End-to-end Statistical Model Checking for ODEs

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LABORATOIRE DES SCIENCES DU NUMÉRIQUE DE NANTES

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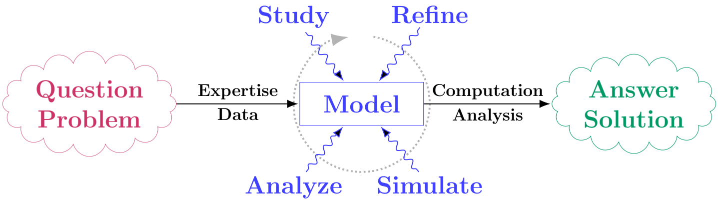
Outline

Outline

Science of Models

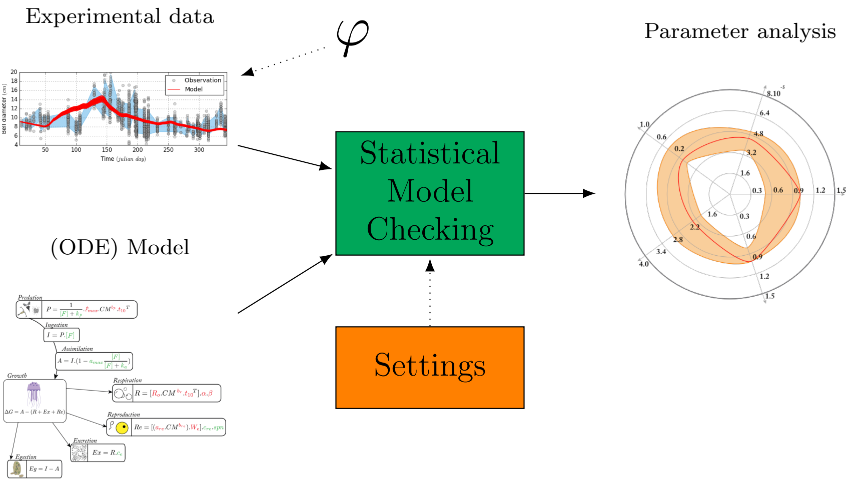


Motivations

Provide mathematical **guarantees** and **tools** for building and analyzing models

- usable by any scientist;
- answering real-life questions.

Example: Parameterization of a jellyfish model [1]



[1] [Ramondec et al. 2020] Probabilistic modeling to estimate jellyfish ecophysiological properties and size distribution. *Scientific Reports*

Formal verification of ODE models

System

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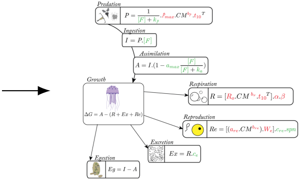
(ODE) Model



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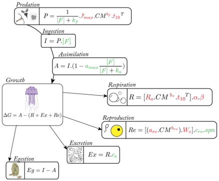

φ

Formal verification of ODE models

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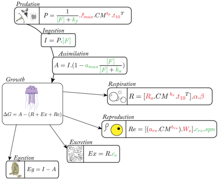

Some models may be verified directly (automata, graphs...).

φ

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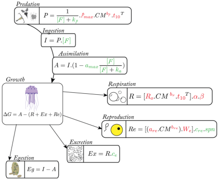

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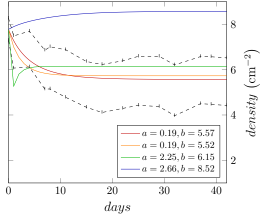

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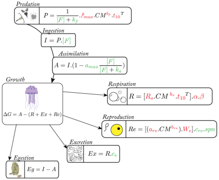

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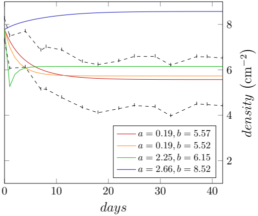

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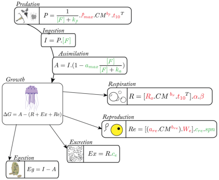

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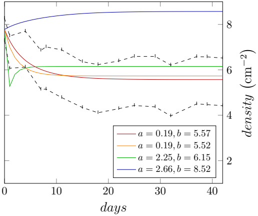

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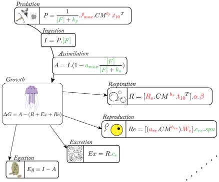

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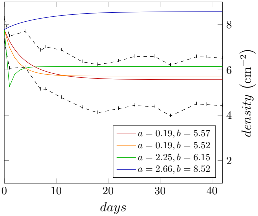
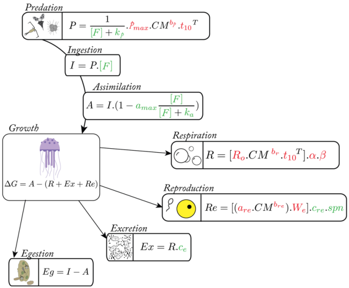


If Model ∼ Traces
⇒ Checking φ on the traces is equivalent to checking it on the model.

φ

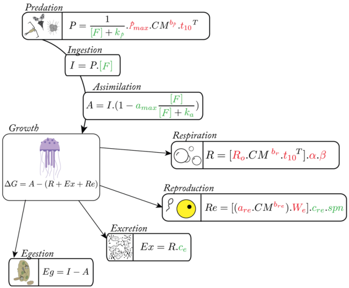
Probabilistic models



Uncertainty and variability

- Several experiments
  ⇒ data uncertainty.
- Family of systems
  ⇒ parameters variability.

Probabilistic models



Uncertainty and variability

- Several experiments
  $\Rightarrow$ data uncertainty.
- Family of systems
  $\Rightarrow$ parameters variability.

$\Rightarrow$ Parametric model with probabilistic parameter values.

Outline

SMC: answering "how good is a model?"

The Monte-Carlo procedure:

1. Randomly generate N samples $(\sigma_1, \ldots, \sigma_N)$ from the model.
2. Check whether the sample i satisfies the property φ.
   $X_i = 1 \Leftrightarrow \sigma_i \models \varphi$
3. Compute the estimator $\hat{p} = \frac{\sum X_i}{N}$.
   $\Rightarrow \mathbb{P}(p \in [\hat{p} - \alpha, \hat{p} + \alpha]) \geq 1 - \theta$

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Central Limit Theorem

- $\hat{p} \sim \mathbb{E}(X)$
  $\Rightarrow \hat{p}$ is a good estimation of $\mathbb{P}(M \models \varphi)$.
- **precision, error.**

Application to ODE models

[Liu et al. 2019] Statistical Model Checking-Based Analysis of Biological Networks.

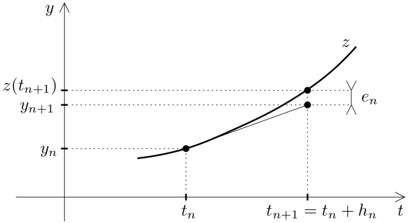
Automated Reasoning for Systems Biology and Medecine

Parameter analysis of ODE models with variability.

Problem: Approximations

Model $\not\approx$ Traces

Approximation error stacks up at each step: $\varepsilon = \max_n e_n$
$\Rightarrow$ SMC estimation does not apply to the original ODE model.



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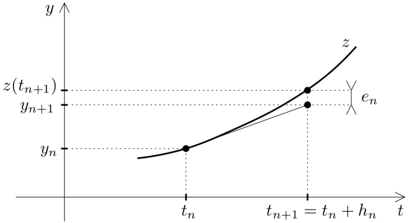

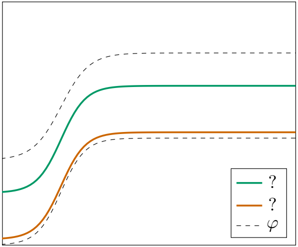

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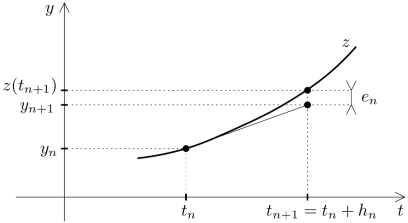

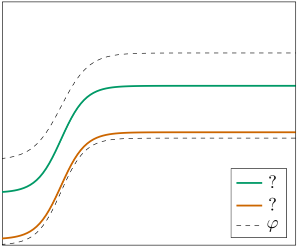

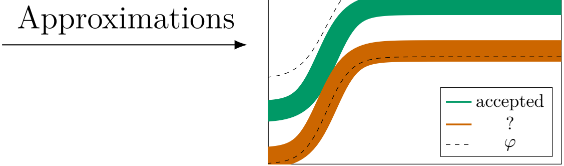

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- Bound approximation error ε on the parameter space.
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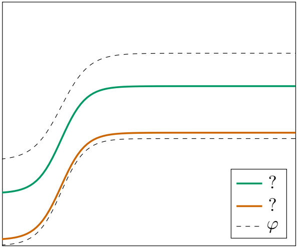

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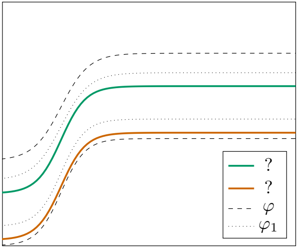

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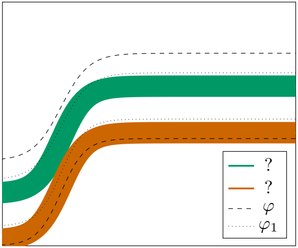

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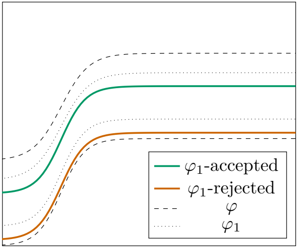

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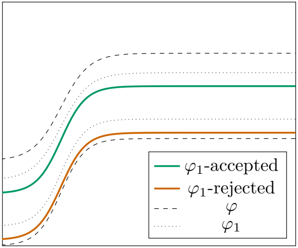

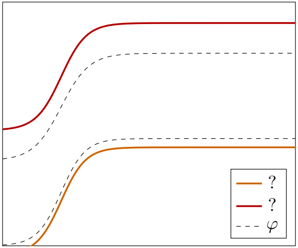

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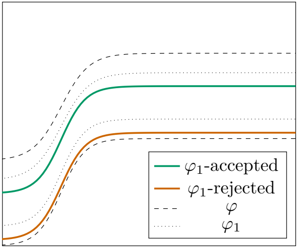

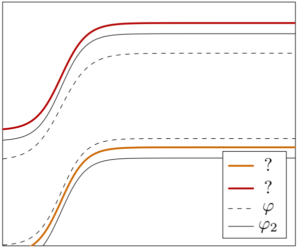

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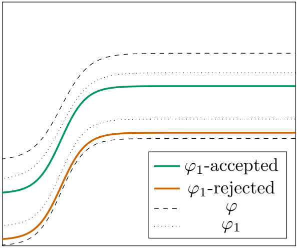

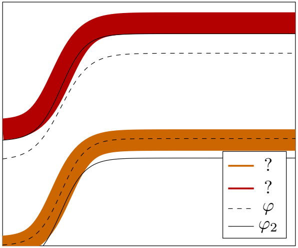

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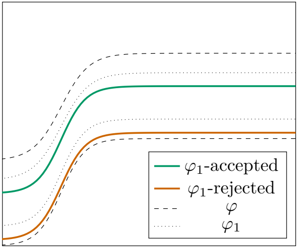

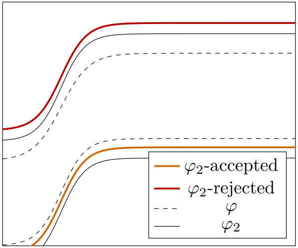

Guarantees: global risk ξ and precision α

Usual SMC

- $n = \frac{\log(2/\xi)}{2\alpha^2}$ simulations.

$\Rightarrow \mathbb{P}(p \in [\hat{p} - \alpha, \hat{p} + \alpha]) \geq 1 - \xi$

In our case (for each property)

- SMC risk $\theta = 1 - \sqrt{1 - \xi} < \xi$
- $n' = \frac{\log(2/\theta)}{2\alpha^2} > n$ simulations

$$\Rightarrow \mathbb{P}(p_1 \in [\hat{p_1} - \alpha, \hat{p_1} + \alpha]) \geq 1 - \theta, \quad \mathbb{P}(p_2 \in [\hat{p_2} - \alpha, \hat{p_2} + \alpha]) \geq 1 - \theta$$

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Theorem 2 (Main theorem).

After performing $N = 2 \times n'$ simulations, the following statements hold:

- $\mathbb{P}(p \in [\hat{p_1} - \alpha, \hat{p_2} + \alpha]) \geq 1 - \xi$;
- $\mathbb{P}(|\hat{p_1} - \hat{p_2}| \leq 3\alpha) \geq 1 - \xi$.

Bonus: extension to reward functions.

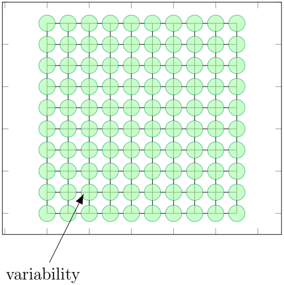
Outline

Generalities

- Parameterization: Find parameter values λ for a generic model.
- Goal: Find good values for λ w.r.t. score ($\mathbb{E}(r)$) of φ-satisfaction.
- Any algorithm:
  - Local search: low execution time / superficial search;
  - **Global** search: more informative / higher execution time;
  - ...

What we do

1. Compute the grid of parameters.
2. Compute the score of each value.
3. Select the best value.



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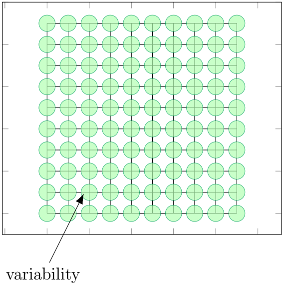

Reminder

It only works if we can bound the error ε!

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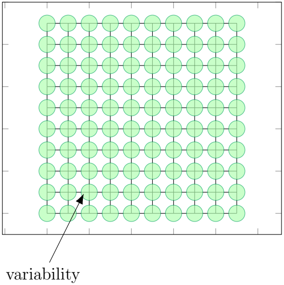

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Proposition

When solving an ODE, the error ε is bounded by a function of the integration step h.

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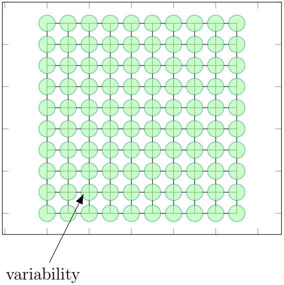

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Lemma 1.

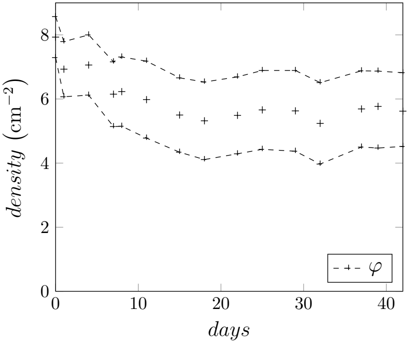
For any arbitrary $\varepsilon > 0$, there exists an integration step h such that

$$0 < \varepsilon_h < \varepsilon, \quad \forall \lambda.$$

Aurelia Aurita[2]

Jellyfish species from the Adriatic Sea.

- $x'(t) = a \cdot x(t) \cdot \left(1 - \frac{x(t)}{b}\right)$
- φ = data $\pm$ standard error



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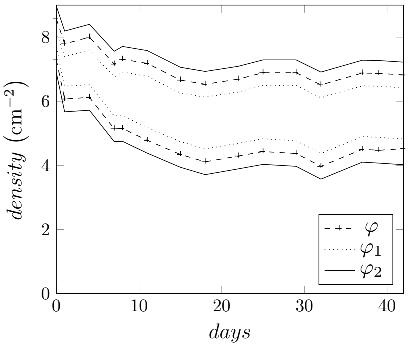
- φ_1 = "$\varphi - \varepsilon$"
- φ_2 = "$\varphi + \varepsilon$"



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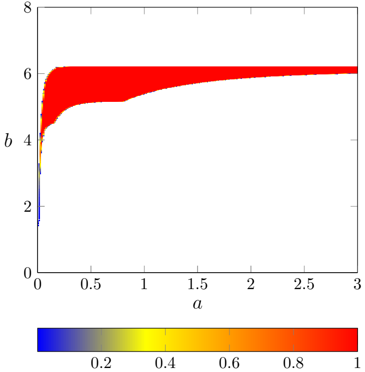
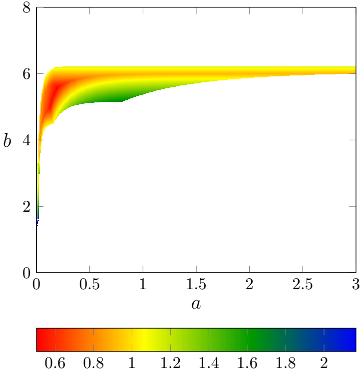
Parameter analysis



Probability of staying in the tunnel.



Expected distance to data.

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Perspectives

Mathematics

- Convergence speed of $\hat{p_1} - \hat{p_2}$.
- Suitable values for ε and h in the general case.

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Modeling

- **Structural properties** of ODE models.
  → stability, attraction, cycles ...
- **Dynamic** discretization of the parameter grid.
  → variance, score

Thank you for your attention !