Eawag
Swiss Federal Institute of Aquatic
Science and Technology

# Model Uncertainties and Parameter Estimation

7.5.2025 — Andreas Scheidegger

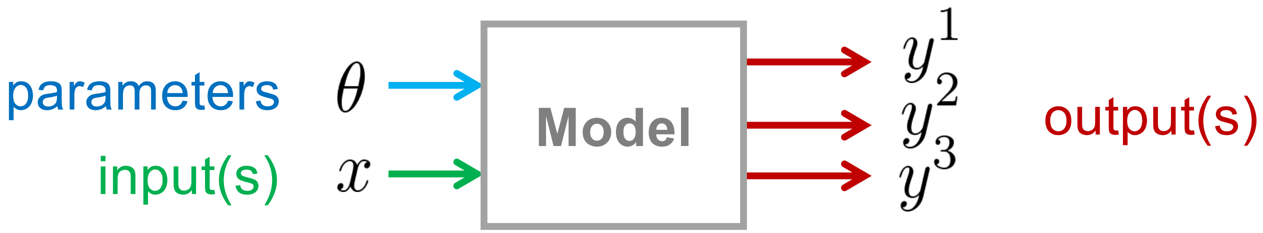
## Goals of today

i. You can identify different *sources* of model *uncertainties*.
ii. You know how *uncertainties* can be *quantified* mathematically.
iii. You can assess different ways to obtain *parameter values*.

# Model uncertainties

## What is a model?

A computer program:



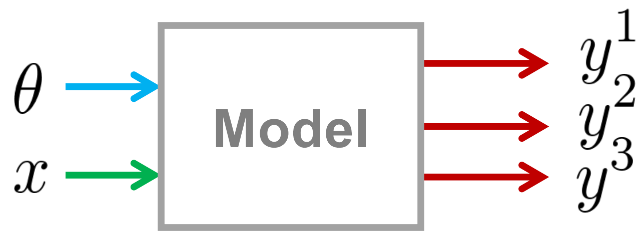

A mathematical function*: $\boldsymbol{y} = m(\boldsymbol{x}; \boldsymbol{\theta})$

*if the model output is stochastic, we often use capital letters: $\boldsymbol{Y} = M(\boldsymbol{x}; \boldsymbol{\theta})$

## Models are wrong: sources of uncertainty

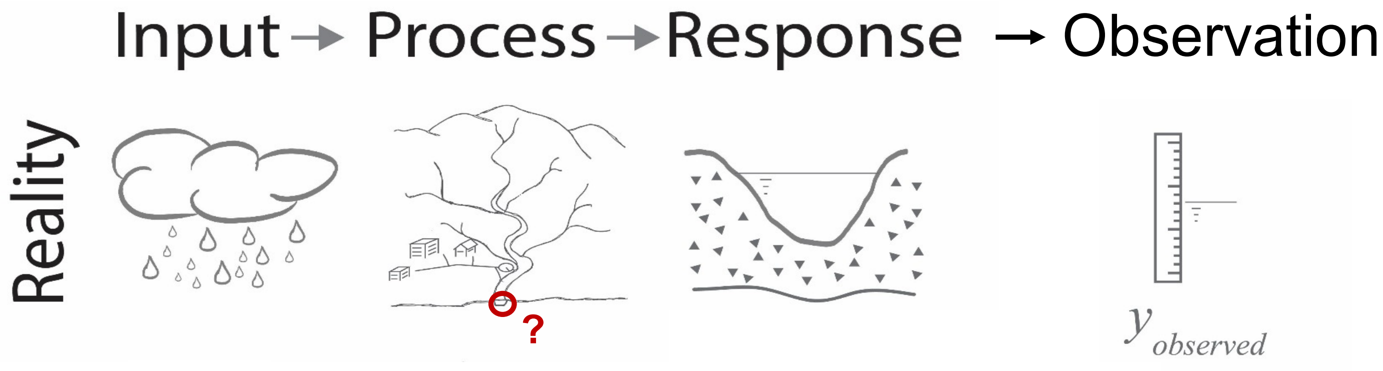
Almost all models suffer from these sources of uncertainty:

1. Input uncertainty
2. Parameter uncertainty
3. Model structure uncertainty
4. Output (measurement) uncertainty
5. (Scenario uncertainty)



# Sources of Model Uncertainty

eawag
aquatic research




Original slide from Omar Wani, thanks!

Adapted from Kavetski, 2018

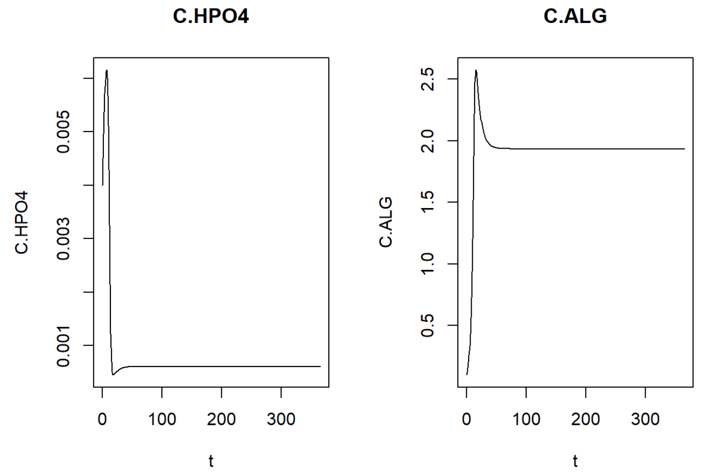
# Sources of uncertainty: Phytoplankton Model

Think about examples for each source of uncertainty:

1. Input uncertainty
2. Parameter uncertainty
3. Model structure uncertainty
4. Output (measurement) uncertainty
5. (Scenario uncertainty)

Which source do you judge the most relevant?

| Process | Substances / Organisms HPO4 $[gP/m^3]$ | ALG $[gDM/m^3]$ | Rate |
|---|---|---|---|
| Growth of algae | $-\alpha_{P,ALG}$ | 1 | $\rho_{gro,ALG}$ |
| Death of algae | | $-1$ | $\rho_{death,ALG}$ |

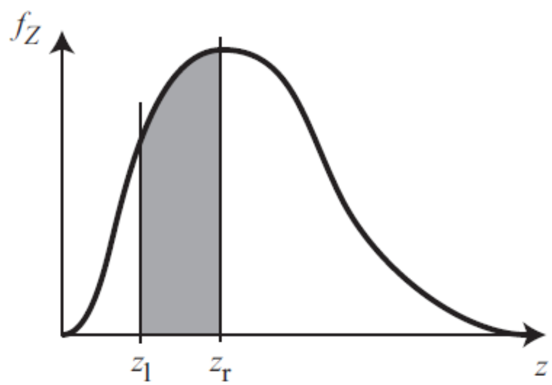


# Descriptions of uncertainties

## How can we describe uncertainties?

1. Guess tomorrow's air temperature in Zurich.
2. How (un)certain are you about your guess?

→ *Probability distributions* are a natural mathematical framework to describe uncertainties.



## Probabilities, are they all the same?

i. What is the probability to throw a five with a dice?

ii. What is the probability to win the Swiss lottery?

} *repeatable* events

iii. What is the probability that it snows tomorrow

iv. What is the probability that it has snowed yesterday on Uetliberg?

} *unique* events

eawag
aquatic research

# Probability interpretations*

These are *interpretations*, the mathematical rules (probability calculus) are always the same!

**Frequentist interpretation:**

- Probability describes the frequency of a random event
- Only applicable if an event can be replicated, e.g. lab experiments, dice, coin flips

**Bayesian or subjective interpretation:**

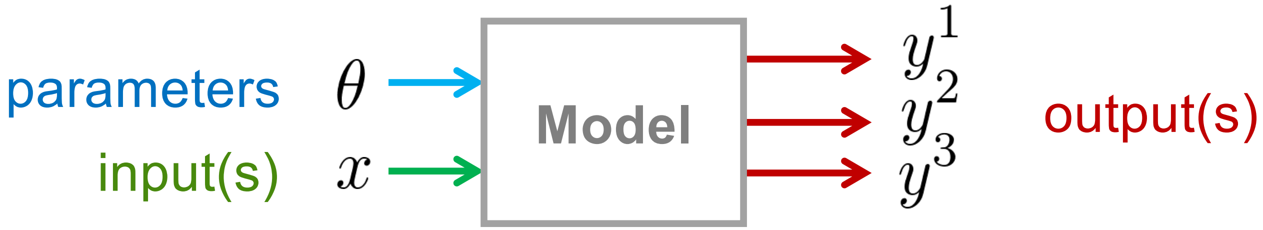
- Probability describes the “knowledge” or “belief” about an event
- Is *subjective* because everybody has different information
- When representing the current state of scientific knowledge, we use “intersubjective” probabilities about which multiple scientists agree.

*This is a deep, philosophical topic, see e.g. https://plato.stanford.edu/entries/probability-interpret/

# Uncertainty Analysis

- Error propagation
- Sensitivity Analysis

# Error Propagation




**I know the *uncertainty of the inputs or parameters*.**

**What is the resulting uncertainty of the *outputs*?**

# Analytical Error Propagation

Given the standard deviation $\sigma_A$ and $\sigma_B$, what is $\sigma_f$ ?

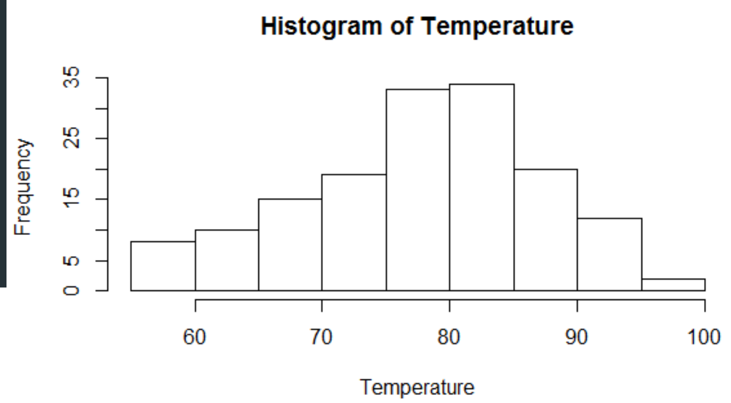
| **Function (model)** | **Variance of output** |
| --- | --- |
| $f = aA \pm bB$ | $\sigma_f^2 = a^2\sigma_A^2 + b^2\sigma_B^2$ |
| $f = AB$ | $\sigma_f^2 \approx (AB)^2 \left[\left(\frac{\sigma_A}{A}\right)^2 + \left(\frac{\sigma_B}{B}\right)^2\right]$ |

For full table see:
https://en.wikipedia.org/wiki/Propagation_of_uncertainty

Based on linear *approximation*!

# Monte Carlo Error Propagation

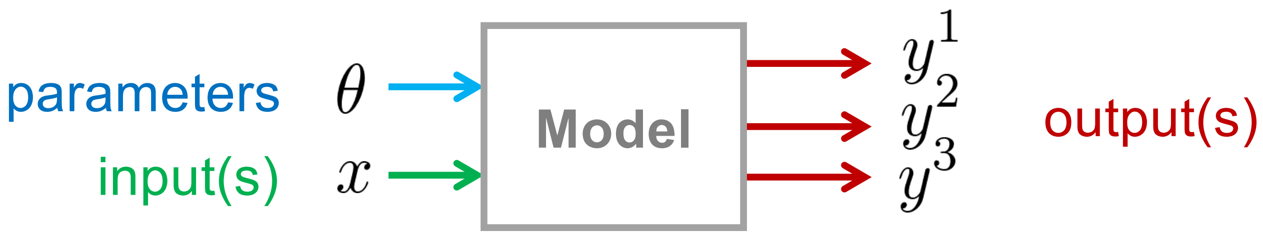
```
y = empty vector

for i in 1:N
    # sample inputs from distributions
    x ~ rnorm(10, 2)            # Normal(μ=10, σ=2)
    θ ~ runif(0, 2)             # Uniform(0, 2)

    # run model
    y[i] = model(x, θ)
end

sd(y)
mean(y)
histogram(y)
```




Exact if *N* goes to infinity

eawag
aquatic research

# Sensitivity Analysis




**How important are the different parameters and/or model inputs for the model output?**

**Factors**

(SA does not distinguish between inputs and parameters)

# Parameter estimation

Where do we get the numbers from?

# How do we get the parameters values?

**Parameters phytoplankton model**

```
# definition of model parameters:

param    <- list(k.gro.ALG   = 0.5,       # 1/d
                 k.death.ALG = 0.1,       # 1/d
                 K.HPO4      = 0.002,     # gP/m3
                 alpha.P.ALG = 0.003,     # gP/gDM
                 A           = 5e+006,    # m2
                 h.epi       = 5,         # m
                 Q.in        = 5,         # m3/s
                 C.HPO4.in   = 0.04,      # gP/m3
                 C.HPO4.ini  = 0.004,     # gP/m3
                 C.ALG.ini   = 0.1)       # gDM/m3
```

Parameter values can be obtained by:

I. Laboratory Experiments

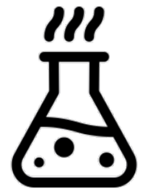
II. Scientific literature

III. Calibration of model output to field observations

## Information on parameter values

**I. Laboratory Experiments**

- Parameter needs a physical interpretation
- Lab conditions are not always transferable to real system



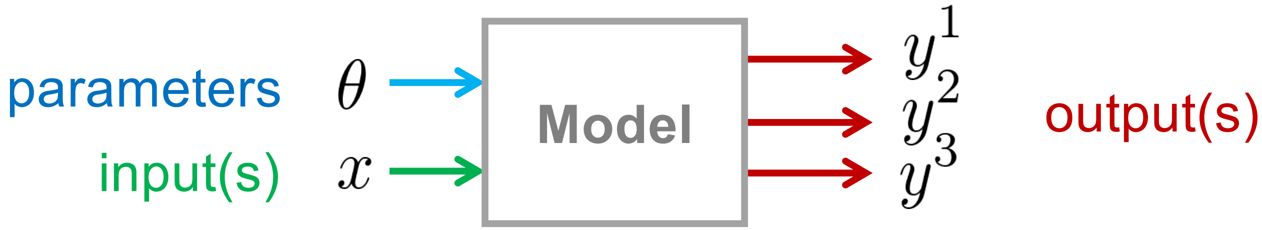
**II. Scientific literature**

- Measured under different conditions, varying methodologies, …
- Only for “famous” parameters possible

**III. Calibration of model output to field observations**

- Result depends on the model
- May not be transferable

# Model Calibration




**What *parameters* *make the* *outputs* most similar to the observations?**

# Demo

Manual Calibration

eawag aquatic research

# Model calibration techniques

i. Manual calibration
ii. Minimizing a loss function
iii. Maximum Likelihood estimation – a special loss function
iv. Bayesian inference – combine field data with other information

# Calibration with loss functions

$$\hat{\theta} = \overbrace{\arg\min_{\theta}}^{\text{take } \theta \text{ at minimum}} \underbrace{L\left(\overbrace{M(x,\theta)}^{\text{model output}}, \overbrace{Y_{\text{obs}}}^{\text{observations}}\right)}_{\text{loss function}}$$

- Any loss function that appears sensible can be used
- Parameter uncertainty cannot be quantified!

# Examples of loss functions

$$\Phi_{\mathrm{SSE}}[\boldsymbol{\theta}] = \sum_{t=1}^{N_t} \left( q_t^{\mathrm{obs}} - q_t^{\mathrm{sim}}[\boldsymbol{\theta}] \right)^2$$

$$\Phi_{\mathrm{RMSE}}[\boldsymbol{\theta}] = \sqrt{\frac{1}{N_t} \Phi_{\mathrm{SSE}}[\boldsymbol{\theta}]}$$

$$\Phi_{\mathrm{NS}}[\boldsymbol{\theta}] = 1 - \left( \frac{\Phi_{\mathrm{RMSE}}[\boldsymbol{\theta}]}{\sigma_{\mathrm{obs}}} \right)^2$$

$$\Phi_{\mathrm{SAE}}[\boldsymbol{\theta}] = \sum_{t=1}^{N_t} \left| q_t^{\mathrm{obs}} - q_t^{\mathrm{sim}}[\boldsymbol{\theta}] \right|$$

# Maximum likelihood estimation

$$\hat{\theta} = \arg\max_{\theta} \underbrace{p_M\left(Y_{\text{obs}} \mid x, \theta\right)}_{\text{Likelihood function}}$$

- The likelihood function is derived from *probabilistic assumptions* about the data generating process.
- Parameter uncertainty can be approximated (see e.g. https://www.sherrytowers.com/mle_introduction.pdf, section 5)

# Likelihood function

A likelihood function $p(\mathrm{data} \mid \theta)$ answers the following question:

"Given a *stochastic* model that generates random data. If the parameters are set to $\theta$, what is probability (density) that the randomly generated data equal the observed $\mathrm{data}$?"

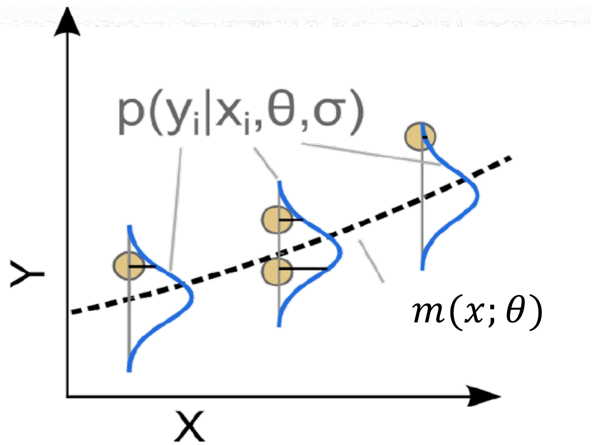
Note, most of our models are deterministic (i.e. non-random).
The most common approach is to assume an additional random error on the output.

# Likelihood function: example of a deterministic model + noise

deterministic model

$$Y_i = \underbrace{m(x;\theta)}_{} + \epsilon_i$$ noise

$$\epsilon_i \sim N(0,\sigma^2)$$




Likelihood for a single observations

$$p_i(y_i|x_i,\theta,\sigma) = \text{pdf of N}(m(x_i;\theta)\,,\sigma^2)$$

i.e. the pdf of a normal distribution with mean = $m(x;\theta)$ and standard deviation $\sigma$.

Likelihood for all observations

$$p(\boldsymbol{y}|\boldsymbol{x},\theta,\sigma) = \prod_i p_i(y_i|x_i,\theta,\sigma)$$

# Demo

Likelihood function

eawag
aquatic research

# Parameter identifyability

$$V = h_{epi} * A$$

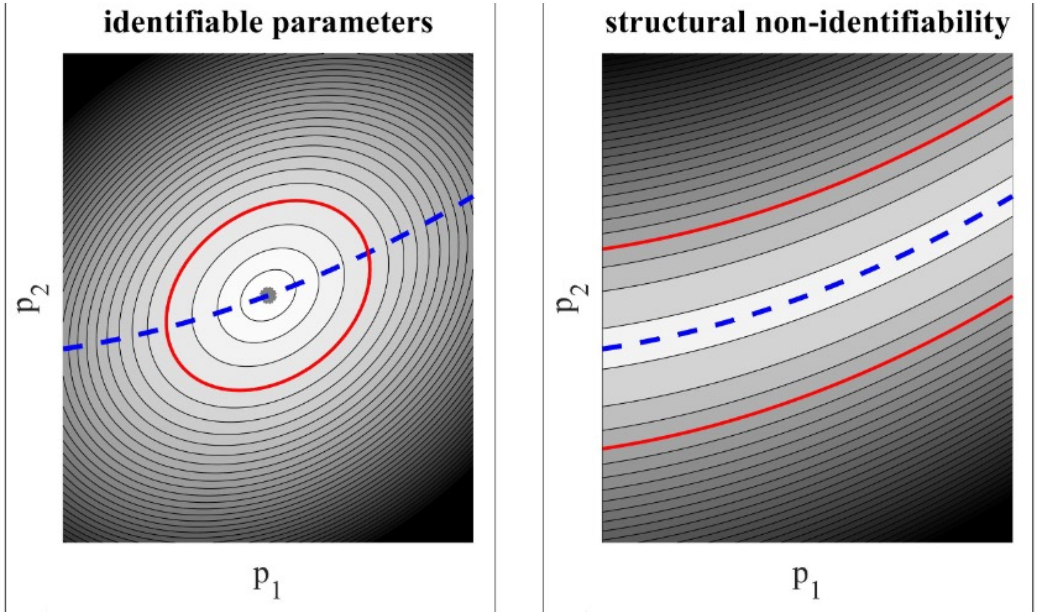
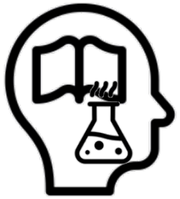



Image from: Wieland, F. G., Hauber, A. L., Rosenblatt, M., Tönsing, C., & Timmer, J. (2021). On structural and practical identifiability. *Current Opinion in Systems Biology*, *25*, 60-69.

# Bayesian inference: combine all information

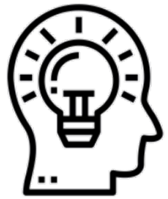


- literature
- lab measurements
- experience

+

- model assumptions
- field data

→



- “updated” knowledge

$$p(\theta) \times p(Y_{obs}|\theta) \propto p(\theta|Y_{obs})$$

**prior distribution** — **likelihood function** (the same as for MLE!) — **posterior distribution**

# Bayesian inference

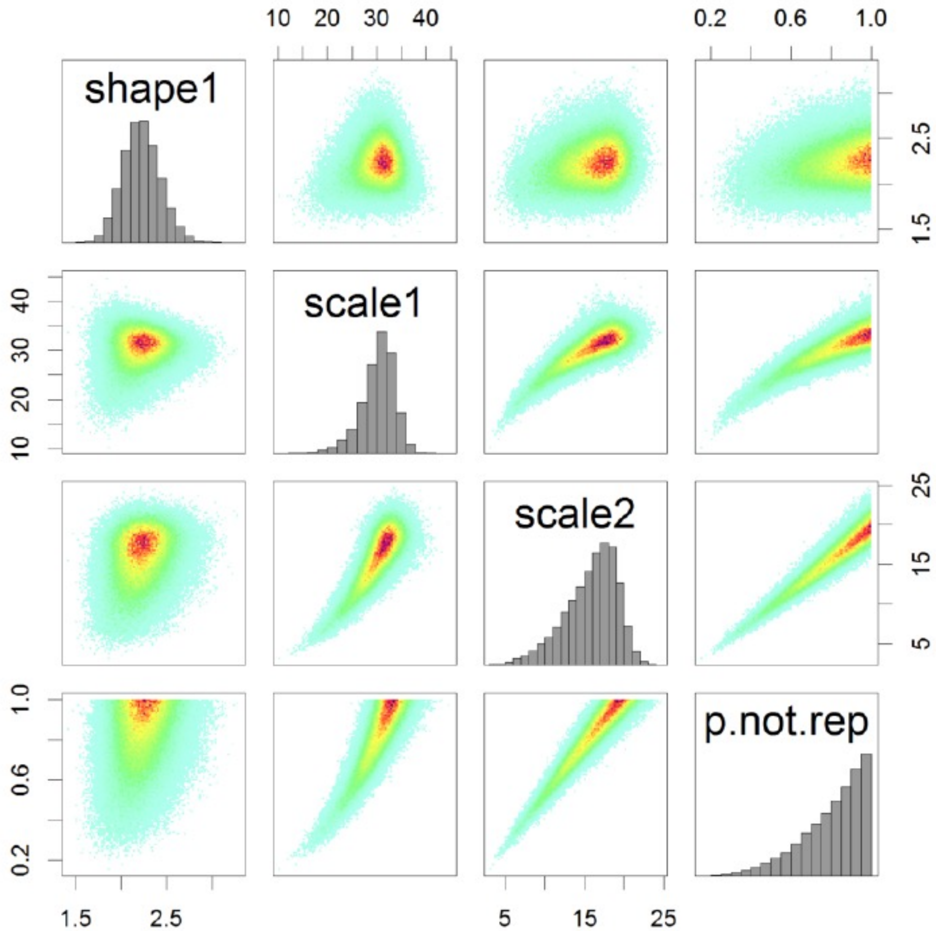
- A principled approach to combine:
  1. Prior information
  2. Data
- Based on subjective probability interpretation
- More intuitive interpretation of uncertainty intervals
- Computationally demanding (need to run the model >1000 times)
- Typically used with Monte Carlo Markov Chain (MCMC) sampling

This is often difficult!

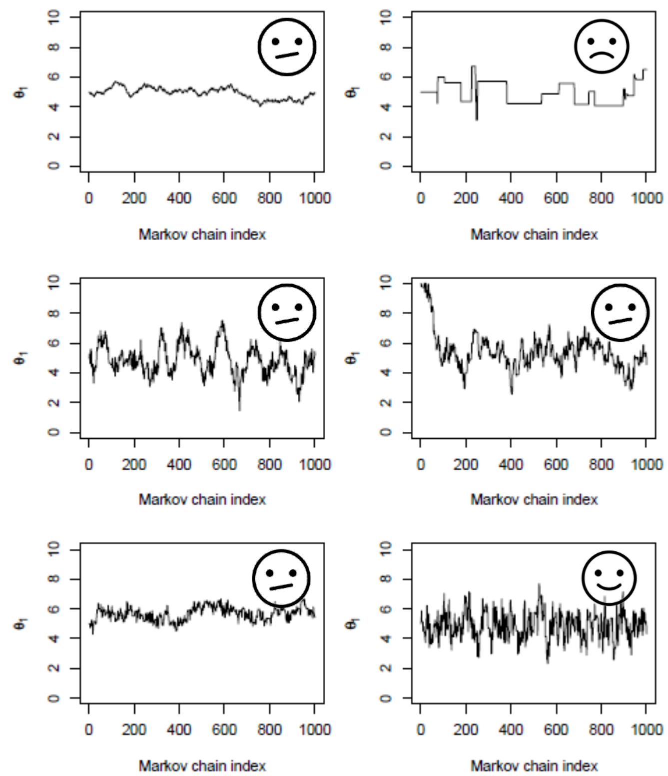
$$p(\theta|Y_{obs}) = \frac{p(Y_{obs}|\theta)p(\theta)}{p(Y_{obs})} = \frac{p(Y_{obs}|\theta)p(\theta)}{\int p(Y_{obs}|\theta')p(\theta')d\theta'}$$

# Monte Carlo Markov Chain sampling

eawag
aquatic research




*One- and two-dimensional marginal of the posterior distribution*




*Diagnostic of MCMC chains.*
*Tuning is important!*

## Multivariate Random Variables

Joint probability: $p(x, y)$

Marginal probability: $p(x) = \int p(x, y)\, \mathrm{d}y$

Conditional probability: $p(x \mid y) = \dfrac{p(x, y)}{p(y)}$

Combining above definitions gives Bayes Theorem:

$$p(x \mid y) = \frac{p(x, y)}{p(y)} = \frac{p(x)\, p(y \mid x)}{p(y)} = \frac{p(x)\, p(y \mid x)}{\int p(x')\, p(y \mid x')\, \mathrm{d}x'}$$

eawag
aquatic research

# Demo

Bayesian Regression

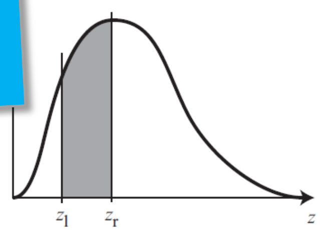
# Summary

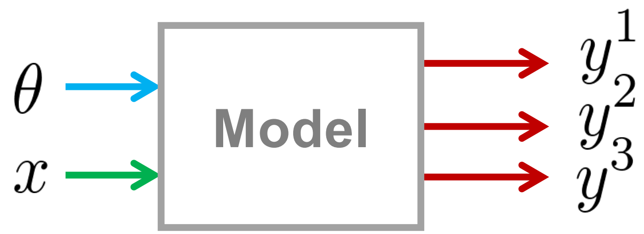
## Model uncertainties

1. Input uncertainty
2. Parameter uncertainty
3. Model structure uncertainty
4. Output (measurement) uncertainty
5. (Scenario uncertainty)

Stop worrying and use Monte Carlo error propagation!

Uncertainties can be described by probability distributions

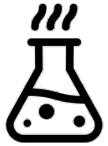


# Parameter values

**Information sources:**

i) literature



ii) laboratory experiments

iii) field measurements

**Model calibration:**

Prior

Bayesian inference

manual calibration

minimize loss function

maximum likelihood estimation