NTNU
Norwegian University of Science and Technology

Tutorial on Uncertainty quantification and sensitivity analysis

Jacob Sturdy
Vinzenz Eck
Leif Rune Hellevik

STARFiSh
STochastic ARterial Flow Simulations
Division of Biomechanics · NTNU

Uncertainty - Random Variables

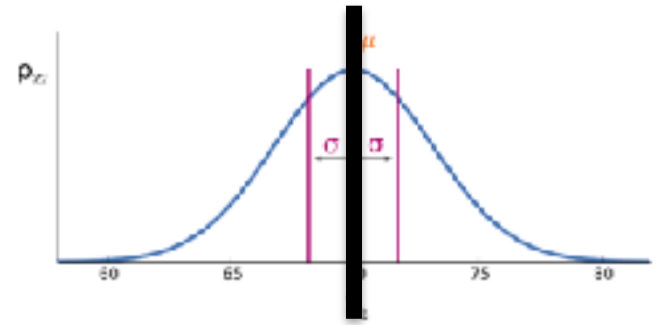
Random variable $\mathbf{Y}$:

Density function $\rho_{\mathbf{Y}}(y)$ $\Pr(Y \leq y) = \int_{-\infty}^{y} \rho_Y(s) ds$

Expected value:

$$\mathbb{E}[\mathbf{Y}] = \int_{\Omega_Y} y \rho_{\mathbf{Y}}(y)\,\mathrm{d}y$$

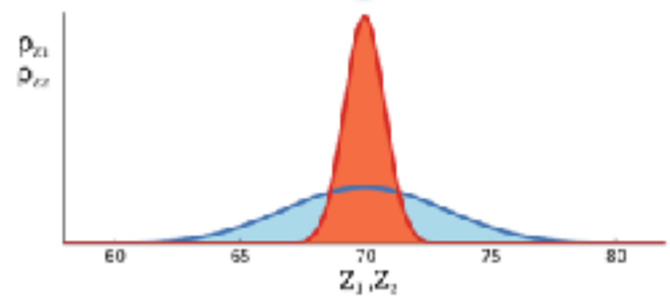
$\mathbb{E}[\mathbf{Y}]$



Variance:

$$\mathrm{Var}[\mathbf{Y}] = \int_{\Omega_Y} (y - \mathbb{E}[\mathbf{Y}])^2 \rho_{\mathbf{Y}}(y)\,\mathrm{d}y$$

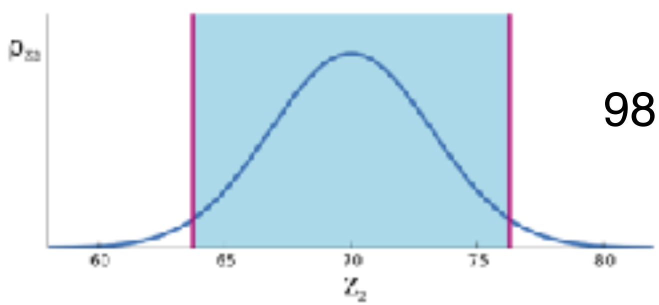
$$\sigma[\mathbf{Y}] = \sqrt{\mathrm{Var}[\mathbf{Y}]}$$



Prediction intervals:

$$\beta = \int_{-\infty}^{y_{[\beta]}} \rho_{\mathbf{Y}}(y)\,\mathrm{d}y$$

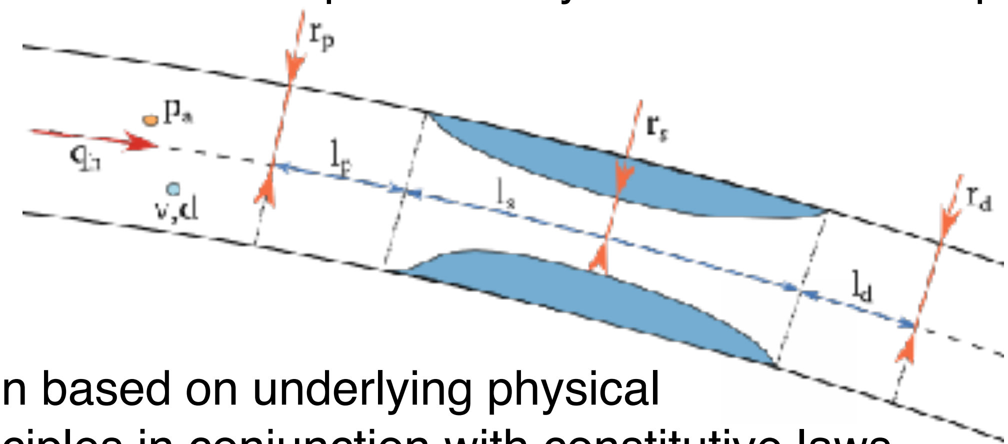
$$I_\beta = \left[y_{[\beta/2]}, y_{[1-\beta/2]}\right]$$



98 % probability

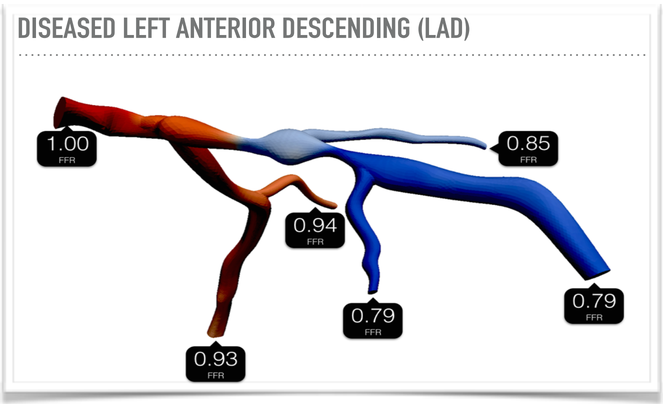
Models, inputs and parameters

Models describe a particular system or relationship



often based on underlying physical principles in conjunction with constitutive laws

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} - \nu\nabla^2\mathbf{u} = -\nabla h.$$



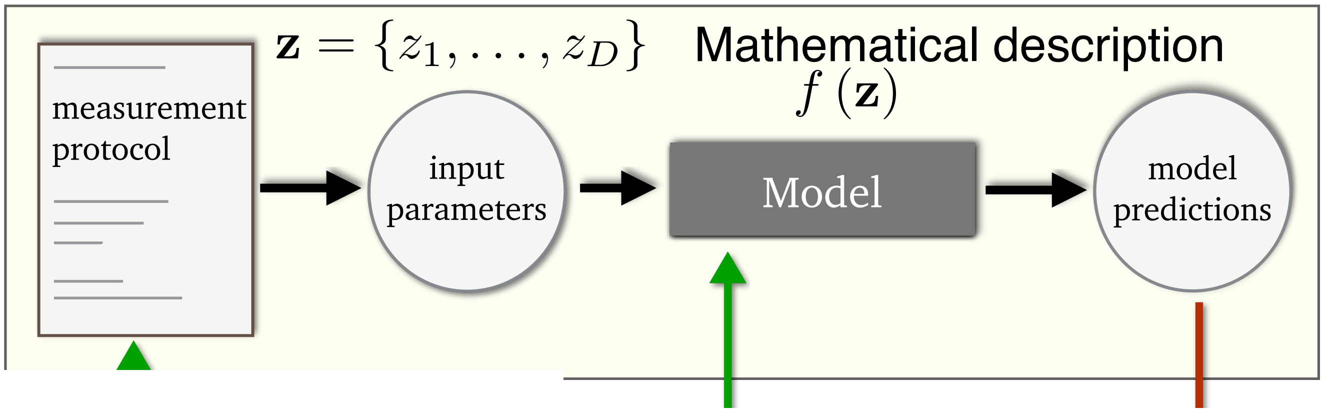
Model predictions depend on time, space and parameters

$$p(t,\mathbf{x},\mathbf{z}) \qquad \tau(t,\mathbf{x},\mathbf{z}) \qquad q(t,\mathbf{x},\mathbf{z})$$

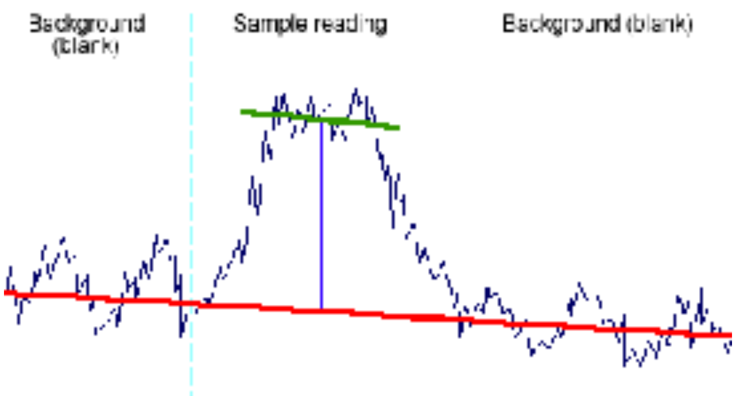
For the purposes of UQSA the focus is on dependence on input parameters $\mathbf{z}$

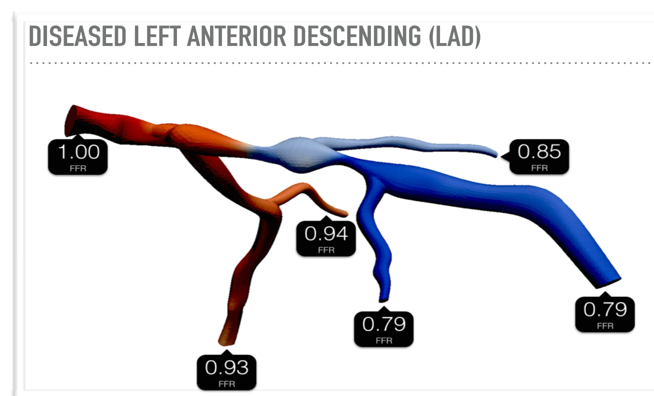
$$p(\mathbf{z}) \qquad \tau(\mathbf{z}) \qquad q(\mathbf{z})$$

Models, inputs and parameters



$y = f(\mathbf{z})$





2 Uncertainty quantification

Many inputs aren't known exactly

$$\mathbf{Z} = \{Z_1, \ldots, Z_D\} \rightarrow f(\mathbf{Z}) \rightarrow \boxed{\mathbf{Y}}$$

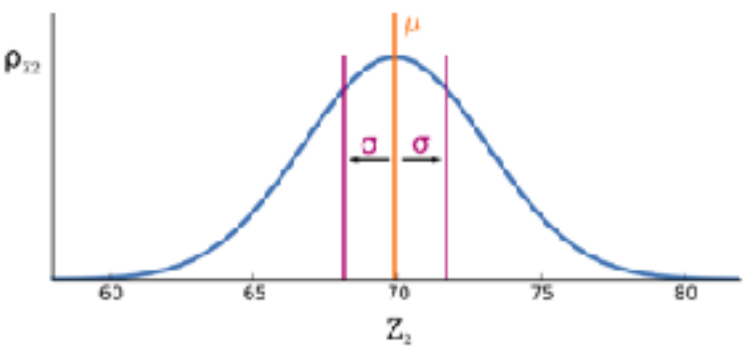
random variables

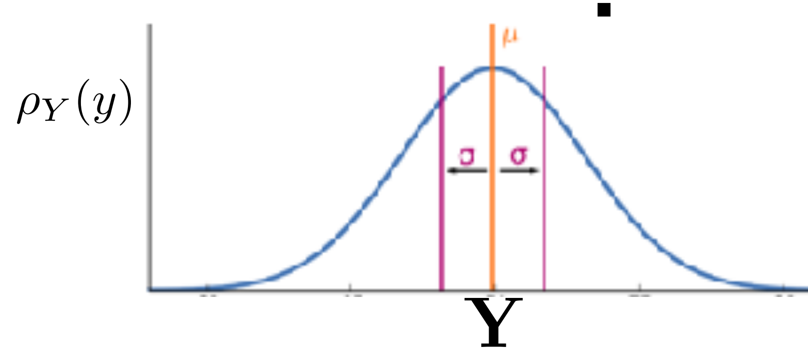
known distributions

random variable

unknown distribution

?





Overview

deterministic system

$\mathbf{z} = \{z_1, \ldots, z_D\}$ → $f(\mathbf{z})$ → $y = f(\mathbf{z})$

input parameter

computational model

model prediction

uncertain

uncertain

$\mathbf{Z} = \{Z_1, \ldots, Z_D\}$ → $f(\mathbf{Z})$ → $\mathbf{Y}$

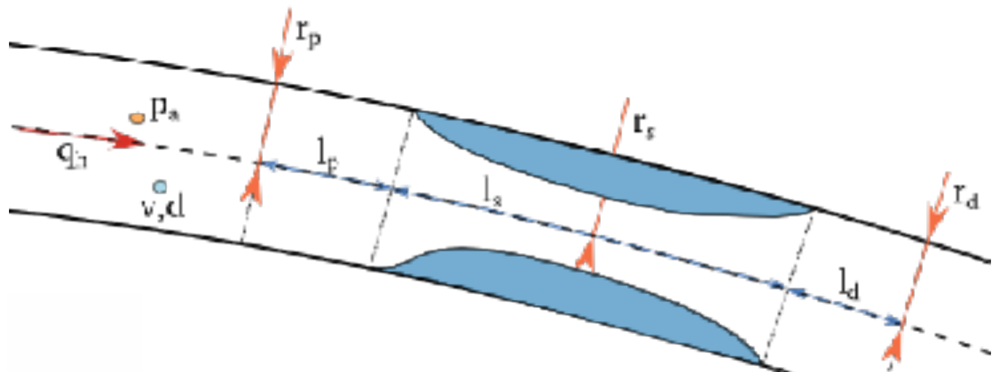
1 How can we describe the uncertainty in model inputs?

3 Account for uncertainty in model simulations

2 How can we assess the uncertainty of **Y** and the sensitivity with respect to **Z**

An example model

Generalisation | **Huo FFR model**



Input parameter

$$\mathbf{z} = \{z_1, \ldots, z_D\} \qquad \mathbf{z} = \{l_\mathrm{p}, l_\mathrm{s}, l_\mathrm{d}, r_\mathrm{p}, r_\mathrm{s}, r_\mathrm{d}, p_\mathrm{a}, q_\mathrm{h}, v, d\}$$

Mathematics describing physics and physiology

$$f(\mathbf{z})$$

$$\Delta p = \frac{q_h^2 d}{2}(\Delta p_\mathrm{convective} + \Delta p_\mathrm{diffusive} + \Delta p_\mathrm{expansion})$$

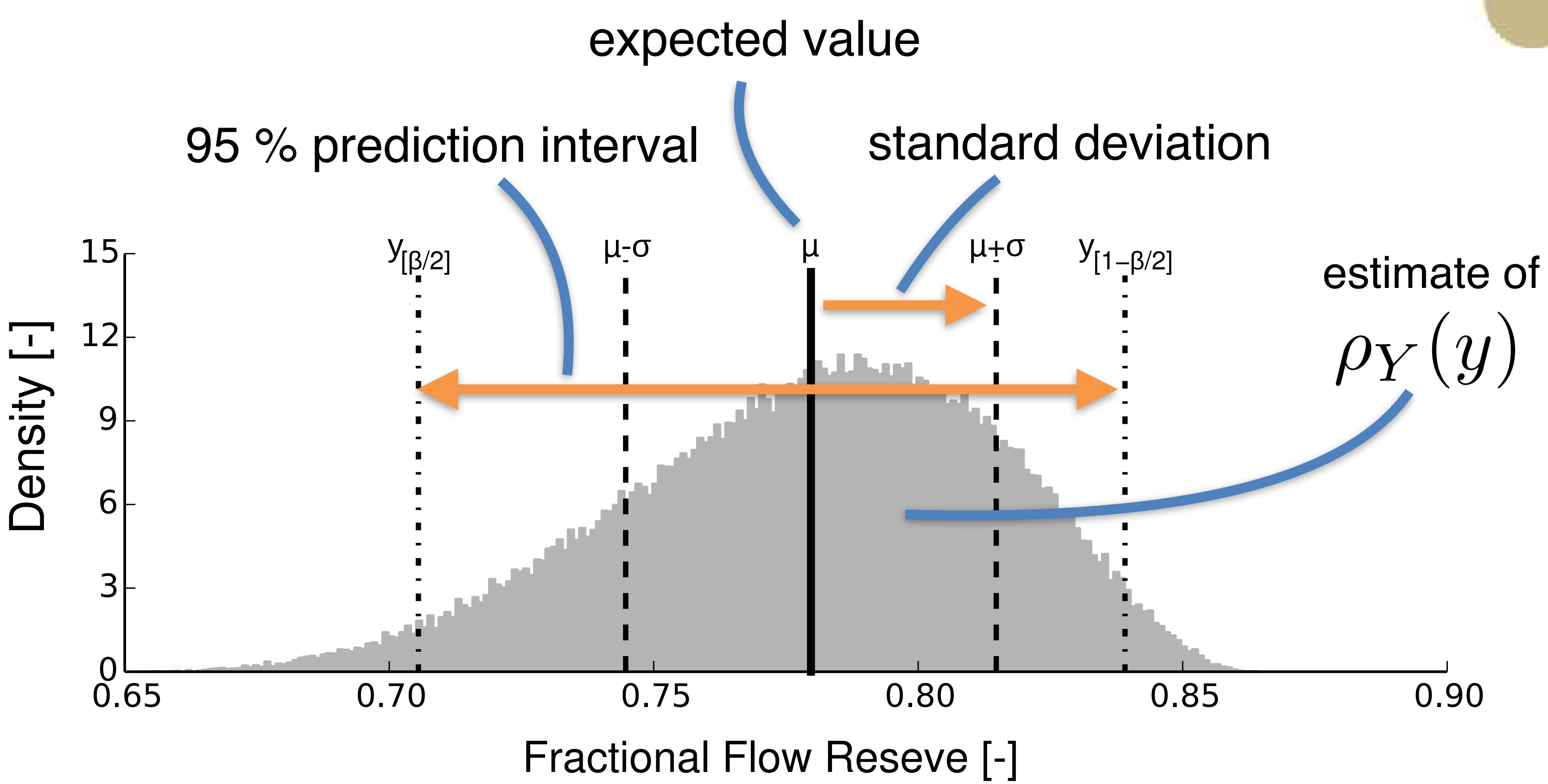
$$\mathrm{FFR} = \frac{p_a - \Delta p}{p_a}$$

Model prediction

$$y = f(\mathbf{z})$$

$$\mathrm{FFR} \in [0,1] \begin{cases} \text{non-significant} & \text{for FFR} > 0.8 \\ \text{significant} & \text{for FFR} < 0.8 \end{cases}$$

2 Huo FFR model prediction



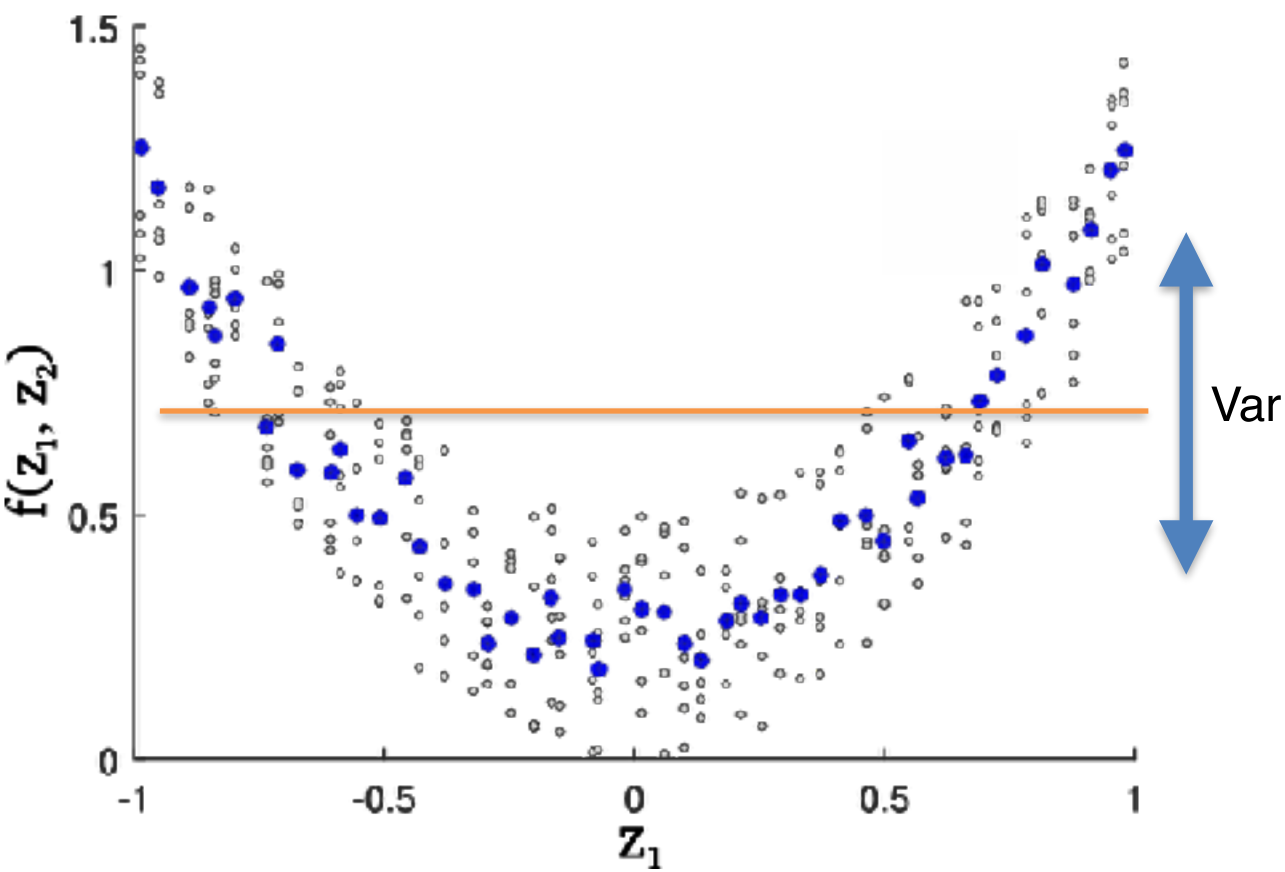
2 Sensitivity analysis

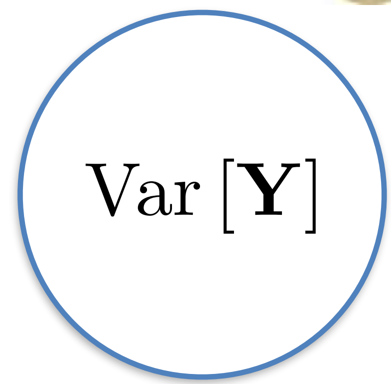
$$\begin{tikzcd} \mathbf{Z} = \{Z_1, \dots, Z_D\} \arrow[r] \arrow[rr, bend left, "?"] \arrow[rr, bend right, "?"'] & f(\mathbf{Z}) \arrow[r] & \boxed{\mathbf{Y}} \end{tikzcd}$$

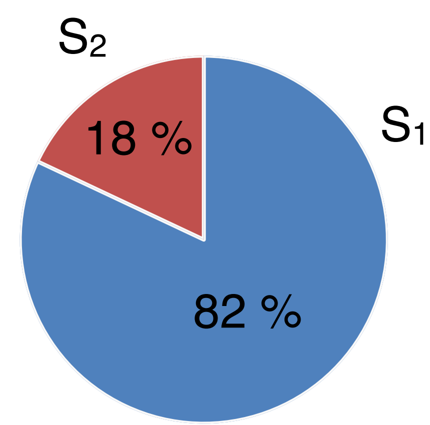
How sensitive is the model prediction to individual uncertain inputs?

2 Sensitivity analysis

first order sensitivity indices $$S_i = \frac{\mathrm{Var}\,[\ \mathbb{E}\,[\mathbf{Y}|Z_i]\ ]}{\mathrm{Var}\,[\mathbf{Y}]}$$







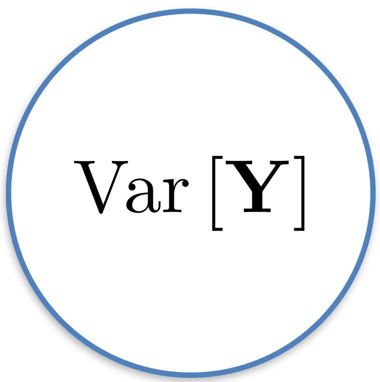
Parameter prioritisatio

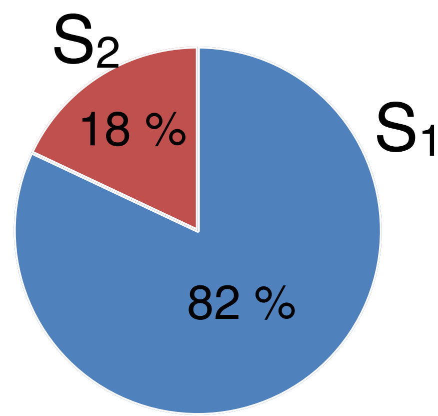
2 Sensitivity analysis

first order sensitivity indices

$$S_i = \frac{\mathrm{Var}\left[\, \mathbb{E}\left[\mathbf{Y} | Z_i\right] \,\right]}{\mathrm{Var}\left[\mathbf{Y}\right]}$$

If additive model, i.e. $y = f(\mathbf{z}) = z_1^2 + z_2$ $\quad \sum_i^D S_i = 1$





parameter prioritisation

2 Sensitivity analysis

$$Y = f_0 + \sum_i f_i + \sum_{ij} f_{ij} + \cdots \qquad f_0 = \mathrm{E}(Y) \qquad f_i = \mathrm{E}(Y|Z_i) - f_0$$

$$E(f_i f_j) = 0 \qquad f_{ij} = \mathrm{E}(Y|Z_i, Z_j) - f_i - f_j - f_0$$

Anova Variance Decomposition

$$\mathrm{Var}\left[\mathbf{Y}\right] = V_1 + V_2 + V_3 + V_{12} + V_{13} + V_{23} + V_{123}$$

$$V_i = \mathrm{Var}[f_i] = \mathrm{Var}[\mathrm{E}(Y|Z_i)] \qquad S_i = \frac{\mathrm{Var}[f_i]}{\mathrm{Var}[Y]}$$

2 Sensitivity analysis

total sensitivity indices S_{Ti}

non - additive model $y = f(\mathbf{z}) = z_1^2 + z_2 + z_3^2 \; z_1$

Anova Variance Decomposition

$$\mathrm{Var}\left[\mathbf{Y}\right] = V_1 + V_2 + V_3 + V_{12} + V_{13} + V_{23} + V_{123}$$

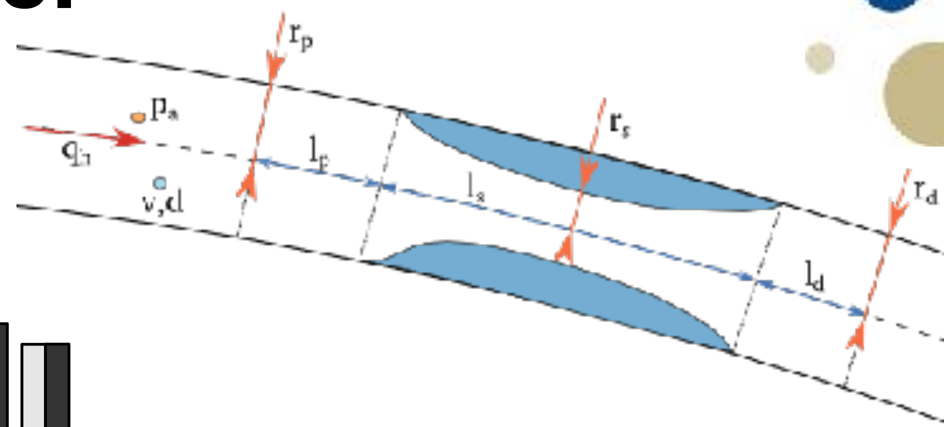
divide by $\mathrm{Var}\left[\mathbf{Y}\right]$

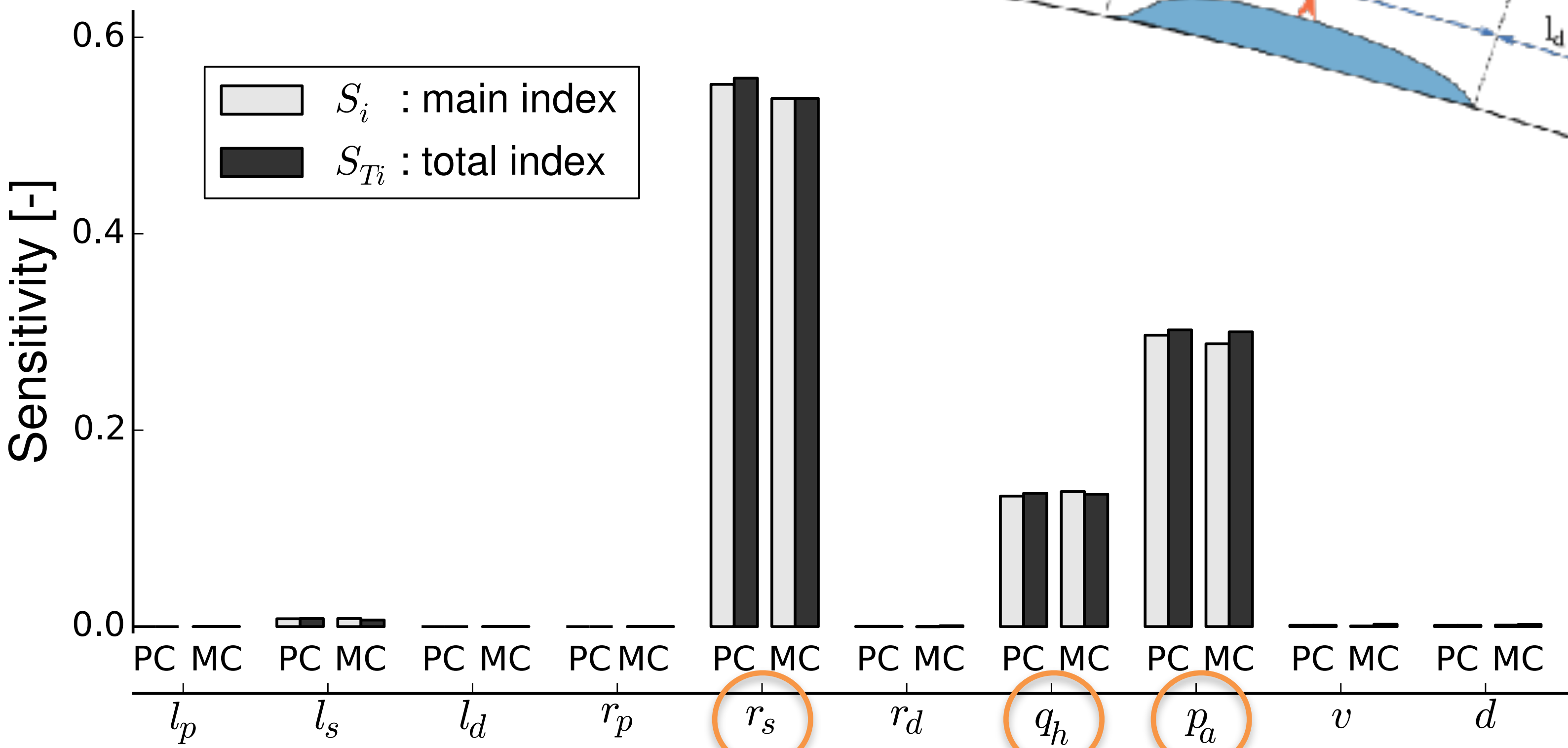
$$1 = S_1 + S_2 + S_3 + S_{12} + S_{13} + S_{23} + S_{123}$$

$$S_{T1} = S_1 + S_{12} + S_{13} + S_{123}$$

parameter fixing

② Huo FFR model





stenosis radius

hyperemic flowrate

arterial pressure

Wave propagation model

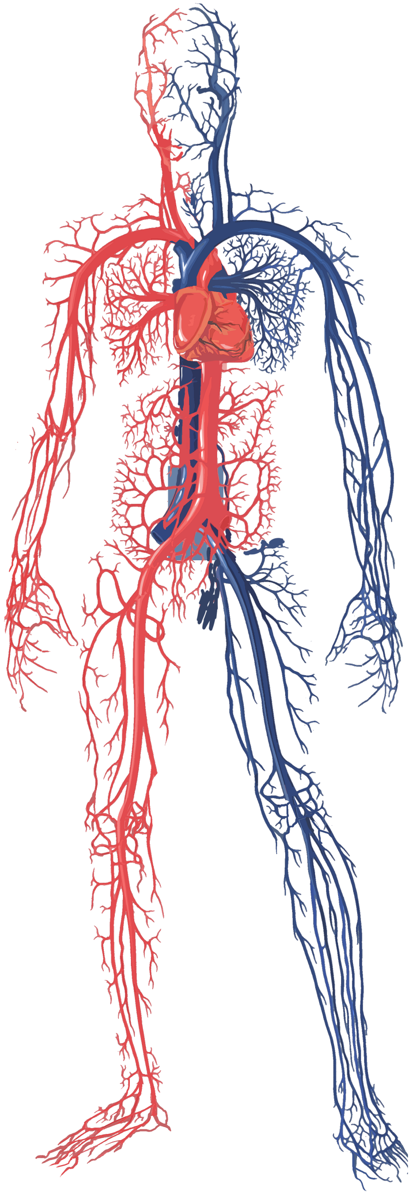
or one-dimensional blood flow model

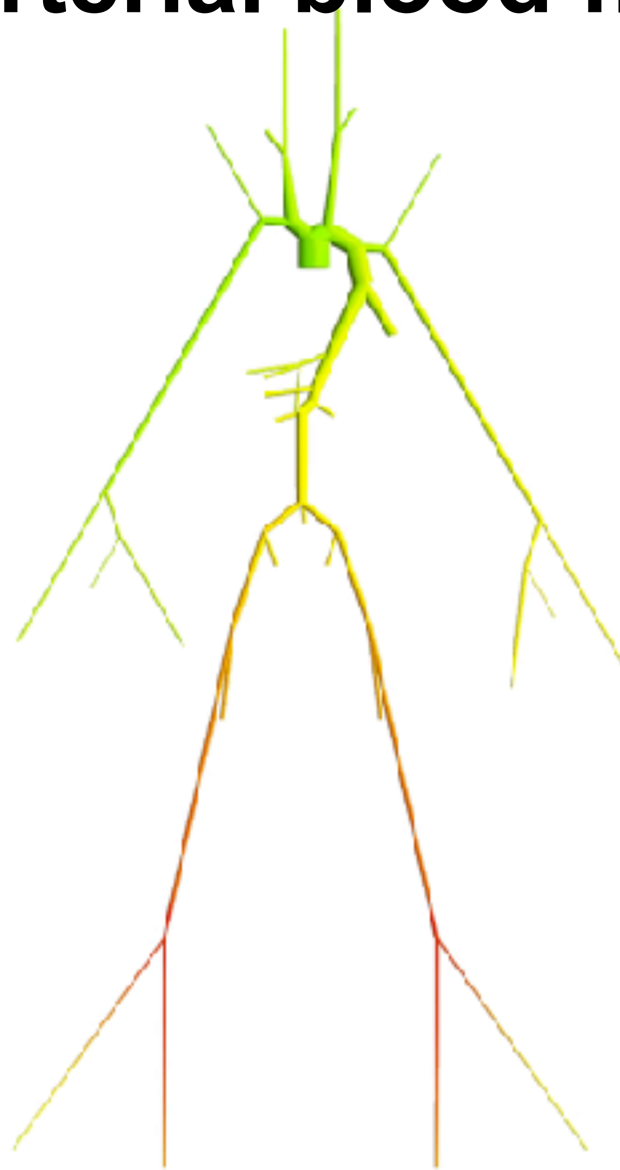
STARFiSh

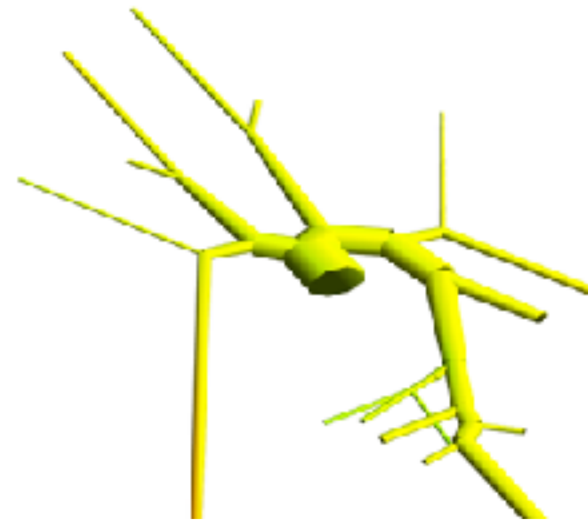
STochastic ARterial Flow Simulations

Open source code available! www.ntnu.no/starfish

Simulating arterial blood flow





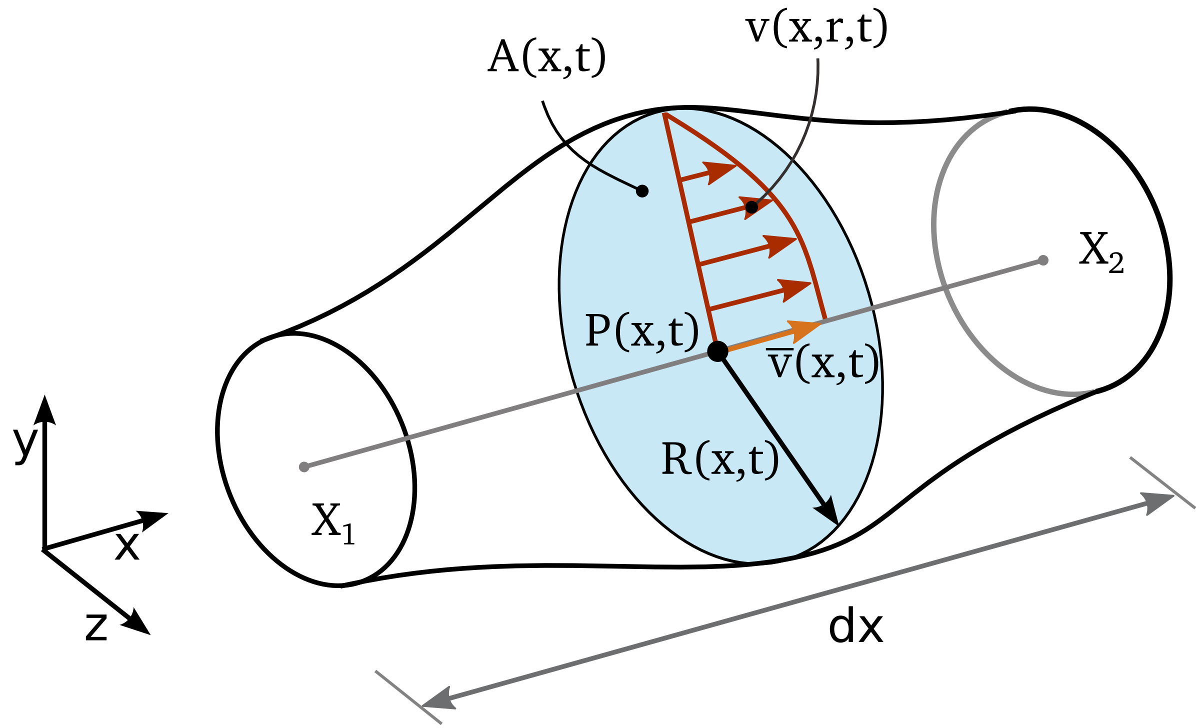


1d model solver equations

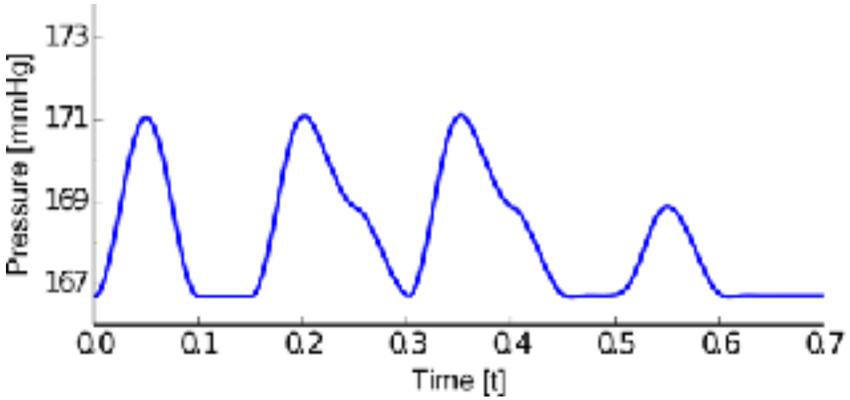
$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = 0$$ conservation of mass

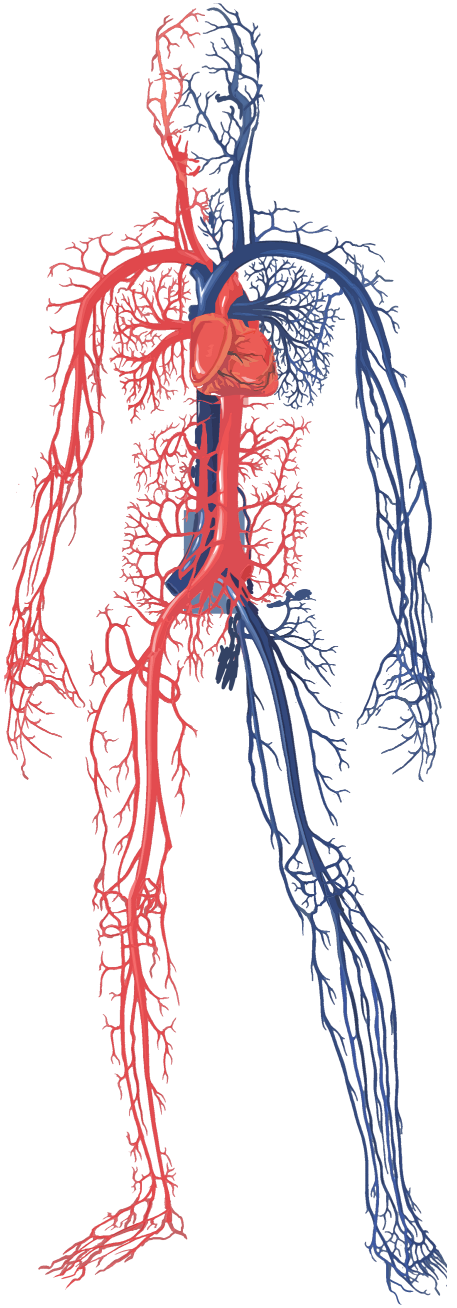
$$\frac{\partial Q}{\partial t} + \delta \frac{\partial}{\partial x}\left(\frac{Q^2}{A}\right) + \frac{A}{\rho}\frac{\partial P}{\partial x} = -2\pi\left(\gamma+2\right)\frac{\mu}{\rho}\frac{Q}{A} + Ag'$$ conservation of momentum

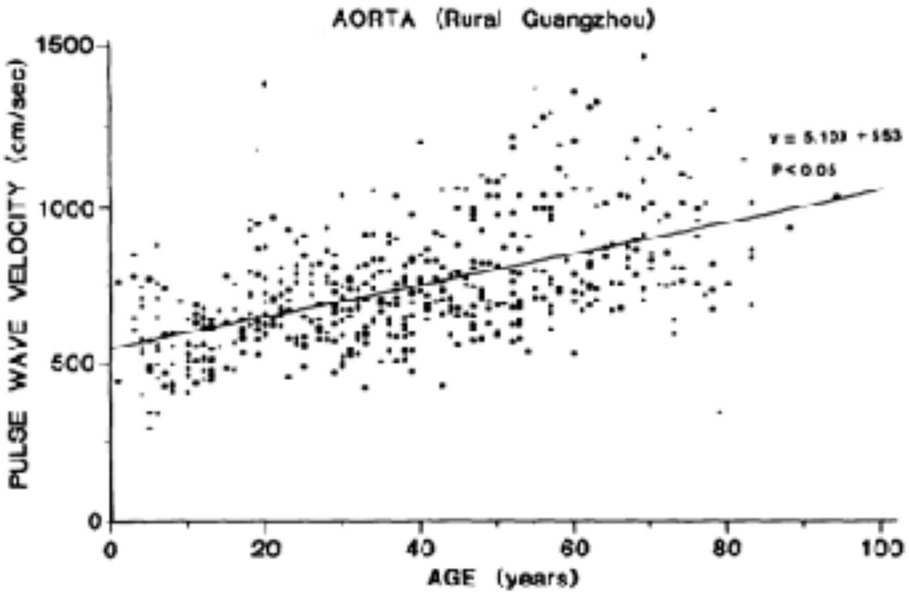
$$A(P) = \ldots \;, \frac{\partial A}{\partial P} = \mathcal{C}(x, P, \ldots)$$ arterial wall / compliance model



Wave propagation





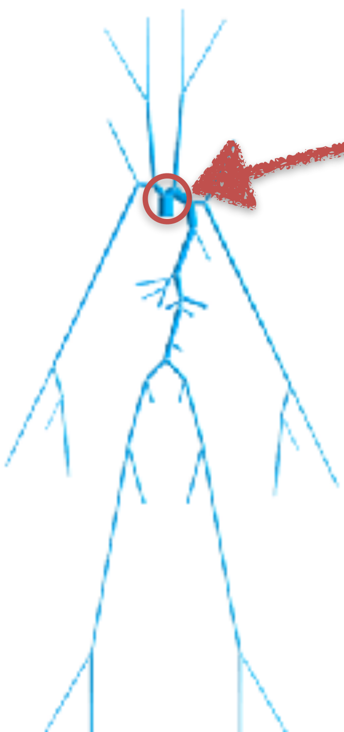


Graph from Avolio et al. 1985

pulse wave velocity ↑

caused by arterial stiffness ↑

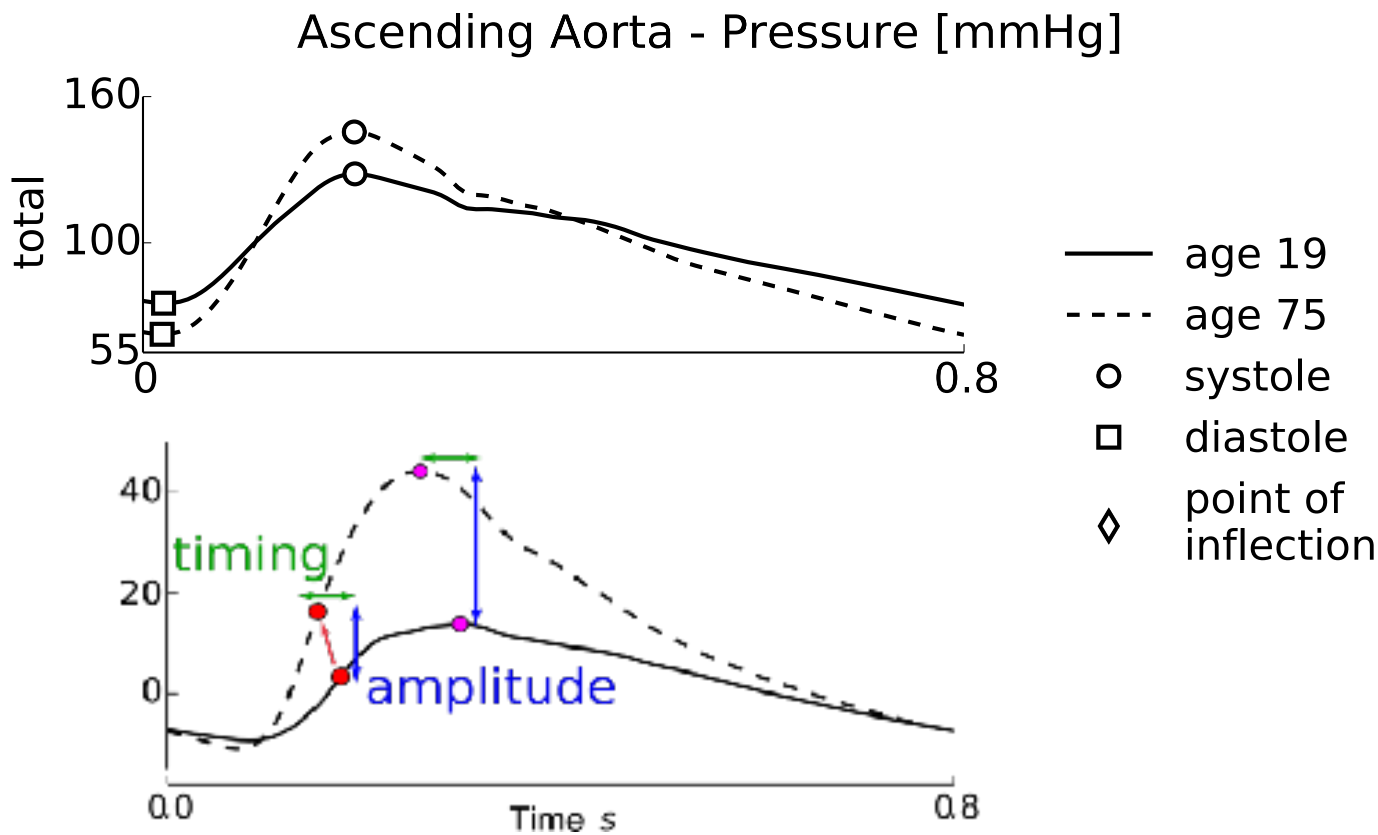
=> pulse pressure ↑



Which arteries are most influential?

sensitivity analysis

Backward pressure wave



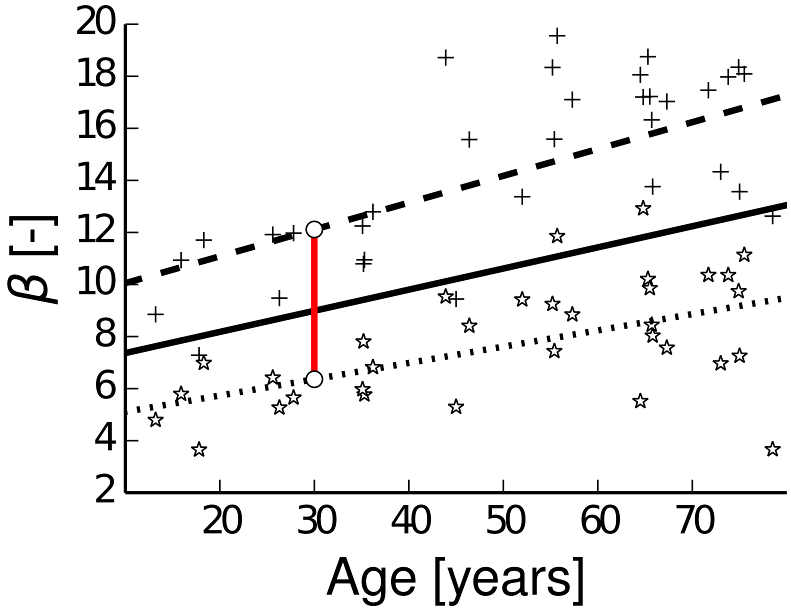
may lead to

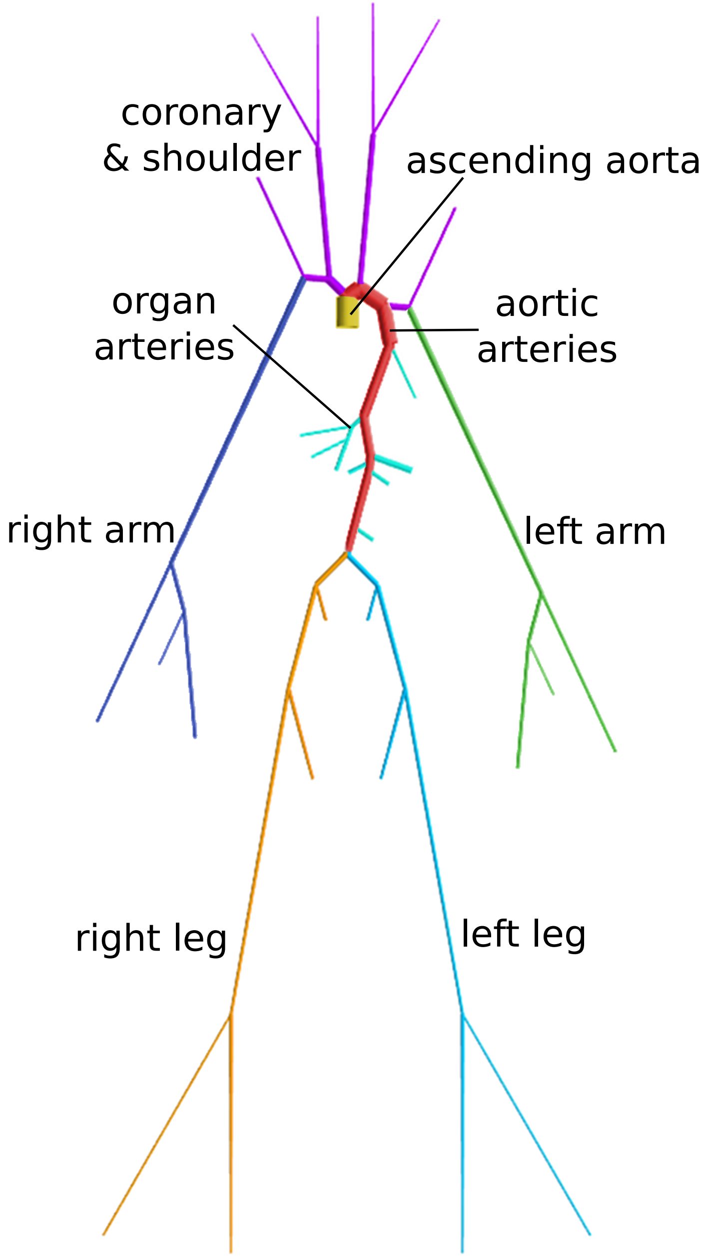
hypertension **hypertrophy of the heart**

8 arterial groups

uncertain arterial stiffness in
8 groups arterial groups

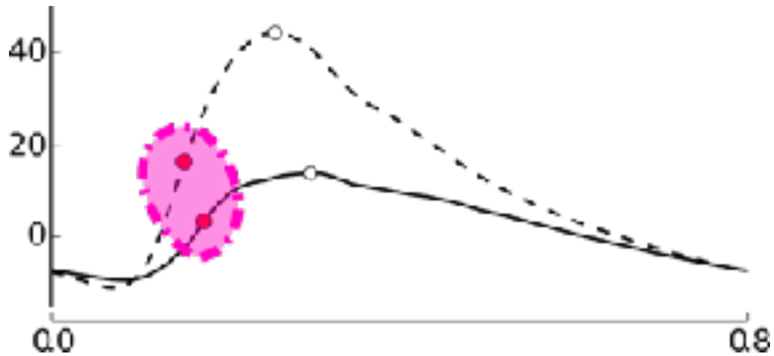
$$\beta = (\beta_1 \ \ \ldots \ \ \beta_8)$$

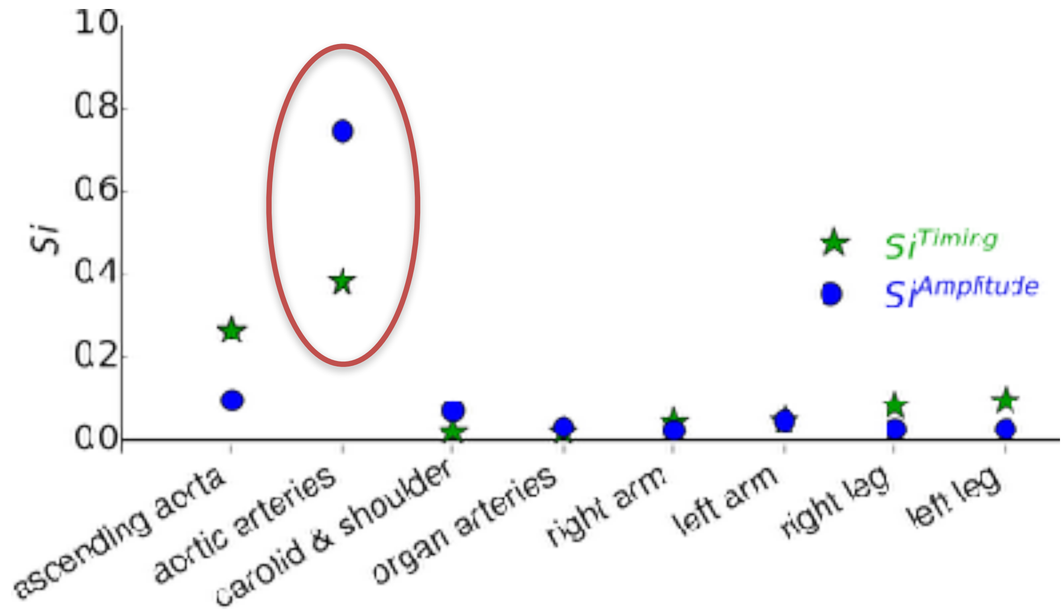




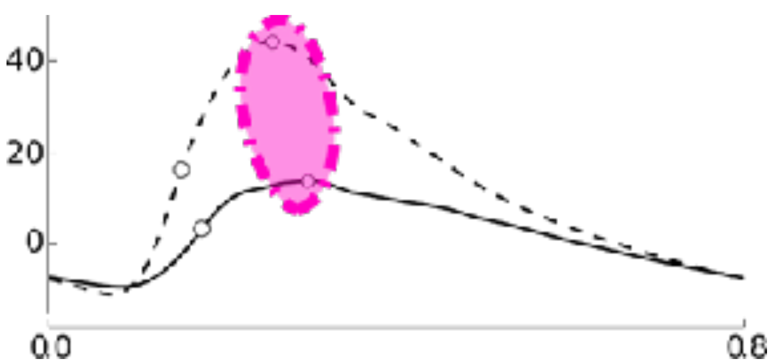
Results **Sensitivity analysis**

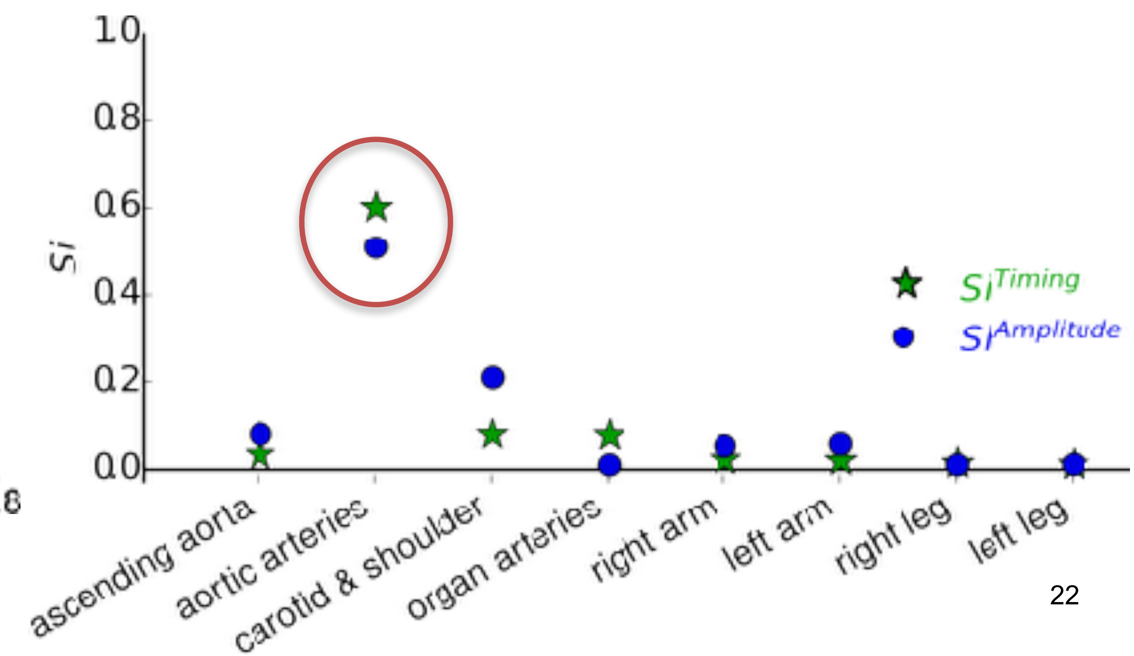
point of inflection





maximum pressure

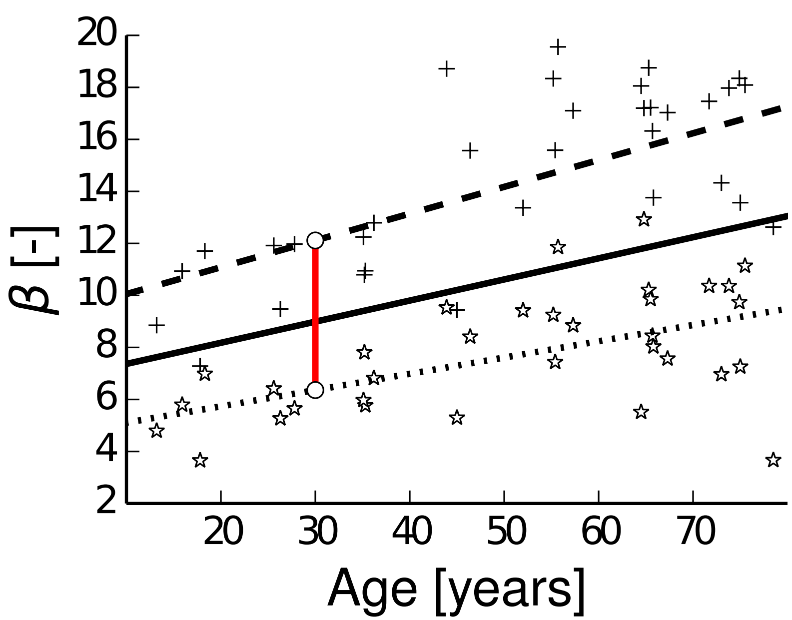


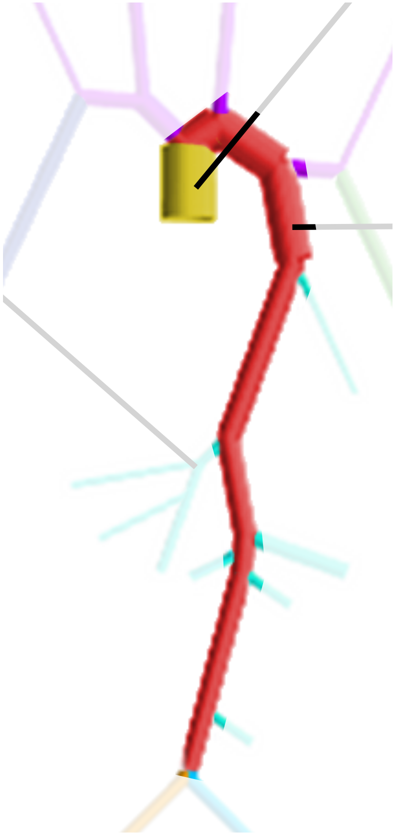


10 aortic arteries

uncertain arterial stiffness in 10 aortic arteries

$$\beta = (\beta_1 \ \ \ldots \ \ \beta_{10})$$





Results **Sensitivity analysis**

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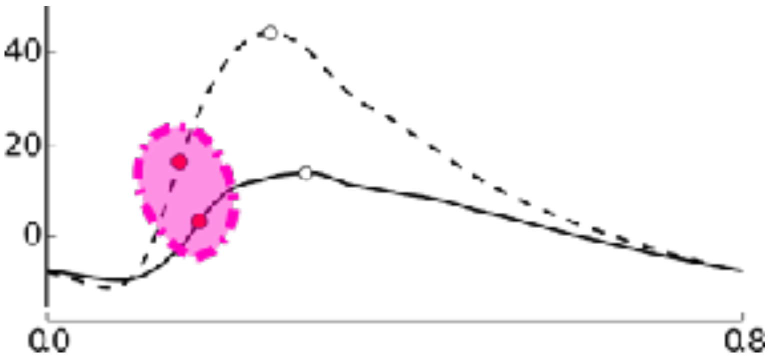
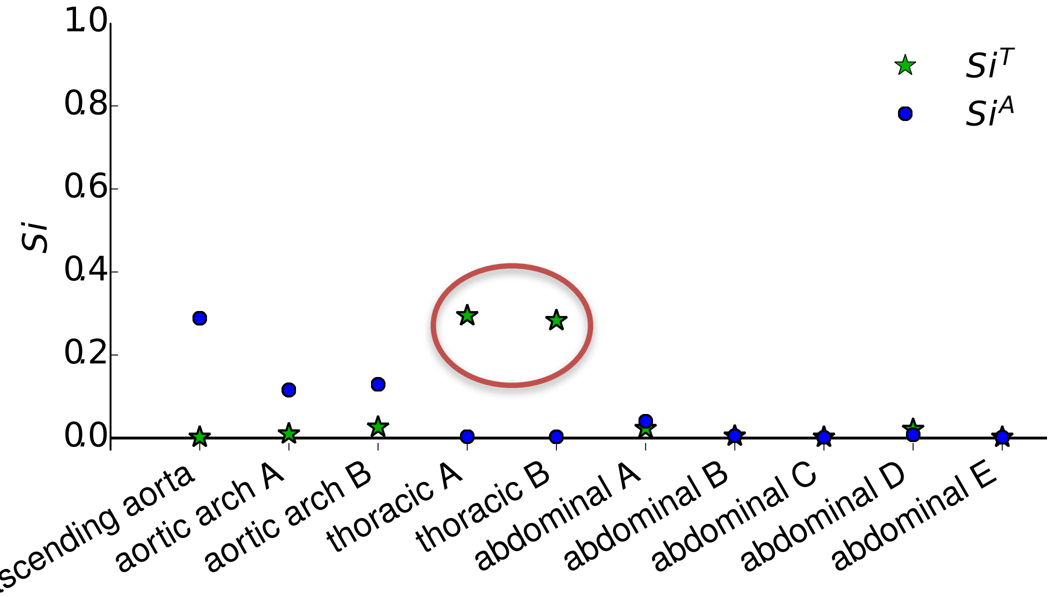
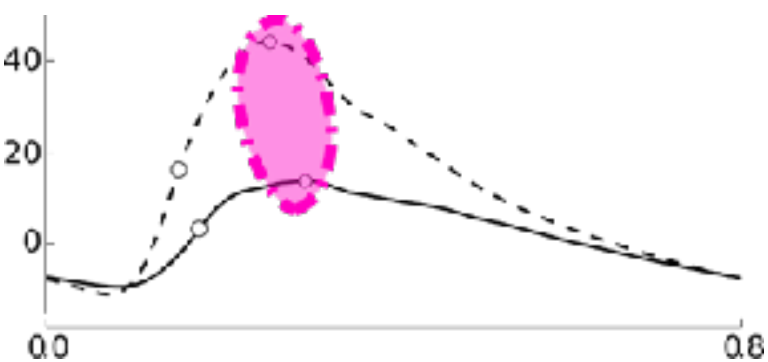
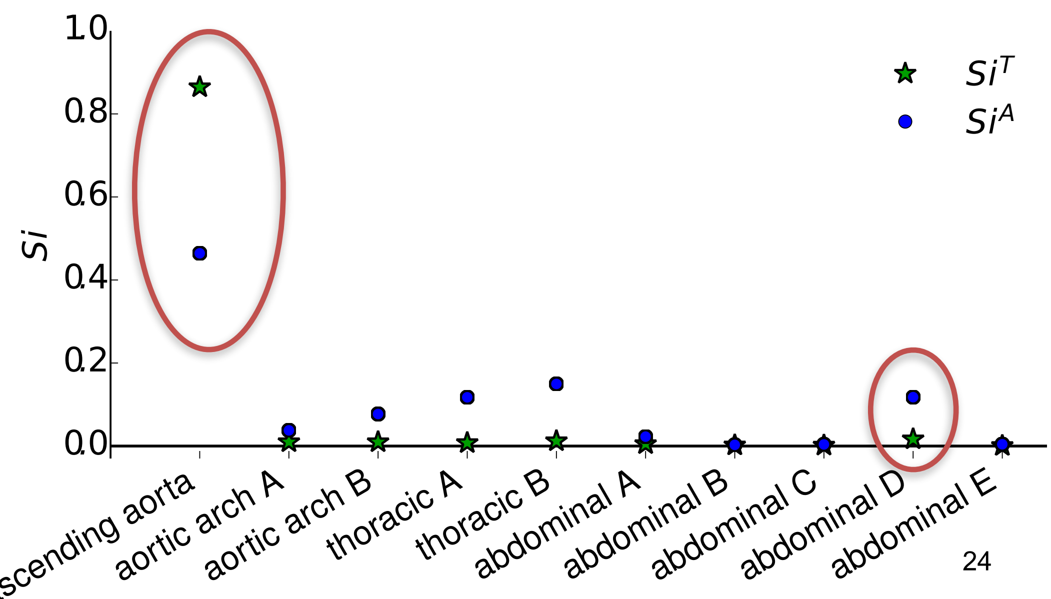


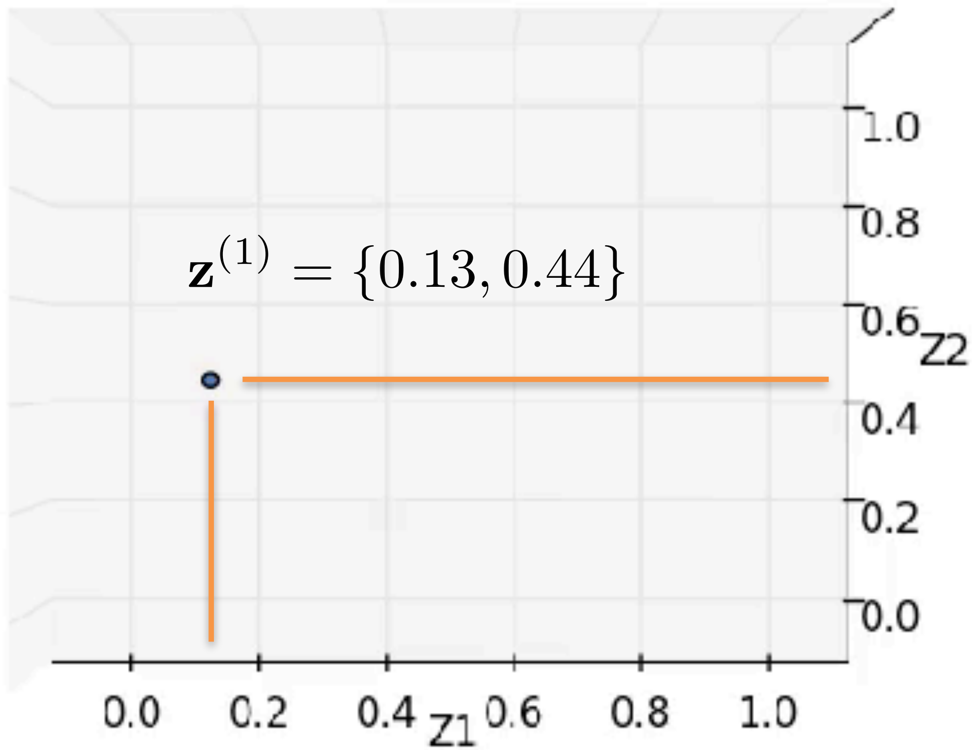


maximum pressure





Sampling



random variable vector

$$\mathbf{Z} = \{Z_1, Z_2\}$$

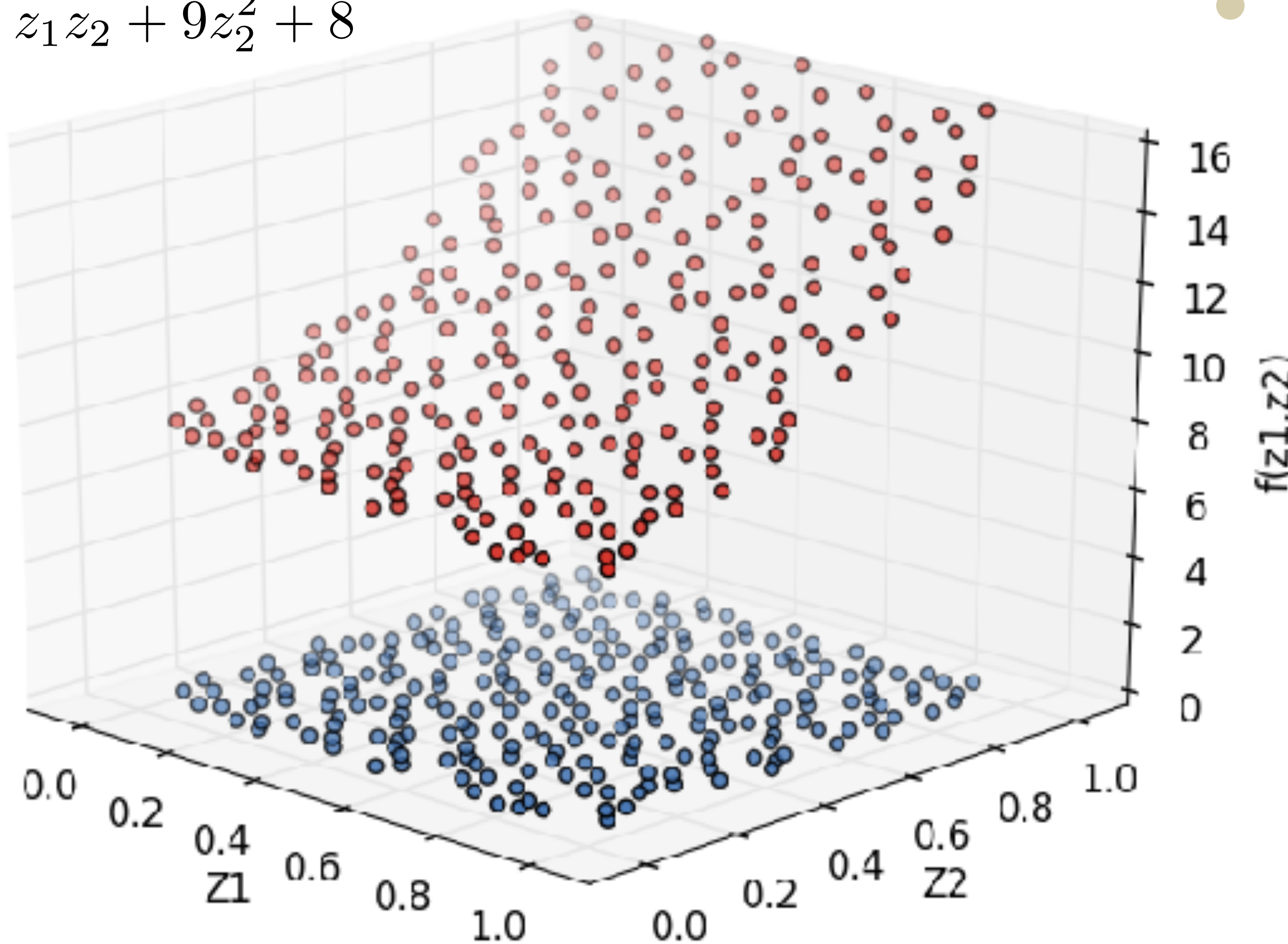
$$Z_1 \sim \mathcal{U}(0,1),\ Z_2 \sim \mathcal{U}(0,1)$$

set of samples

$$\left\{\mathbf{z}^{(s)}\right\}_{s=1}^{N_s}$$

Model evaluation

$$f(\mathbf{z}) = -z_1 + z_1 z_2 + 9z_2^2 + 8$$

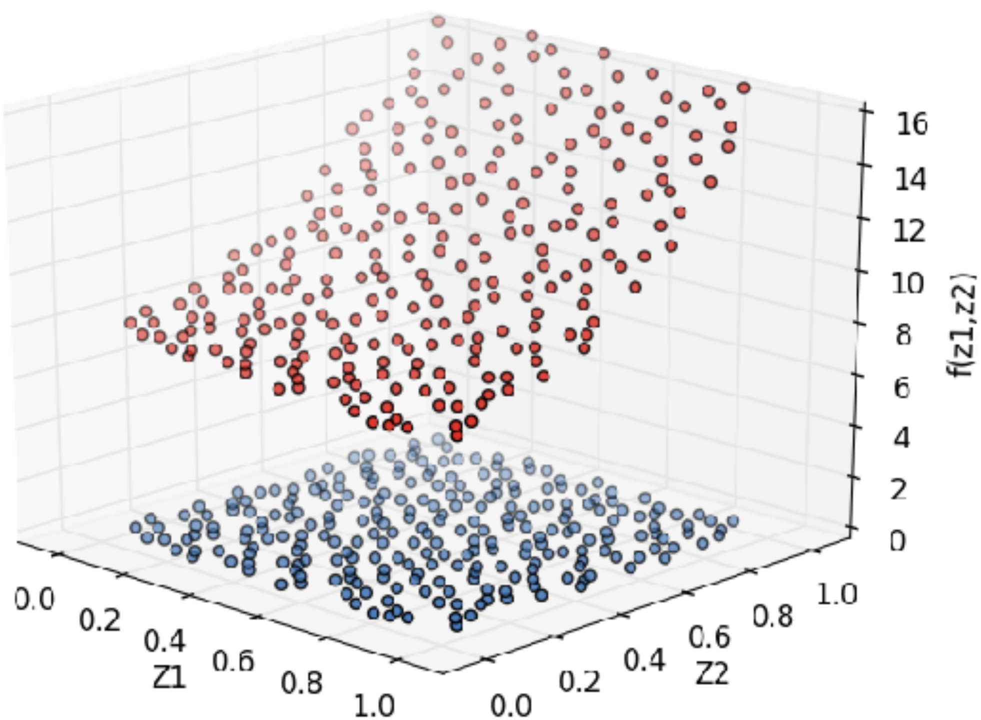


$$\left\{\mathbf{z}^{(s)}\right\}_{s=1}^{N_s} \rightarrow \mathbf{y}^{(s)} = f\left(\mathbf{z}^{(s)}\right) \rightarrow \left\{\mathbf{y}^{(s)}\right\}_{s=1}^{N_s}$$

Monte Carlo method

Idea: use all model evaluations directly

$$\left\{\mathbf{y}^{(s)}\right\}_{s=1}^{N_\mathrm{s}}$$



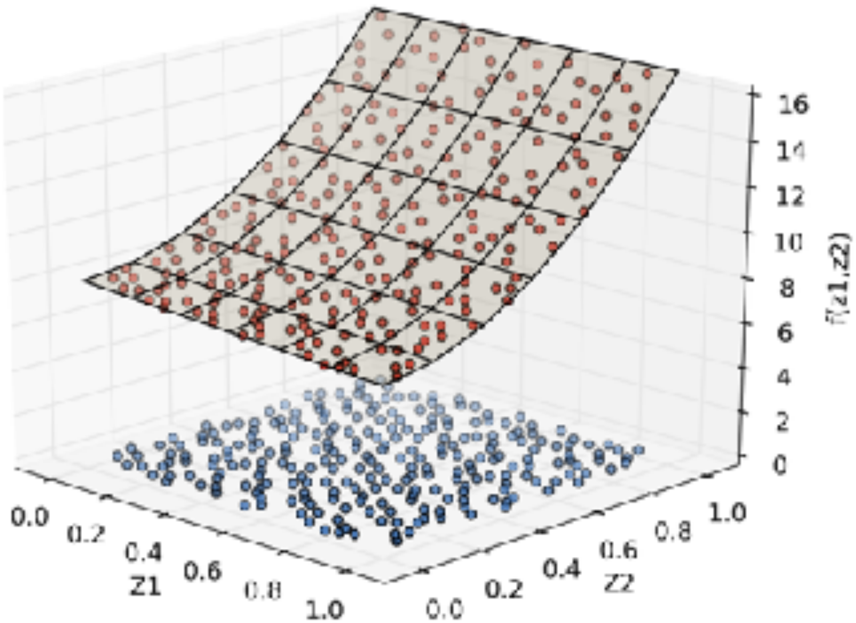
e.g.:

expected value

$$\mathbb{E}\left[\mathbf{Y}\right] \approx \frac{1}{N_\mathrm{s}} \sum_{s=1}^{N_\mathrm{s}} \mathbf{y}^{(s)}$$

Polynomial chaos

Idea: approximation with a spectral expansion



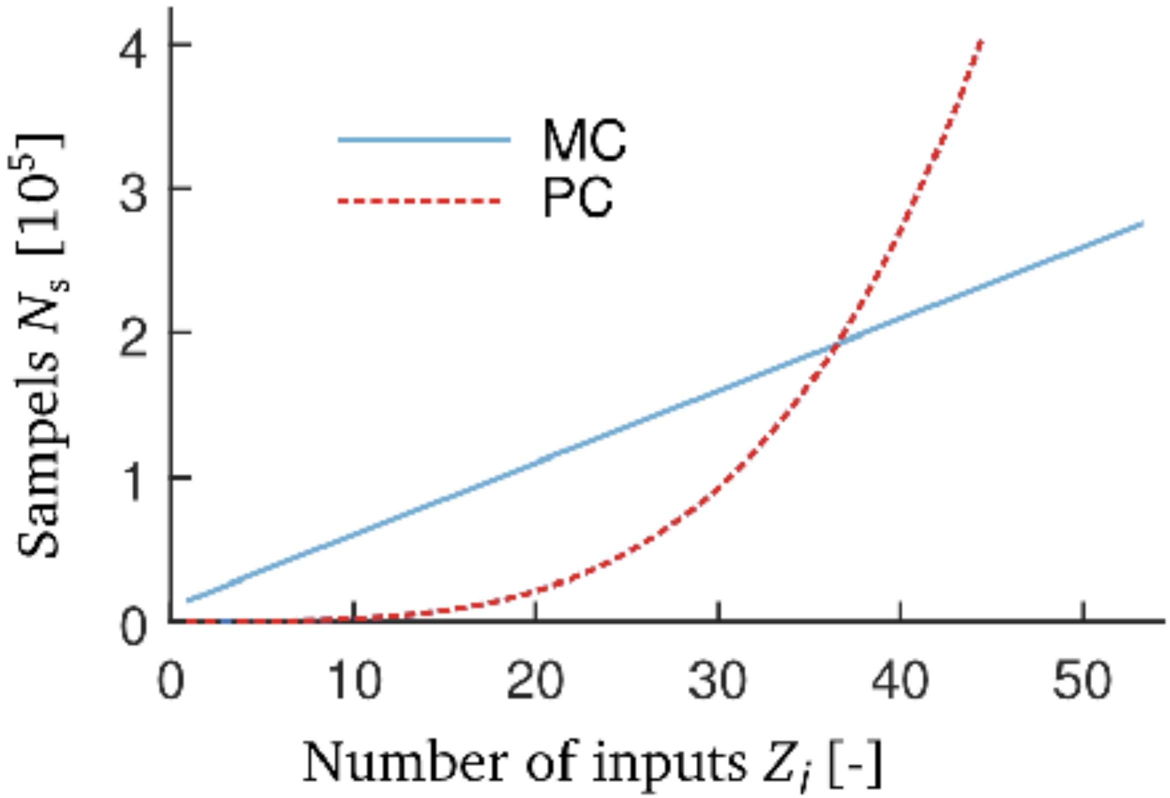
expansion coefficients

$$f(\mathbf{Z}) \approx \hat{f}(\mathbf{Z}) = \sum_{n=0}^{N_p} c_n \Phi_n(\mathbf{Z})$$

orthogonal polynomials

e.g.: expected value $\mathbb{E}\left[\mathbf{Y}\right] \approx c_0$

Monte Carlo vs polynomial chaos

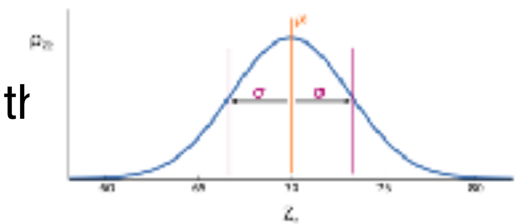


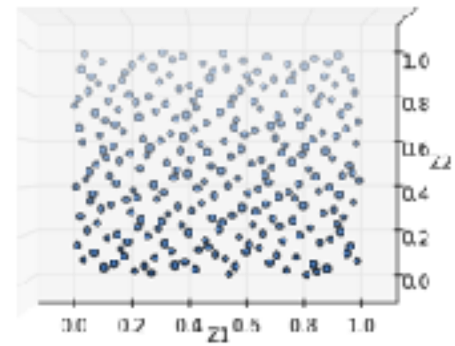
6 steps to UQ and SA

1. Identification of the output of interest

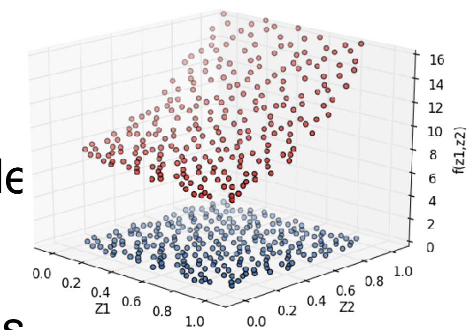
$$\mathrm{FFR} \in [0,1] \begin{cases} \text{non/significant} & \text{for FFR} > 0.8 \\ \text{sigificant} & \text{for FFR} < 0.8 \end{cases}$$

2. Identification and assessment of th
distribution of the uncertain inputs



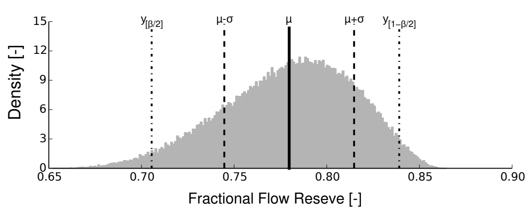


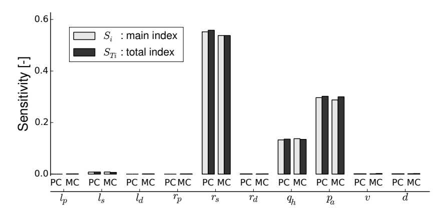
3. Sampling of the input space



4. Evaluation of the deterministic mode

5. Calculation of UQ and SA measures





6. Assessment of convergence of UQ and SA measures