First steps towards the development of a tool for sensitivity analysis and uncertainty propagation studies for steady-state thermal-hydraulic simulations of research reactors

R. Schönecker
Forschungs-Neutronenquelle Heinz Maier Leibnitz/TUM
Institut Laue-Langevin/ILL
ronja.schoenecker@frm2.tum.de

Motivation

- **Calculation of steady-state thermal-hydraulic (SSTH) safety margins:** Required for investigation of potential new fuel element designs for FRM II and RHF within conversion efforts

- **Consideration of uncertainties:**
  - uncertainties in model inputs (e.g. manufacturing tolerances)
  - uncertainties due to modeling assumptions (e.g. fluid properties, geometry)
  - numerical uncertainties

➢ **Inclusion of sensitivity analysis and uncertainty propagation studies in SSTH safety margin calculations**

Sampling-based sensitivity analysis

Introduction

- Consider a response y which is a function of multiple parameters $x_1, \dots x_M$ i.e. $y = f(x_1, \dots x_M)$
- Naive way to define sensivities of y with respect to any of the x_m: Use of derivatives, i.e. $\frac{dy}{dx_m}$
- **Problems:**
  - Investigation of local effects only
  - Derivatives cannot be obtained easily if the response function is too complicated
  - Derivatives cannot be obtained at all if the response function is unknown
- **Alternative approach:** Application of sampling-based (statistical) methods
- **Advantages:**
  - Full exploration of parameter space possible
  - No need to calculate the derivatives: → independence of response
- Goal: replace derivatives with statistical quantities which can be obtained by sampling

Sampling-based sensitivity analysis

Mathematical background

- Consider a response y which is a function of a single parameter x, i.e. $y = f(x)$
- **Absolute first-order sensitivity index (SI):**

$$\left(S_{y,x}^{1}\right)_{abs} = \frac{\mathrm{Cov}[y,x]}{\mathrm{Var}[x]} = \frac{dy}{dx}(\mu) \qquad (1)$$

- Normalization with mean values of x and y yield relative first-order SI:

$$\left(S_{y,x}^{1}\right)_{rel} = \left(S_{y,x}^{1}\right)_{abs} \cdot \frac{\overline{x}}{\overline{y}} \qquad (2)$$

- Eqs. (1) and (2) applicable to all parameters of y if they are statistically independent

The tool

Application mode 1: embedded model evaluation

Input

General info:
- Model specification (python/PLTEMP)
- Batching yes/no?
- Specification of response
- Number of samples

Parameter info:
- Specification of parameter
- Specification of distribution

Python code

1. Sampling of parameters

For each batch:

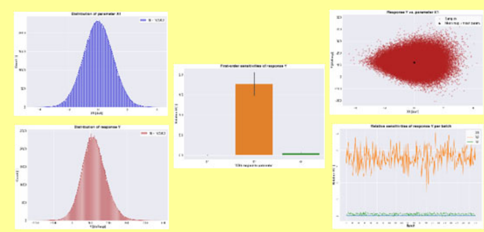
2. Model evaluation
3. Calculation of batch SI

4. Calculation of average SI
5. Post-Processing

Output

Files:
- Sampled parameters / obtained responses
- (Co-)variance terms per batch
- SI per batch + average SI (csv)

Plots:



The tool

Application mode 2: use of external data

Input

General info:
- Specification of input csv file
- Batching yes/no?
- Specification of response
- Number of samples

Parameter info:
- Specification of parameter
- Specification of distribution

→

Python code

1. Sampling of parameters

For each batch:

2. Model evaluation
3. Calculation of batch SI

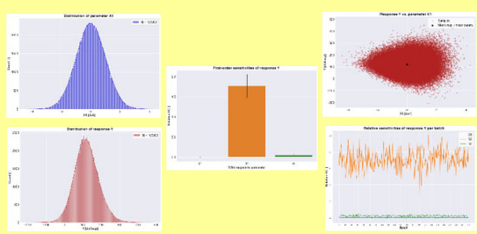
4. Calculation of average SI
5. Post-Processing

→

Output

Files:
- Sampled parameters / obtained responses
- (Co-)variance terms per batch
- SI per batch + average SI (csv)

Plots:



Application example 1: python model (1)

First-order response with four equally sampled parameters

- **Input:**

  - Response: $y = x_1 + 2x_2 + 3x_3 + 4x_4$
  - Parameters: $x_1, x_2, x_3, x_4 \in N(1,1)$

  Note: $\bar{y} = y(\bar{x}) = 10$

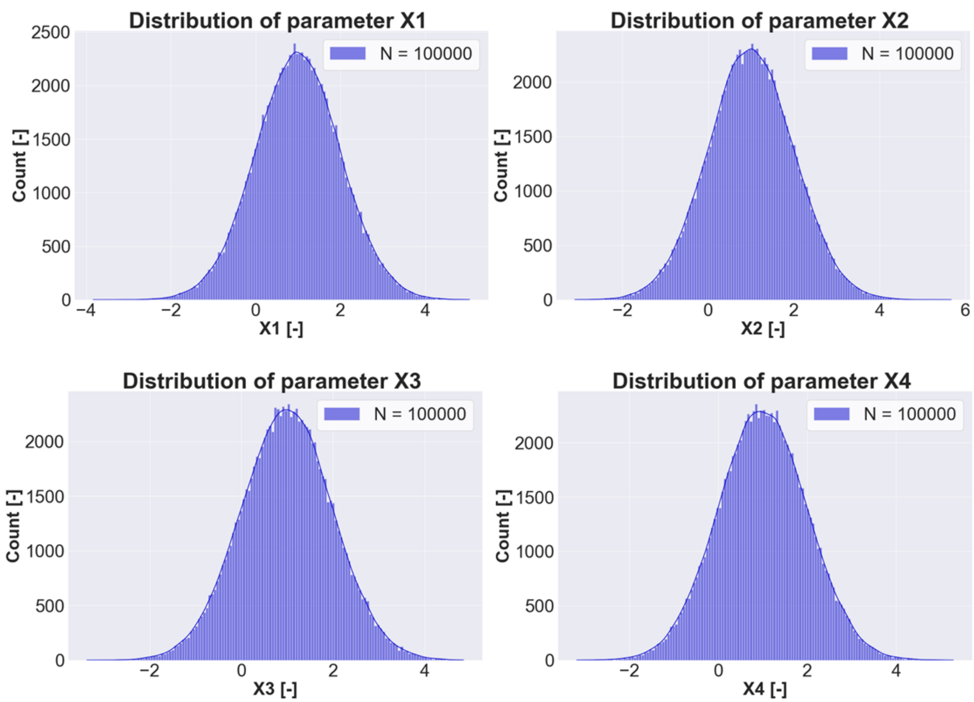
- **Expected results for the first-order SI** (obtained from derivatives)**:**

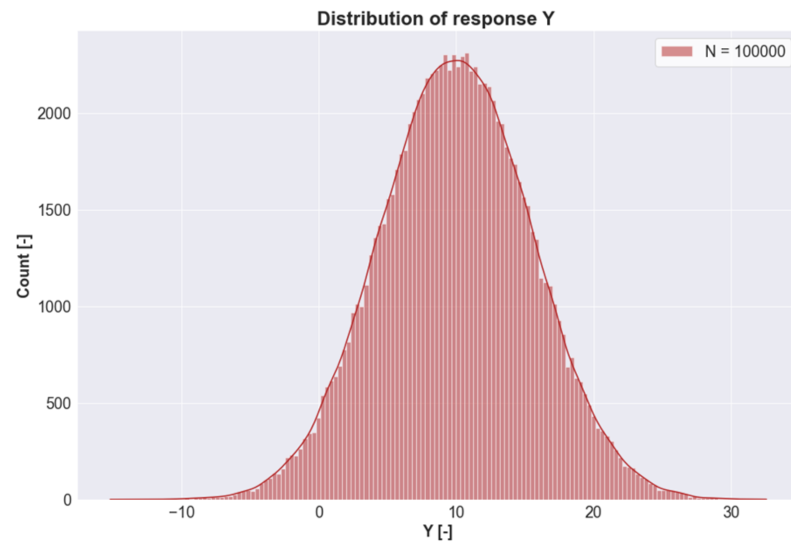
Parameter	Absolute SI	Relative SI
x_1	1	0.1
x_2	2	0.2
x_3	3	0.3
x_4	4	0.4

Application example 1: python model (2)

First-order response with four equally sampled parameters

- **Output:** **Histograms of sampled parameter and obtained response values:**

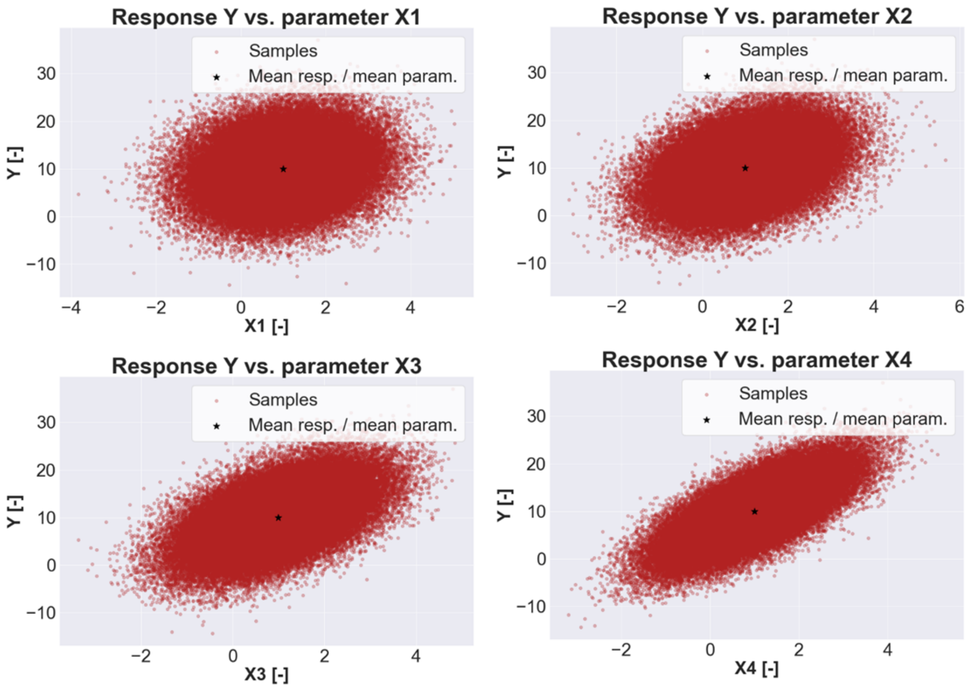




Application example 1: python model (3)

First-order response with four equally sampled parameters

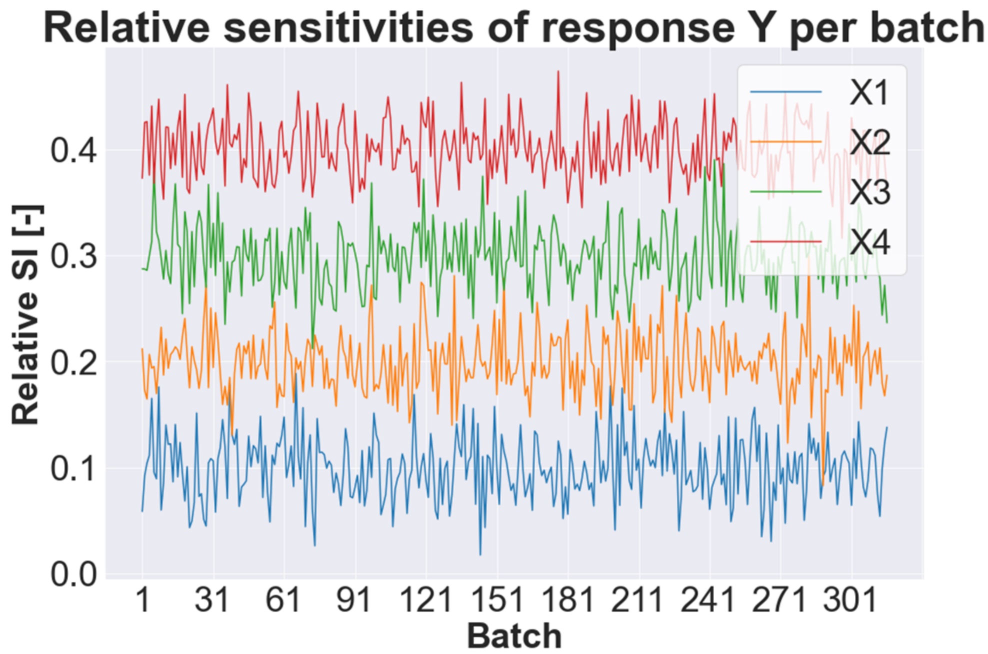
- **Output:** **Scatterplots and relative SI comparison:**



Application example 1: python model (4)

First-order response with four equally sampled parameters

- **Output:** **Relative sensitivity per batch:**



Application example 1: python model (5)

First-order response with four equally sampled parameters

- **Conclusions:**
  - correct sampling and model evaluation by the tool
  - consistency of scatterplots and relative SI
  - agreement between obtained SI and expected results
  - reasonable choice of sample size

Application example 1: PLTEMP model (1)

PLTEMP model of a FRMII cooling channel (hypothetical)

- **PLTEMP:**
  SSTH code for fast assessment of T/H performance and safety margins of research reactors (ANL)

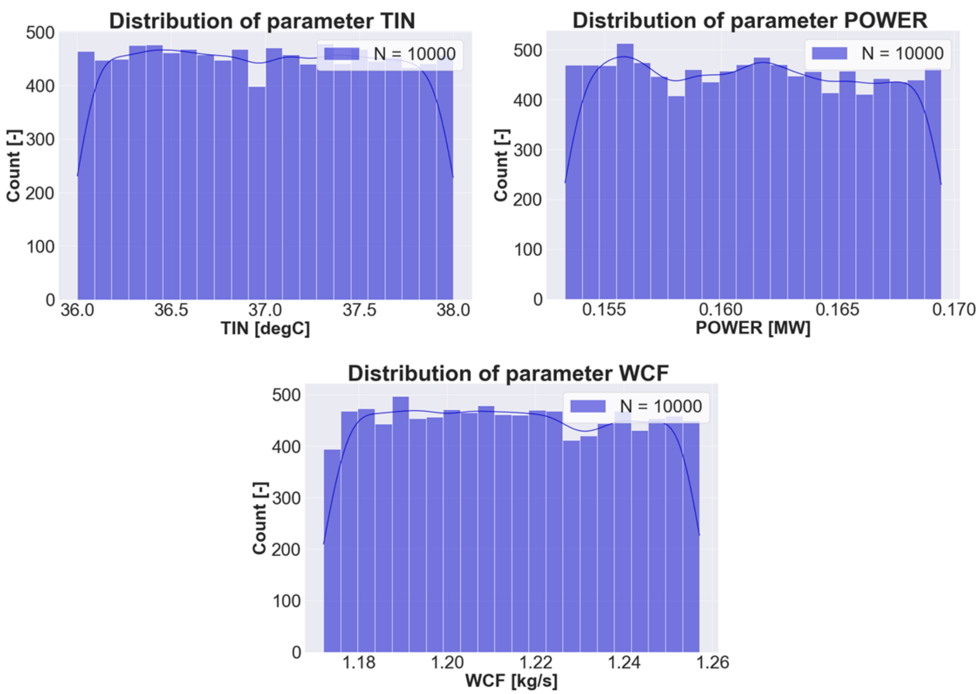
- **Input:**

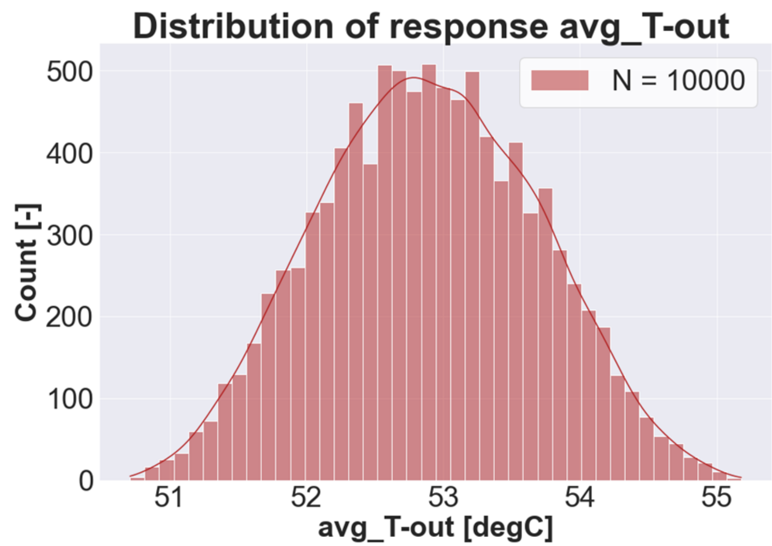
- Response:	average coolant outlet temperature in cooling channel of FRM II		
- Parameters: (arbitrary)	coolant inlet temperature:	nominal value +/- 1°C	(uniform)
	deposited power:	nominal value +/- 5%	(uniform)
	channel mass flow rate:	nominal value +/- 3.5%	(uniform)

Application example 1: PLTEMP model (2)

PLTEMP model of a FRMII cooling channel (hypothetical)

- **Output:** **Histograms of sampled parameter and obtained response values:**

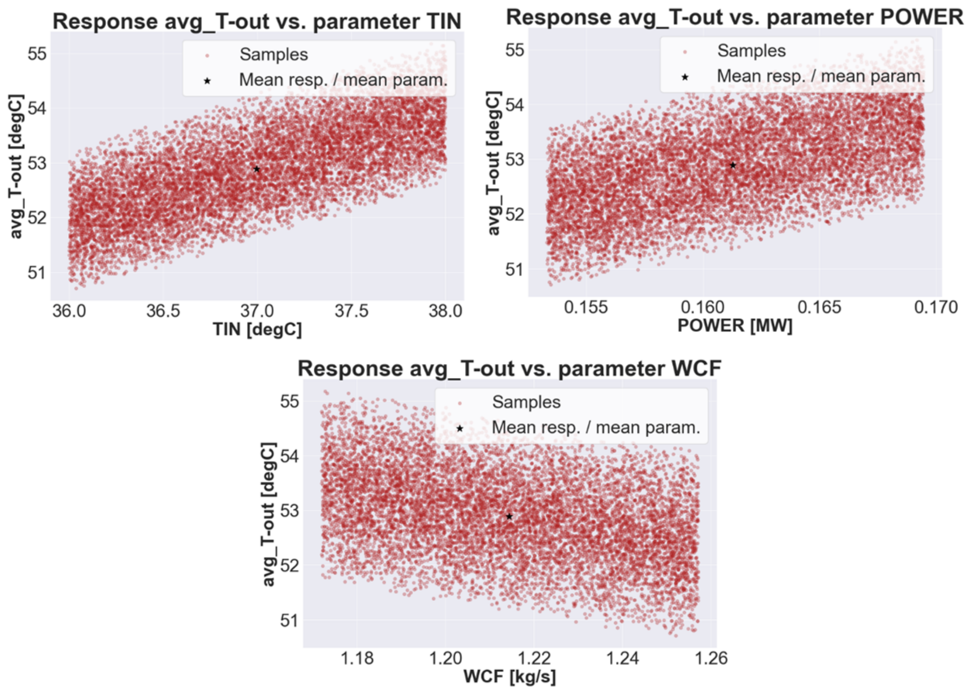


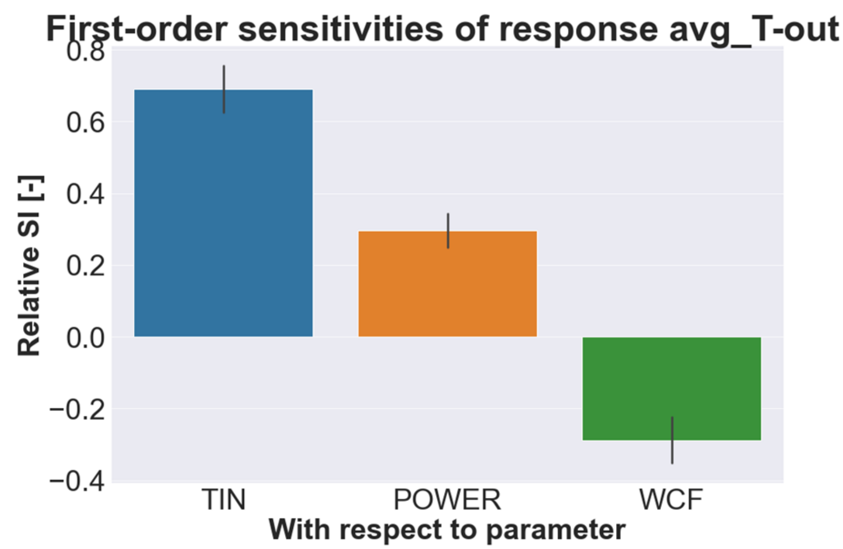


Application example 1: PLTEMP model (3)

PLTEMP model of a FRMII cooling channel (hypothetical)

- **Output:** **Scatterplots and relative SI comparison:**

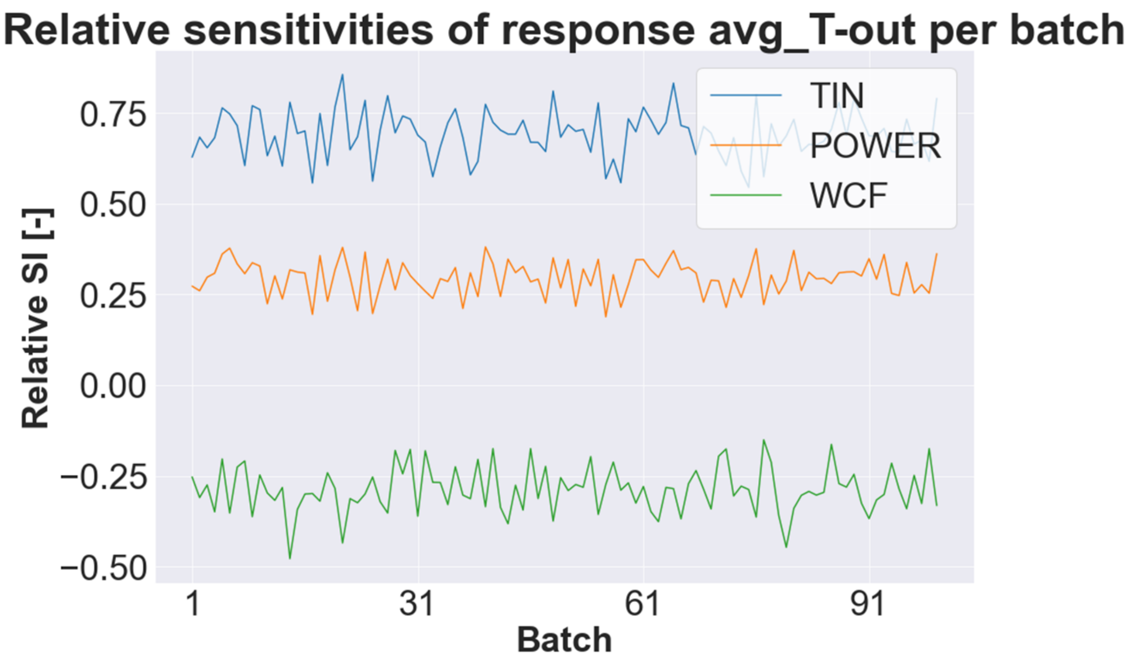




Application example 1: PLTEMP model (4)

PLTEMP model of a FRMII cooling channel

- **Output:** **Relative sensitivity per batch:**



Application example 1: PLTEMP model (5)

PLTEMP model of a FRMII cooling channel

- **Conclusions:**
  - SI reflect expected behavior of the response:

    Inlet temperature, power ↑ → outlet temperature ↑

    Mass flow rate ↑ → outlet temperature ↓

  - most influential parameter: inlet temperature

Summary and outlook

- **Done:**
  Implementation of a tool for first-order sensitivity analysis of python models, PLTEMP models and external data

- **Ongoing work:**
  Inclusion of second-order sensitivity analysis

- **Outlook:**
  - Inclusion of uncertainty propagation
  - Coupling with Ansys CFX

INSTITUT LAUE LANGEVIN THE EUROPEAN NEUTRON SOURCE

NEUTRONS FOR SOCIETY

Special thanks to all co-authors:

- W. Petry, C.Reiter (TUM)
- F. Thomas, Y. Calzavara (ILL)
- P. Bianchini (MMP)

FRM II
Forschungs-Neutronenquelle
Heinz Maier-Leibnitz

Application example 1: python model (1)

First-order response with four equally sampled parameters

Slide version with equation

- **Input:**

  - Response: $y = x_1 + 2x_2 + 3x_3 + 4x_4$
  - Parameters: $x_1, x_2, x_3, x_4 \in N(1,1)$

  Note: $\bar{y} = y(\bar{x}) = 1 + 2 \cdot 1 + 3 \cdot 1 + 4 \cdot 1 = 10$

- **Expected results for the first-order SI:**

$$\left(S^1_{y,x_1}\right)_{abs} = \frac{dy}{dx_1}(\mu_1) = \frac{dy}{dx_1} = 1 \qquad \left(S^1_{y,x_1}\right)_{rel} = \left(S^1_{y,x_1}\right)_{abs} \cdot \frac{\overline{x_1}}{\bar{y}} = 1 \cdot \frac{1}{10} = 0.1$$

$$\left(S^1_{y,x_2}\right)_{abs} = \frac{dy}{dx_2}(\mu_2) = \frac{dy}{dx_2} = 2 \qquad \left(S^1_{y,x_2}\right)_{rel} = \left(S^1_{y,x_2}\right)_{abs} \cdot \frac{\overline{x_2}}{\bar{y}} = 2 \cdot \frac{1}{10} = 0.2$$

$$\left(S^1_{y,x_3}\right)_{abs} = \frac{dy}{dx_3}(\mu_3) = \frac{dy}{dx_3} = 3 \qquad \left(S^1_{y,x_3}\right)_{rel} = \left(S^1_{y,x_3}\right)_{abs} \cdot \frac{\overline{x_3}}{\bar{y}} = 3 \cdot \frac{1}{10} = 0.3$$

$$\left(S^1_{y,x_4}\right)_{abs} = \frac{dy}{dx_4}(\mu_4) = \frac{dy}{dx_4} = 4 \qquad \left(S^1_{y,x_4}\right)_{rel} = \left(S^1_{y,x_4}\right)_{abs} \cdot \frac{\overline{x_4}}{\bar{y}} = 4 \cdot \frac{1}{10} = 0.4$$