Uncertainty quantification and sensitivity analysis of multi-parameter models

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Outline

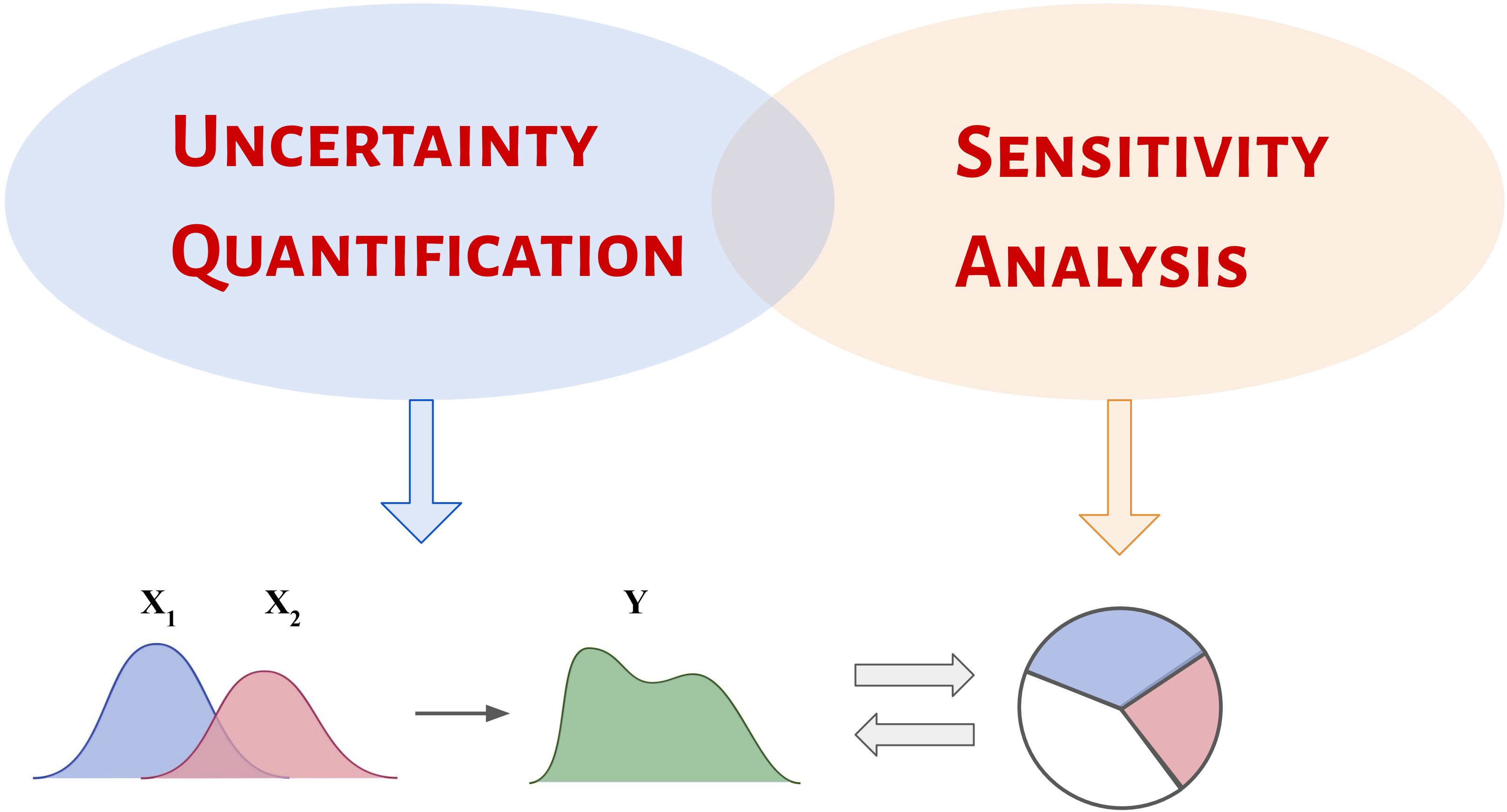
- General overview of some of the main methods
- Which methods are used when
- What are the limitations

Uncertainty Quantification

Quantification of uncertainties in model outputs resulting from uncertainties in model input parameters

Sensitivity Analysis

Quantification or ranking of the importance of model inputs to selected outputs of interest.

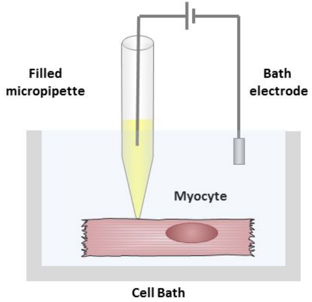

Uncertainty Quantification
Sensitivity Analysis
X_1
X_2
Y

There are several sources of uncertainty in numerical models

Experimental

Measurement setup

Technique

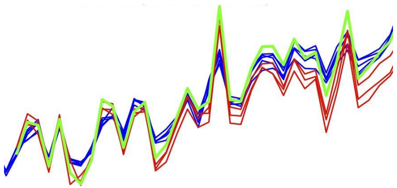


Parametric

Unknown

Not measurable

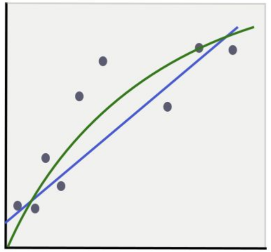
Stochastic



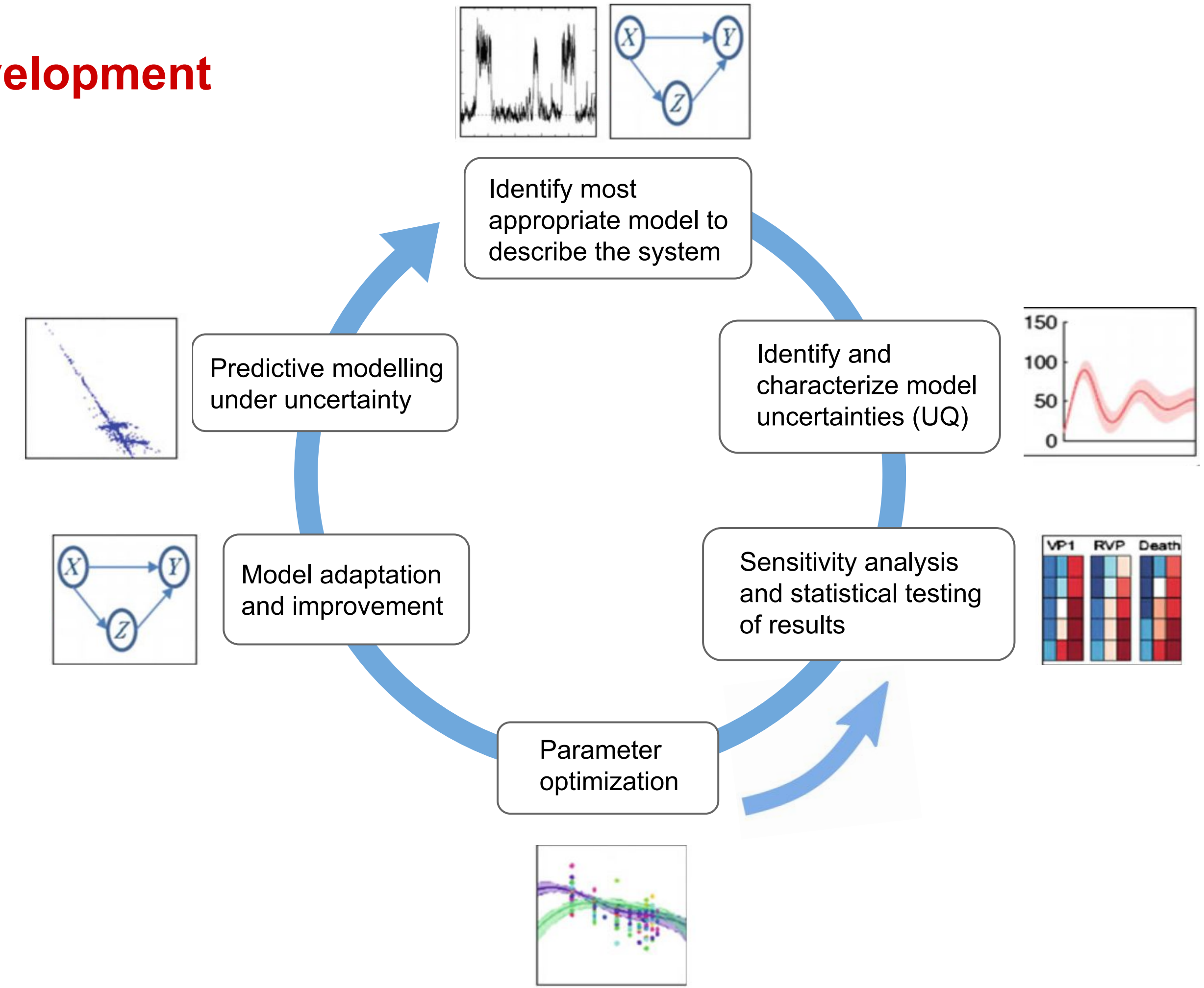
Structural

Model adequacy

Unknown underlying physics



Model development life cycle



General notation

Model: $Y = f(X)$

Input variables (model parameters): $X=(X_1, X_2, \dots, X_n)$

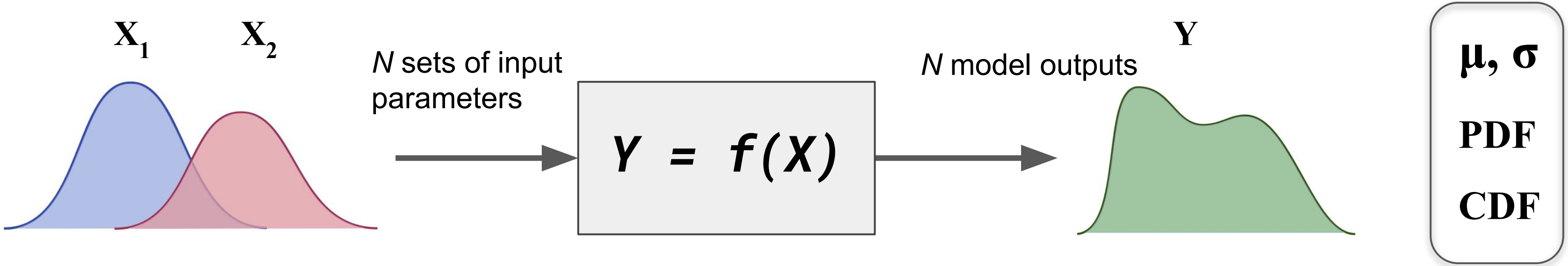
Output variables: $(Y_1, Y_2, \dots, Y_k)$

Number of input variables: n

Number of samples: N

Uncertainty Quantification

Uncertainty in input variables propagates through the model to the output



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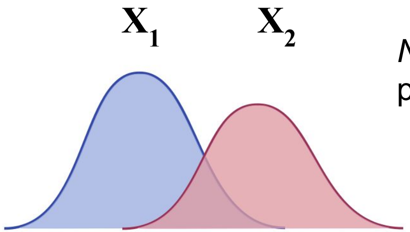
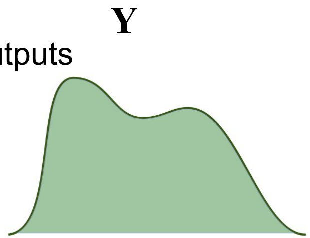


N sets of input parameters

$$Y = f(X)$$

N model outputs



μ, σ

PDF

CDF

Defined *a priori*

Uniform distribution

$$f(x) = \frac{1}{b-a},$$

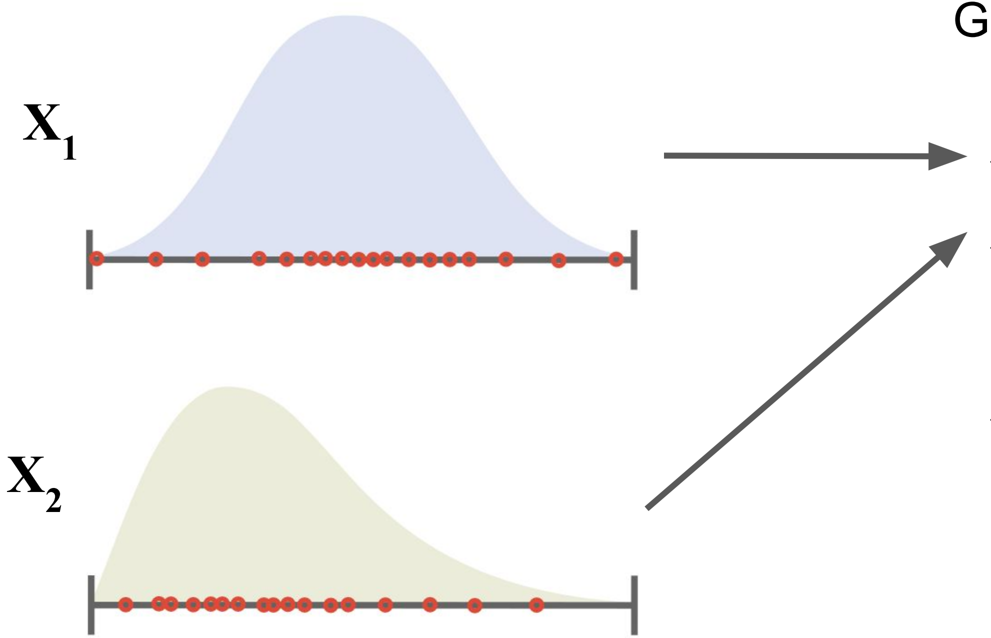
$$a < x < b, -\infty < a < b < +\infty$$

Normal distribution

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}},$$

$$-\infty < x < +\infty$$

Sampling methods can be used when the uncertainties cannot be calculated analytically



Generate N random samples

$$\left.\begin{array}{l} \{\, X_1^{(1)}, X_1^{(2)}, \ldots, X_1^{(N)} \,\} \\ \{\, X_2^{(1)}, X_2^{(2)}, \ldots, X_2^{(N)} \,\} \\ \vdots \\ \{\, X_n^{(1)}, X_n^{(2)}, \ldots, X_n^{(N)} \,\} \end{array}\right]$$

n vectors of N samples

Sampling based UQ follows some criteria

1. Input space is (pseudo) randomly sampled
2. *N* random samples drawn from the specified PDF
3. Sampling must cover entire input parameter space
4. Sampled numbers follow the desired PDF when enough samples are drawn
5. Test for "random number quality"

Random sampling

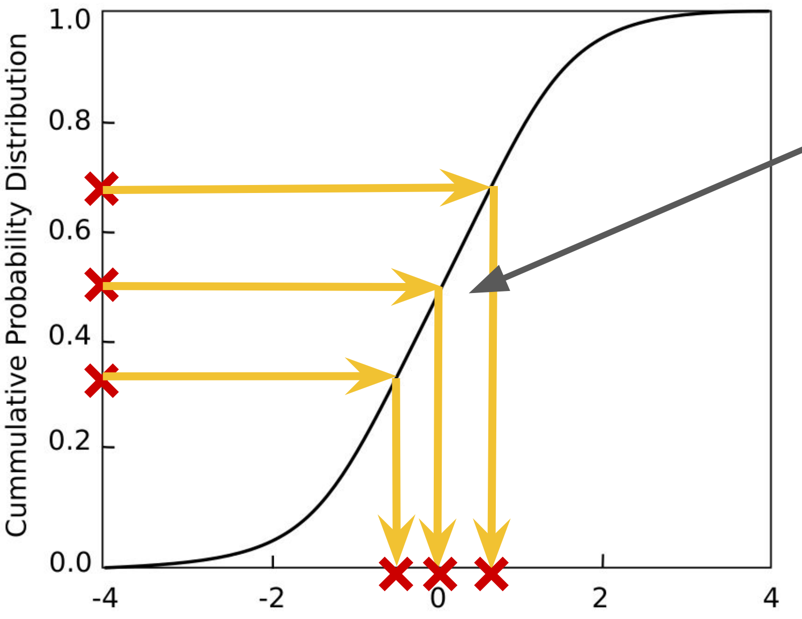
Latin Hypercube

Monte Carlo is a common method for random sampling

Monte Carlo method → a broad class of computational algorithms that relies on repeated random sampling to generate sequences of numbers that are used to solve (often deterministic) problems.

Monte Carlo simulation → samples from a probability distribution of each input variable to produce a large number of possible outcomes; it uses repeated sampling to obtain the statistical properties of a model (i.e., its behavior).

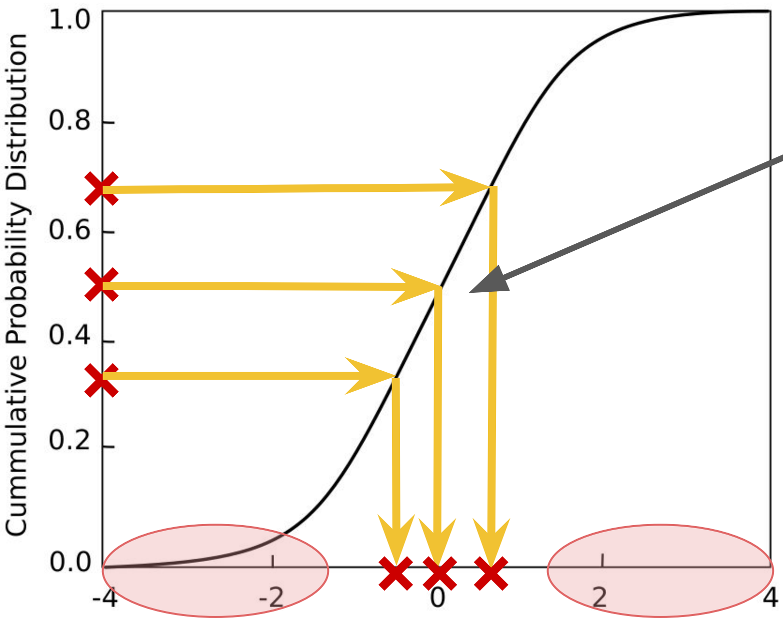
Monte Carlo method



The most likely values lie in the range where the curve is the steepest

Memoryless

Monte Carlo method

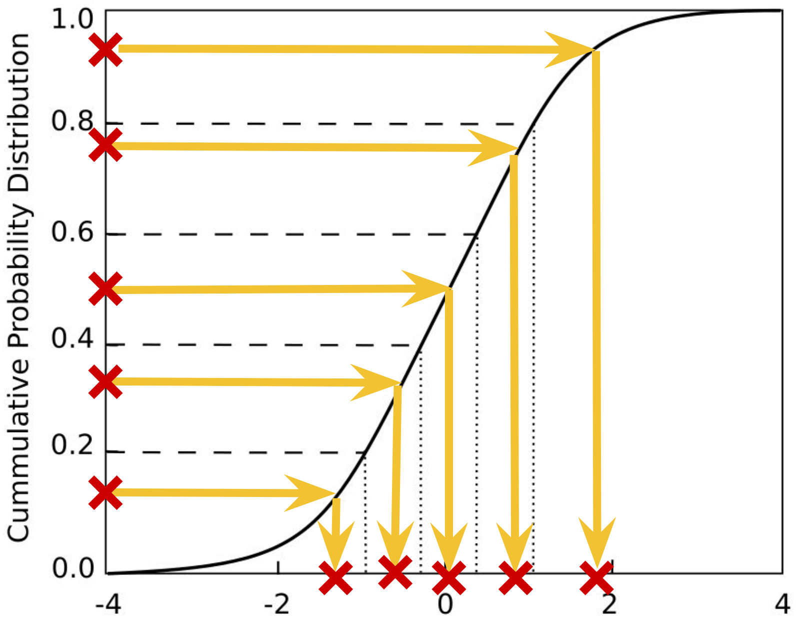


Under-represented

The most likely values lie in the range where the curve is the steepest

Memoryless

Latin-hypercube sampling



LHS introduces *stratification* of the CDF

One sample inside each stratification

Ensures an even coverage of the entire CDF

Recreates PDF with less samples compared to the MC approach

METAMODELLING

- ➔ Metamodels can be used to reduce computational cost of complex models
- ➔ Replace the model with a simpler model (surrogate) that can accurately emulate the behavior of the system

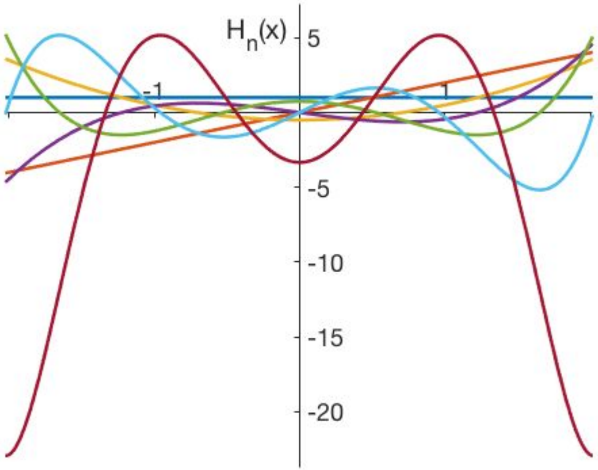
$$f' \approx f$$

- ➔ The search curve of the surrogate model can be used to make predictions of the model output
- ➔ Dimensionality reduction

Polynomial Chaos Expansion is one of the most common methods

- ➔ PCE aims at approximating a computational model response using a set of orthogonal polynomials of the input variables.
- ➔ Different basis functions can be used for different input uncertainty distributions, eg. Hermite, Legendre, and Laguerre polynomials

Hermite polynomials



PCE is based on spectral representation of uncertainty

➔ PCE aims at approximating a computational model response using a set of orthogonal polynomials of the input variables.

$$\hat{f}(w) = \sum_{k=0}^{P} C_k \Phi_k(\xi(w))$$

$$C_k = \int_{\Omega} \hat{f}(\xi)\rho(\xi)\Phi_k(\xi)d\xi$$

$$\xi = (\xi_1, \cdots, \xi_{1n})$$

PCE is based on spectral representation of uncertainty

➔ PCE aims at approximating a computational model response using a set of orthogonal polynomials of the input variables.

Random basis of orthogonal functions

$$\hat{f}(w) = \sum_{k=0}^{P} C_k \boxed{\Phi_k(\xi(w))}$$

$$C_k = \int_{\Omega} \hat{f}(\xi)\rho(\xi)\Phi_k(\xi)d\xi$$ **?**

PCE coefficients (spectral modes)

$$\xi = (\xi_1, \cdots, \xi_{1n})$$

n-dimensional vector of random variables

Intrusive PCE

➔ all dependent variables and random parameters in the governing equations are replaced with their polynomial chaos expansions

➔ Difficult, time consuming, and computationally expensive

Non-intrusive PCE

➔ obtain approximations of the polynomial coefficients without making any modifications to the deterministic code

➔ Main approaches are: sampling based, collocation based, and quadrature methods

Non-intrusive point collocation PC allows to determine C_k by solving a linear system

$$\hat{f}(w) = \sum_{k=0}^{P} C_k \Phi_k(\xi(w))$$

1. Replace the variables $f(x)$ of interest with chosen polynomial expansions with $P+1$ modes.

Non-intrusive point collocation PC allows to determine C_k by solving a linear system

$$\boxed{\hat{f}(w)} = \sum_{k=0}^{P} C_k \Phi_k(\xi(w))$$

1. Replace the variables *f(x)* of interest with chosen polynomial expansions with $P+1$ modes.
2. Choose $P+1$ random points of the input space, and evaluate model at those points (left-hand side of equation)

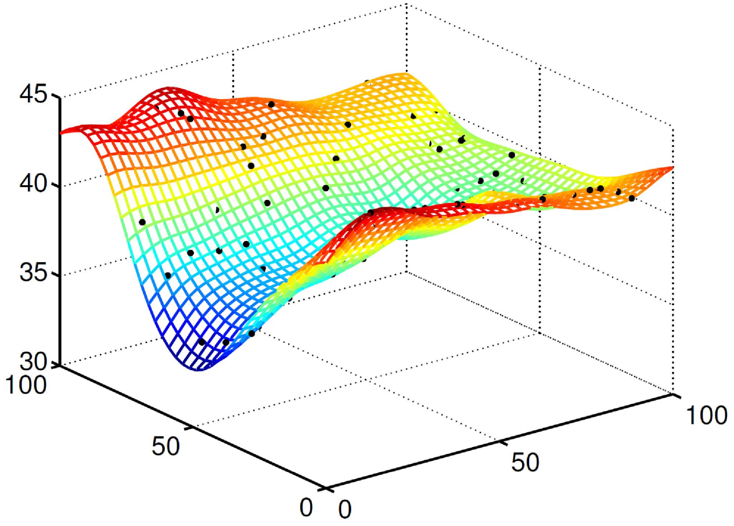
Non-intrusive point collocation PC allows to determine C_k by solving a linear system

$$\boxed{\hat{f}(w)} = \sum_{k=0}^{P} C_k \Phi_k(\xi(w))$$

$$\begin{bmatrix} \Phi_0(\xi_0) & \Phi_1(\xi_0) & \dots & \Phi_P(\xi_0) \\ \Phi_0(\xi_1) & \Phi_1(\xi_1) & \dots & \Phi_P(\xi_1) \\ \vdots & \vdots & \ddots & \vdots \\ \Phi_0(\xi_n) & \Phi_1(\xi_n) & \dots & \Phi_P(\xi_n) \end{bmatrix} \times \boxed{\begin{bmatrix} C_0 \\ C_1 \\ \vdots \\ C_P \end{bmatrix}} = \begin{bmatrix} \hat{f}(\xi_0) \\ \hat{f}(\xi_{01}) \\ \vdots \\ \hat{f}(\xi_{0n}) \end{bmatrix}$$

1. Replace the variables $f(x)$ of interest with chosen polynomial expansions with $P+1$ modes.
2. Choose $P+1$ random points of the input space, and evaluate model at those points (left-hand side of equation)
3. Solve linear system to determine the coefficients Ck (spectral modes)

Point collocation requires expanded system to be satisfied at a set of points



[http://www.sudret.ibk.ethz.ch/research/past-projects/polynomial-chaos-kriging.html]

➔ search curve matches exactly the model where the function is evaluated to construct the curve

➔ MC, LHS, etc. can be used to increase number of samples and accuracy of approximation

➔ If several collocation points are taken (N>(P+1)), Least Squares can be used to solve the linear system

Sensitivity Analysis

Local SA → parameters are varied one-at-a-time with very small perturbations (eg., 0.1%)

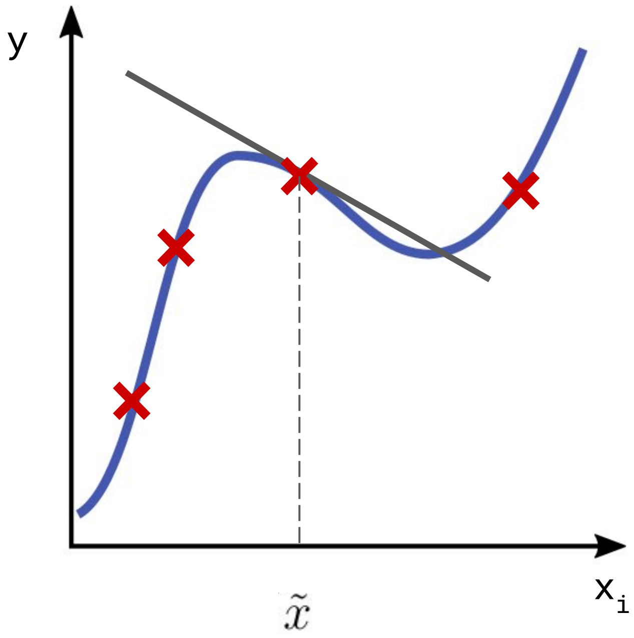
Global SA → all parameters varied simultaneously over the entire input parameter space

Screening

Variance-based

Sampling-based

Local SA estimates the local effects of small perturbations in inputs, by varying inputs one at a time

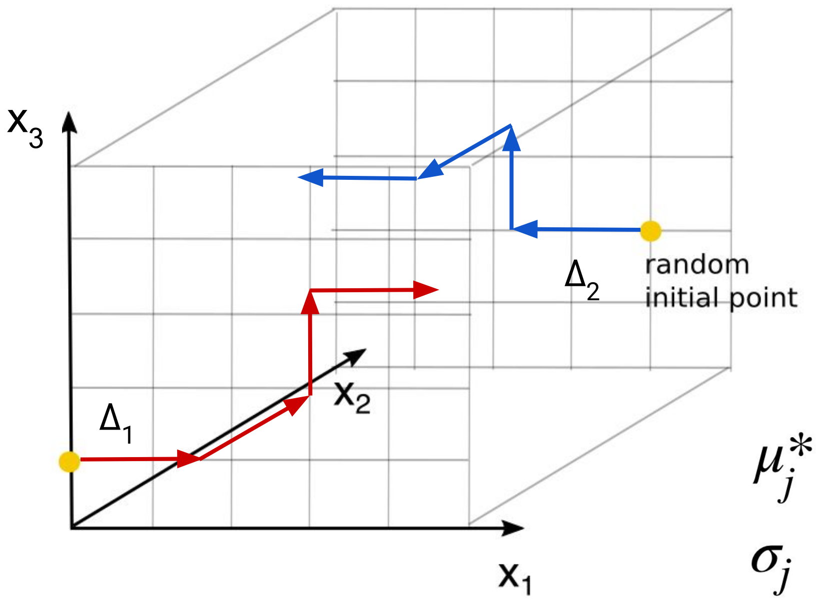


Partial Derivatives

$$S_i = \frac{\partial f(\tilde{x})}{\partial x_i}$$

Screening methods offer a qualitative type of GSA methods at a low computational cost

Morris method (screening)



$$E_j^{(i)} = \frac{f(\tilde{\mathbf{X}}) - f(\mathbf{X})}{\Delta}$$

$\mu_j^* \rightarrow$ overall importance

$\sigma_j \rightarrow$ nonlinear/interaction effects

➔ Allows to rank variables in order of their importance

Sampling-based SA rely on random sampling of the input parameter space to calculate statistical moments of the model responses

Regression analysis

General Linear Models, MLR, MVLR

Correlation analysis

Pearson and Spearman correlation coefficients

Variance decomposition

Sobol method, FAST/eFAST

Multivariate Linear Regression

$$\begin{bmatrix} y_{11} & y_{12} & \dots & y_{1k} \\ y_{21} & y_{22} & \dots & y_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ y_{n1} & y_{n2} & \dots & y_{nk} \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{12} & \dots & x_{2p} \\ 1 & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{np} \end{bmatrix} \times \begin{bmatrix} \beta_{01} & \dots & \beta_{0k} \\ \beta_{11} & \dots & \beta_{1k} \\ \vdots & \ddots & \vdots \\ \beta_{p1} & \dots & \beta_{pk} \end{bmatrix} + \begin{bmatrix} \epsilon_{11} & \dots & \epsilon_{1k} \\ \epsilon_{21} & \dots & \epsilon_{2k} \\ \vdots & \ddots & \vdots \\ \epsilon_{n1} & \dots & \epsilon_{nk} \end{bmatrix}$$

$$\mathbf{Y} = \mathbf{X} \cdot \mathbf{B} + \mathbf{E}$$

Multivariate Linear Regression

$$\begin{bmatrix} y_{11} & y_{12} & \dots & y_{1k} \\ y_{21} & y_{22} & \dots & y_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ y_{n1} & y_{n2} & \dots & y_{nk} \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{12} & \dots & x_{2p} \\ 1 & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{np} \end{bmatrix} \times \begin{bmatrix} \beta_{01} & \dots & \beta_{0k} \\ \beta_{11} & \dots & \beta_{1k} \\ \vdots & \ddots & \vdots \\ \beta_{p1} & \dots & \beta_{pk} \end{bmatrix} + \begin{bmatrix} \epsilon_{11} & \dots & \epsilon_{1k} \\ \epsilon_{21} & \dots & \epsilon_{2k} \\ \vdots & \ddots & \vdots \\ \epsilon_{n1} & \dots & \epsilon_{nk} \end{bmatrix}$$

$$\hat{\mathbf{Y}} = \mathbf{X} \cdot \hat{\mathbf{B}}$$

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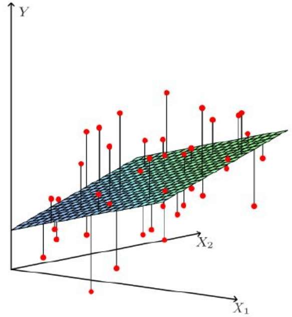
$$\hat{\mathbf{Y}} = \mathbf{X} \cdot \hat{\mathbf{B}}$$

Least squares:

$$\hat{\mathbf{B}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$



Normalization:

$$SRC_j = \hat{\beta}_j \sqrt{\frac{Var(X_j)}{Var(Y)}}$$

⇧ **|SRC|** ⇧ **sensitivity**

Goodness of fit can be estimated with the coefficient of determination

$$R^2 = \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}$$

- ➔ measures the extent to which the regression model can match the observed data;
- ➔ Regression coefficients provide measure of importance only if X_i are independent; otherwise, variable rankings are unreliable;
- ➔ Regression gives quantitative SA only if the model is perfectly linear, i.e., R^2 is close to 1.

Correlation analysis measures the strength of association between two variables

$$\rho_{X_jY} = \frac{\textbf{Cov}(X_j, Y)}{\sqrt{\textbf{Var}(X_j)\textbf{Var}(Y)}}$$

$$-1 \leq \rho_{x_iy} \leq 1$$

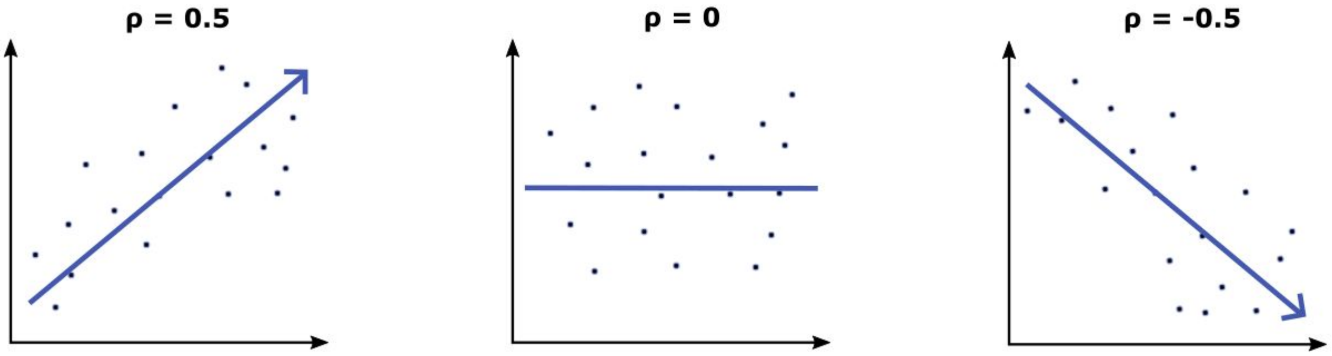
Pearson CC

(Linear trends)

Measure of the **joint variability** of $\mathrm{X_j}$ and Y, normalized to their variances.

Detects trends in data, without making assumptions on causality.

Correlation coefficient can be used a sensitivity index



↑ **|ρ|** ↑ **sensitivity**

- ➔ Provides measure of importance of X_i given that variables are **uncorrelated**;
- ➔ Non-zero ρ does not preclude the existence of a well-defined nonlinear association between X_i and y.

For nonlinear monotonic trends, we can do a **Rank transformation** of the data to compute the correlation coefficients

X	Rank(X)
95	2
120	6
98	3
102	4
87	1
111	5

$$\rho_{\hat{X}_j Y} = \frac{\mathbf{Cov}(\hat{X}_j, Y)}{\sqrt{\mathbf{Var}(\hat{X}_j)\mathbf{Var}(Y)}}$$

Spearman CC

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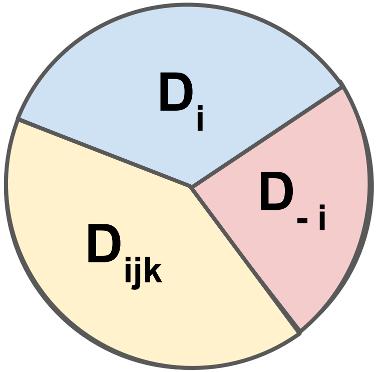
$$\rho_{\hat{X}_j Y} = \frac{\mathrm{Cov}(\hat{X}_j, Y)}{\sqrt{\mathrm{Var}(\hat{X}_j)\mathrm{Var}(Y)}}$$

Spearman CC

Linear regression → **Standard Rank Regression Coefficients**

Variance-based SA is based on variance decomposition into fractions attributable to the main effects of each input variable, plus the interactions among variables



First-order effects → main effect of X_i alone

Higher-order effects → interactions among several variables

Complementary effects → effects of other variables except X_i

Total-order effects → first-order + higher-order effects

Sobol method of variance decomposition partitions the output variance into terms of increasing order associated to each input

$$f = f_0 + \sum_i f_i(X_i) + \sum_{i<j} f_{ij}(X_i, X_j) + \cdots + f_{12\cdots n}(X_1, \cdots, X_n),$$

Variance:

$$\int f^2 dX - f_0^2 = \sum_{s=1}^{n} \sum_{i_1<\cdots<i_s}^{n} \int f^2_{i_1\cdots i_s} dx_{i_1} \cdots dx_{i_s}.$$

For orthogonal summands:

$$\mathrm{Var}(Y) = \sum_{s=1}^{n} \sum_{i_1<\cdots<i_s}^{n} D_{i_1\cdots i_s}(Y) =$$

$$= \sum_{i=1}^{n} D_i(Y) + \sum_{i<j}^{d} D_{ij}(Y) + \cdots + D_{1,\ldots,n}(Y)$$

Sobol indices are ratios of variances and thus are **positive** by definition

First-order indices

$$S_i = \frac{D_i(Y)}{D(Y)},$$

Higher-order indices

$$S_{i_1 \cdots i_s} = \frac{D_{i_1 \cdots i_s}(Y)}{D(Y)}$$

Total-order indices

$$S_i^T = S_i + \sum_{i<j} + \sum_{j \neq i, k \neq i, j<k} S_{ijk} + \cdots = \sum_{l \in \# i} S_i$$

$$\sum_{s=1}^{n} \sum_{i_1 < \cdots < i_s}^{n} S_{i_1 \cdots i_s} = \sum_{i}^{n} S_i + \boxed{\sum_{i<j}^{n} S_{i \ldots j}} = 1 \longrightarrow \sum_{i=1}^{n} S_i \simeq 1$$

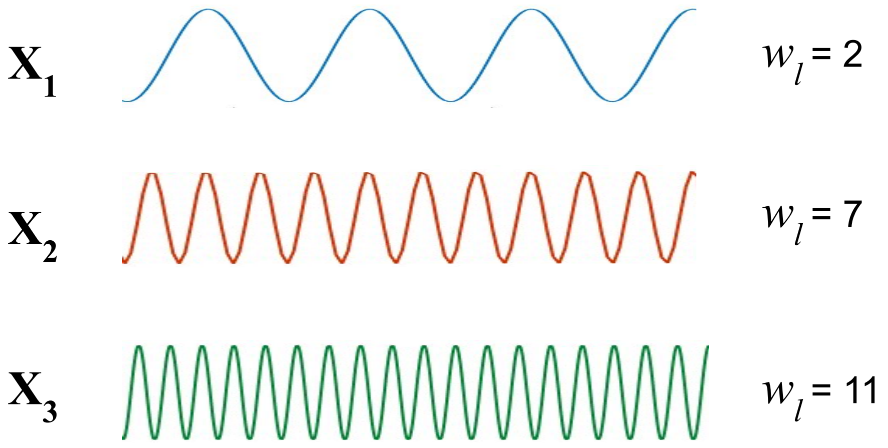
≃ 0

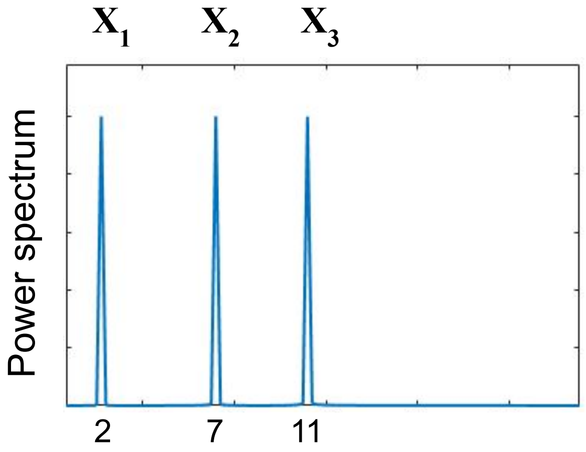
Additive

Fourier Amplitude Sensitivity Test is a variance-based SA method

➔ Each inputs is varied at a specific fundamental frequency w_l (**unique identifier** of the parameter)

➔ Frequency spectrum shows each fundamental w_l and its harmonics





The first part is to re-formulate the model in terms of periodically varying input variables

1. Assign fundamental frequencies w_l to each input

➔ w_l are integers

➔ w_l are (approximately) incommensurate

2. Replace each X_l by parametric sinusoidal functions

$$x_l(s) = G_l(\sin w_l s)$$

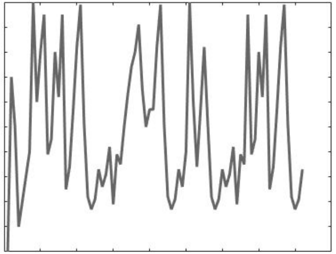
$$-\infty < s < +\infty$$

3. Discretization

$$s_k = \frac{2k\pi}{N}, k = 1, ..., N$$

4. Evaluate model for each sampled frequency

$$Y = f(X)$$

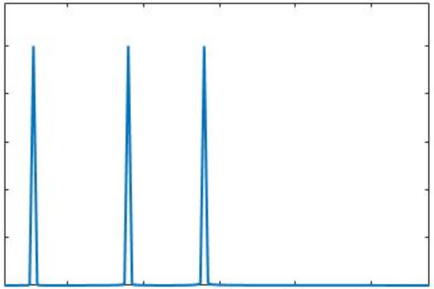


The second part is to perform Fourier analysis on model results to determine which frequencies propagated more ‘strongly’

5. Fourier analysis

$$A_{pw_i} = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(s)\cos(pw_l s)ds$$

$$B_{pw_i} = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(s)\sin(pw_l s)ds$$



6. Calculate variances

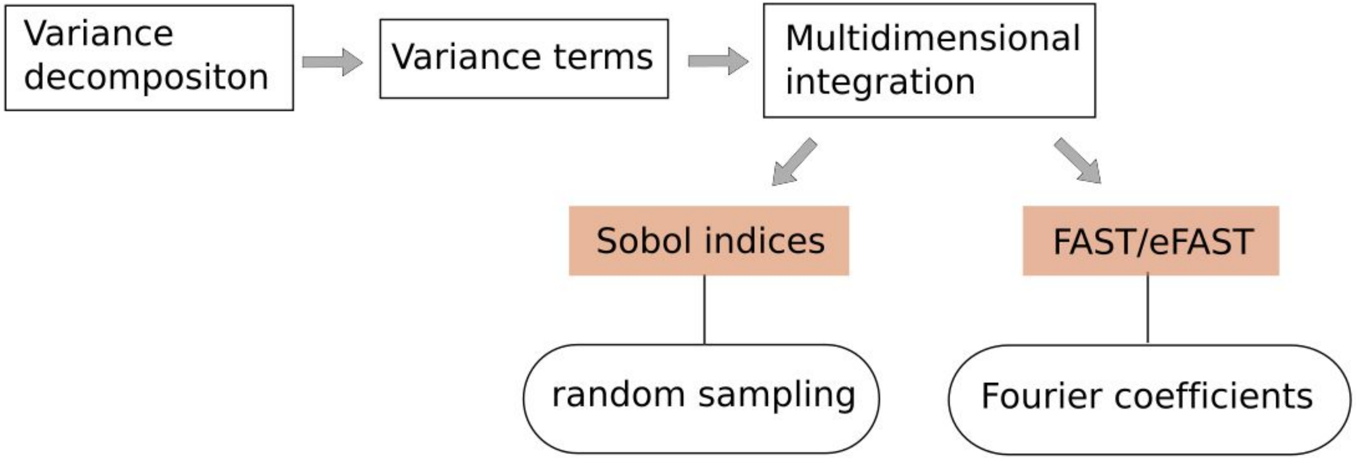
$$\sigma_l^2 = 2\sum_{p=-\infty}^{+\infty}(A_{pw_l}^2 + B_{pw_l}^2)$$

$$\sigma^2 = 2\sum_{j=-\infty}^{+\infty}(A_j^2 + B_j^2)$$

7. Calculate sensitivity indices

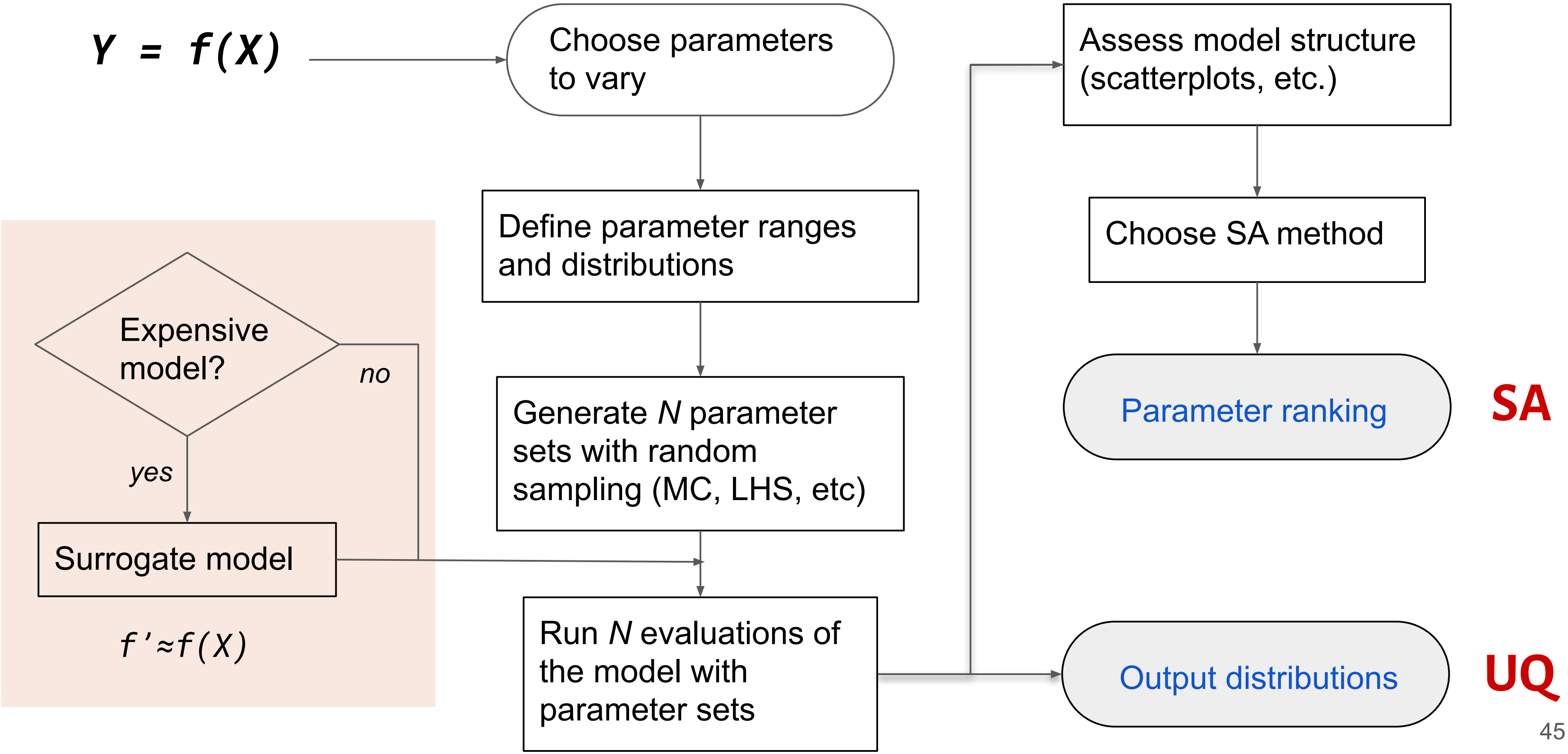
$$S^*_{w_l} = \frac{\sum_{p=-(N/2-1)}^{N/2}(A^*_{pw_l}|^2 + B^*_{pw_l}|^2)}{\sum_{j=-(N/2-1)}^{N/2}(A^*_j|^2 + B^*_j|^2)} = \frac{(\sigma_i^*)^2}{(\sigma^*)^2}$$

Variance-based methods



- ➔ FAST is more computational efficient as compared to the Sobol method (requires less samples for convergence)
- ➔ Sobol seems to provide more accurate estimates of the variance
- ➔ FAST cannot compute total-order indices

General UQ/SA framework



Conclusions & synthesis

- ➔ It is more and more accepted that good model development practice requires acknowledgement of model uncertainties
- ➔ There are multiple different ways to perform SA in multi-parameter models
- ➔ Methods of sensitivity analysis can give quite different results, and therefore should ideally be performed complementarily
- ➔ The best choice of method should be based on the type of model and on the nature of the data
- ➔ For computationally expensive models, it is often necessary to replace the model with a metamodel that can emulate the behavior of the system with much less complexity
- ➔ UQ and SA are valuable tools for understanding how models work