1:n
    for j=1:k
        m1 = (k+1)*(i-1);
        r1 = m1 + j ;
        ix = find (X(r1,:) - X(r1+1,:)) ; % find the non-zero value
        if length(ix) > 1
            warning('there is more than one factor changed')
            return
        end
```

y: Substrate

sy= y(t=0.3h)

Morris method for sensitivity analysis

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step 4: Compute elementary effects

y: oxygen

sy= y(t=0.3h)
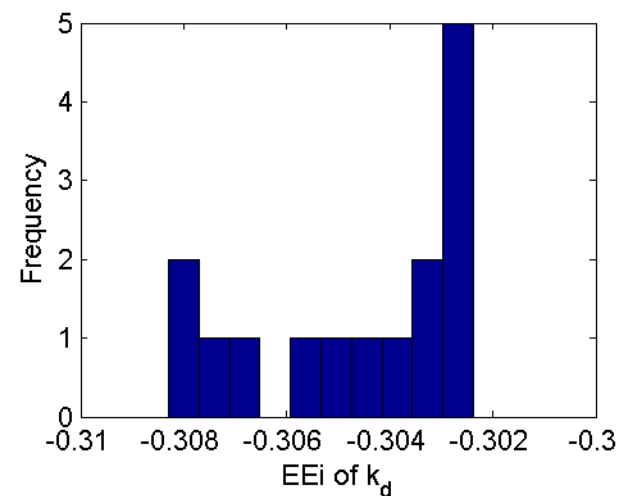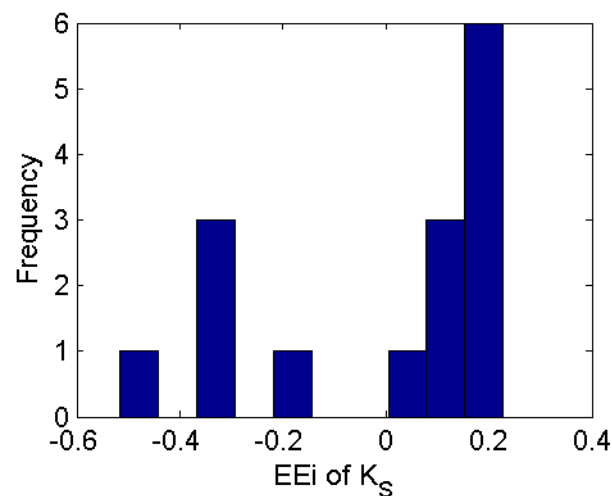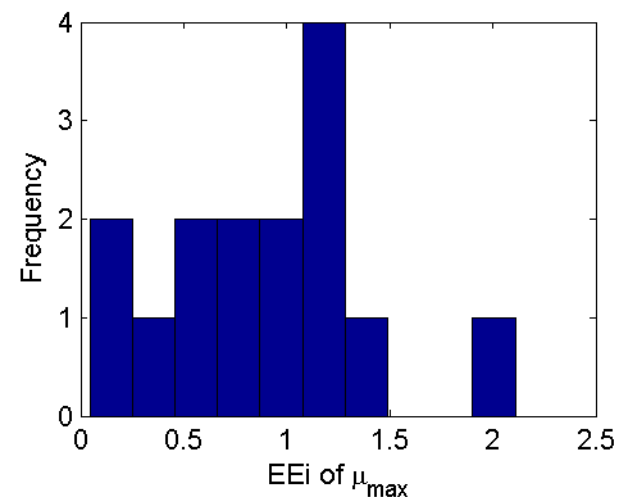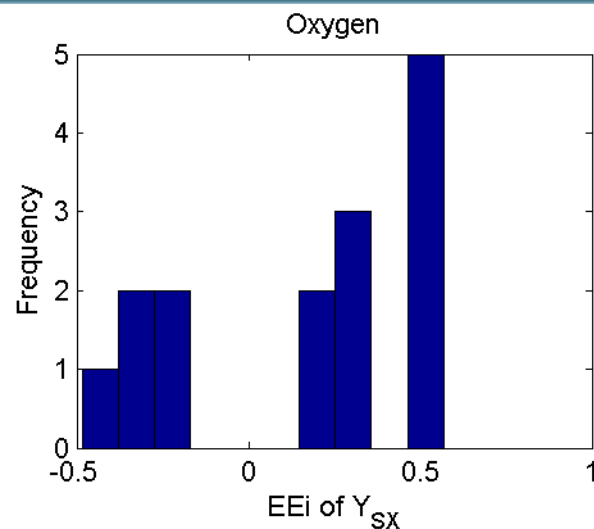
Morris method for sensitivity analysis

step 4: Compute elementary effects

Y: biomass

sy= y(t=0.3h)

Morris method for sensitivity analysis
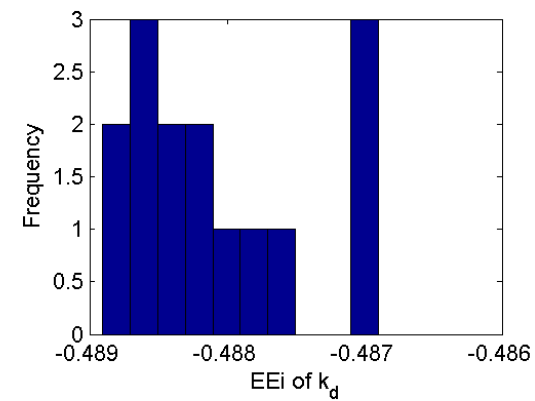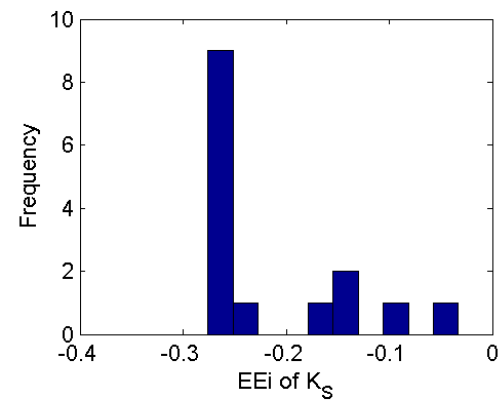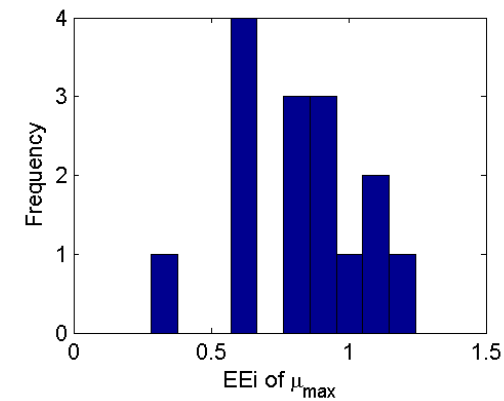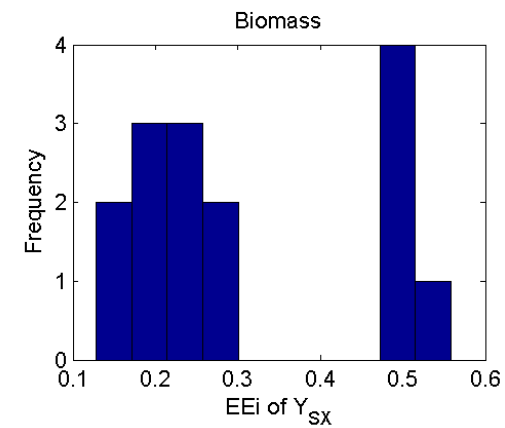
step 4: Compute elementary effects

y: our

sy= y(t=0.3h)

Morris method for sensitivity analysis
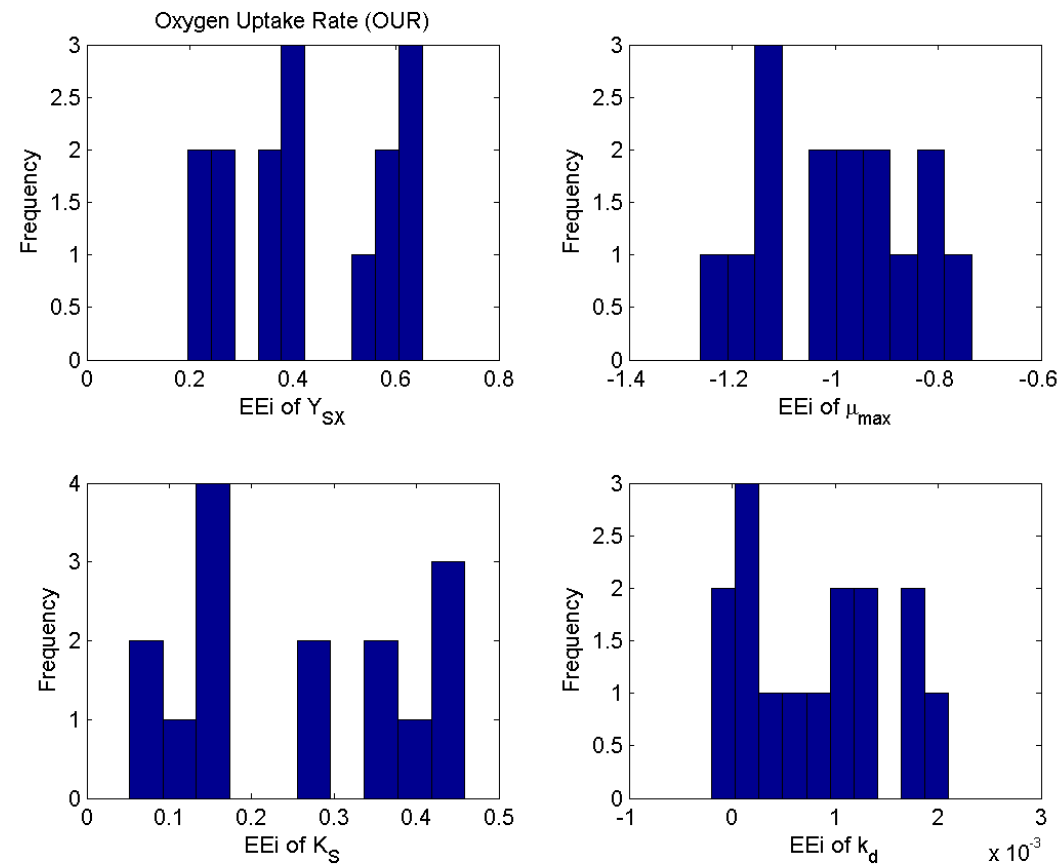
step 5: Rank parameter significance

Morris: consider standard error on the mean of EEi(sem). Use this to form a wedge!
Parameters inside the wedge insignificant, outside significant. (plotmorrissim.m)

Positive:
• Visually appealing!
• consider the quality of estimating mean Eei
• Combines info of mean and sigma of Eei
Negative
• Becomes cumbersome for models with many parameters!
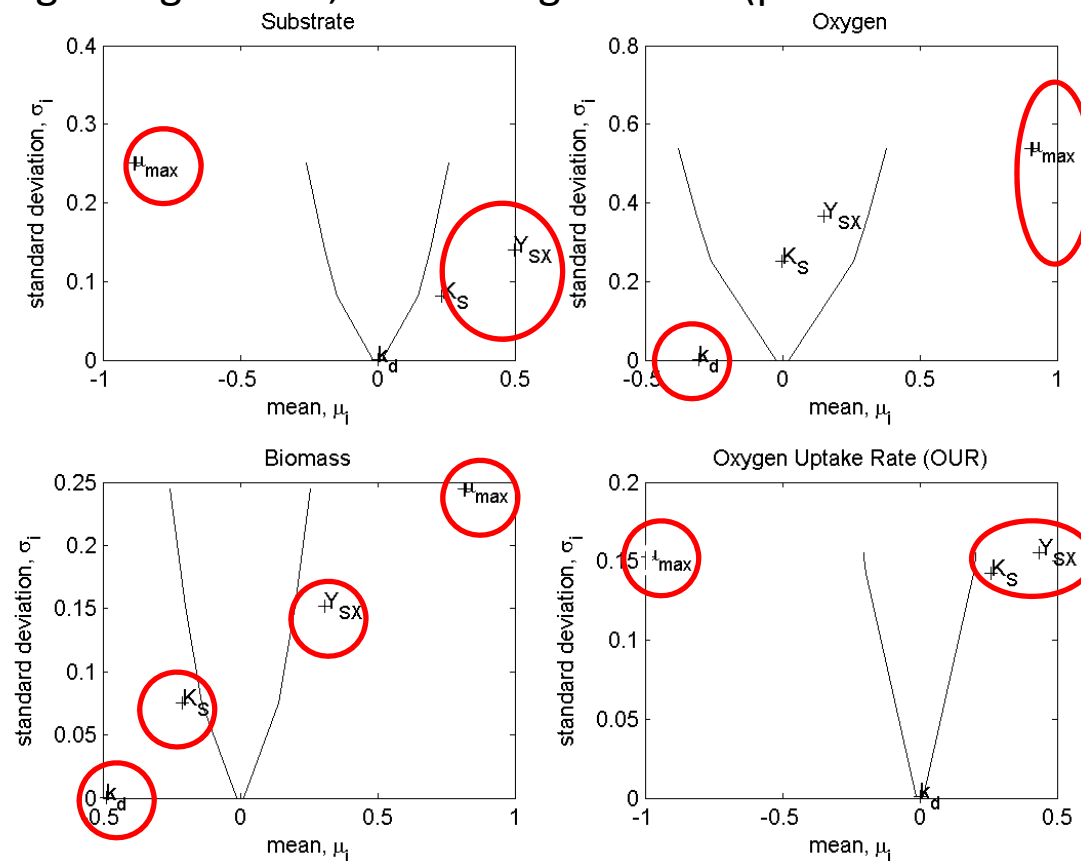
Morris method for sensitivity analysis

step 5: Rank parameter significance

Saltelli: Focus on the absolute measure of the mean of EEi and rank them!

	Substrate	Rank*	Oxygen	Rank	Biomass	Rank	OUR	Rank
Y_{SX}	0.50	2	0.15	3	0.31	3	0.43	2
μ_{max}	-0.89	1	0.90	1	0.81	1	-0.99	1
K_S	0.23	3	0.00	4	-0.21	4	0.26	3
k_d	0.00	4	-0.30	2	-0.49	2	0.00	4

Positive:
• Helps ranking parameter importance with single measure!

Drawback:
•Ignores information in standard deviation

Quality check: compare the results of Morris with SRC or other SA methods

sy= y(t=0.3h)

	substrate Morris, μ_i	SRC	oxygen Morris, μ_i	SRC	biomass Morris, μ_i	SRC	our Morris, μ_i	SRC
Y_{SX}	0.50	0.38	0.15	-0.14	0.31	0.47	0.43	0.36
μ_{max}	-0.89	-0.85	0.90	0.85	0.81	0.79	-0.99	-0.89
K_S	0.23	0.22	0.00	-0.03	-0.21	-0.21	0.26	0.16
k_d	0.00	0.01	-0.30	-0.09	-0.49	-0.20	0.00	0.04

Bottom line: The results of Morris and SRC agree well with each other with one exception (Ysx on Oxygen)! Empirical evidence that senstivity analysis results are reliable!

To sum up

Morris method allows screening of the importance of model parameters (inputs) on the outputs

It is robust wrt type II error (identifying a non-important parameter as important)

The original method considers one type of model output. The extended method is applicable to a model with many outputs (thanks to sigma-scaling of EEi)

Recommended as efficient screening method prior to more detailed and computationally exhaustive methods, such as Sobol's variance decomposition.

Exercise 1: Repeat Morris method of sensitivity analysis

AEROBIC GROWTH OF MICROORGANISM

Exercise details

- Do the exercise individually

- Use the matlab scripts introduced earlier using the OUR example

- Follow the steps outlined above in the example (slide # 23)

- and learn by doing! For example to learn Morris sampling theory in detail, first read the accompanying paper and then check the morris code. you may do the following:

    - Open the morrissampling.m

    - Set r equal to 1. investigate the resulting samples (X and Xval)

    - Set r equal to 2. investigate the resulting samples (X and Xval)

    - In the same manner, change the p parameter to 6 and repeat above steps.

    - Write down the results on a paper and compare them with the theory of morris sampling (see the paper).

Morris method for sensitivity analysis

Exercise 1: Repeat Morris method of sensitivity analysis

SIMPLE FERMENTATION MODEL

Exercise details

- Do the exercise individually

- Use the matlab scripts introduced earlier using the OUR example, BUT this time use the fermentation model!

- Adopt the scripts if necessary for your exercise!

- Follow the steps outlined above in the example (slide # 23)

- and learn by doing!

- We will be around to help you out!....

Morris method for sensitivity analysis