Likelihood-Free Inference

— An Introduction to My Research —

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Program

Overview of my research interests

Efficient inference for simulator-based models

Program

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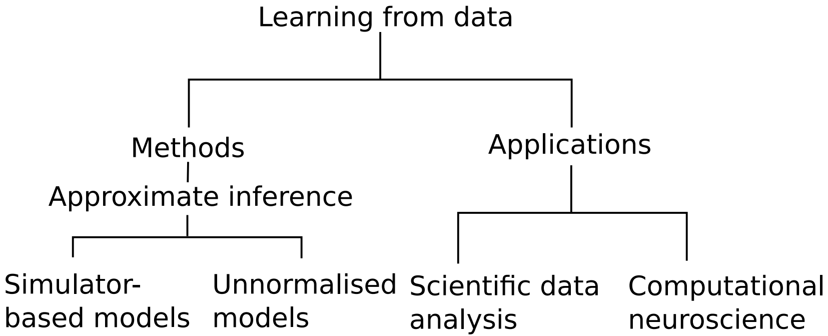
Efficient inference for simulator-based models

My research interests in brief



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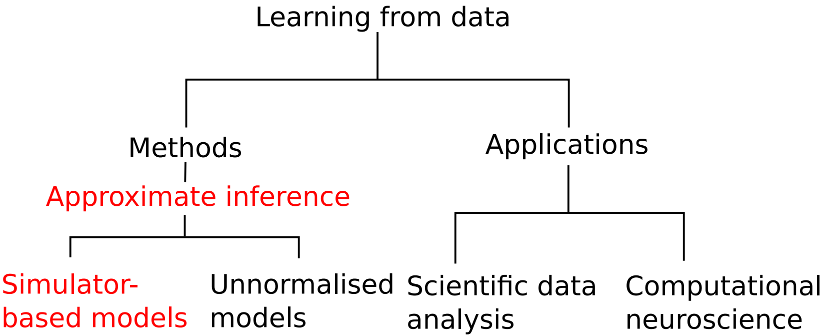
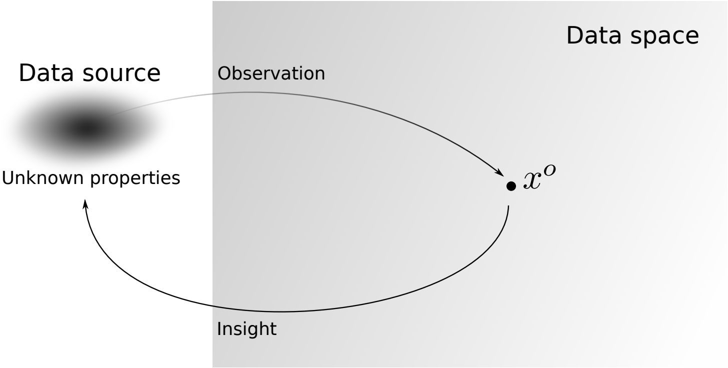


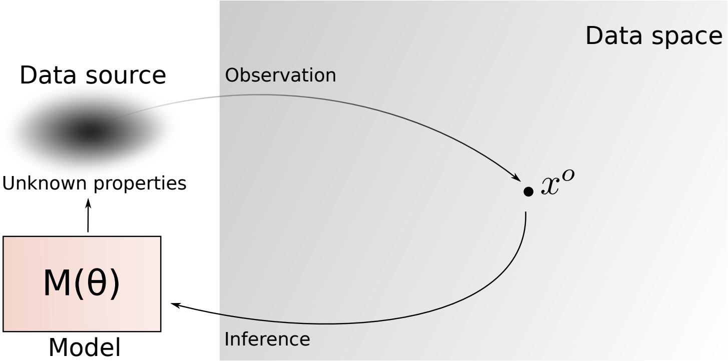
Learning from data

- Goal: Using observed data x^o, learn about their source
- Enables decision making, predictions, ...



General approach

- Set up a model with potential properties θ (parameters)
- See which θ are in line with the observed data x^o



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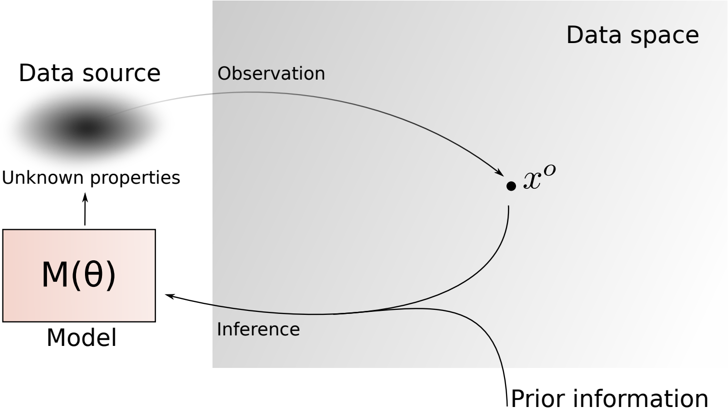
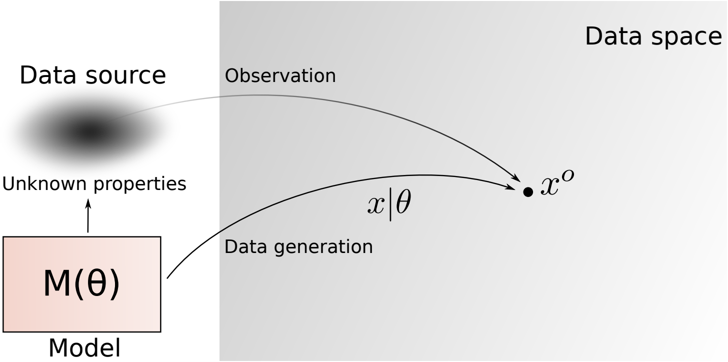


The likelihood function

- Measures agreement between θ and the observed data x^o
- Probability to generate data like x^o if hypothesis θ holds



Performing statistical inference

- If $L(\theta)$ is known, inference is straightforward
- Maximum likelihood estimation

$$\hat{\theta} = \mathrm{argmax}_\theta \, L(\theta)$$

- Bayesian inference

$$p(\theta|x^o) \propto p(\theta) \times L(\theta)$$

$$\text{posterior} \propto \text{prior} \times \text{likelihood}$$

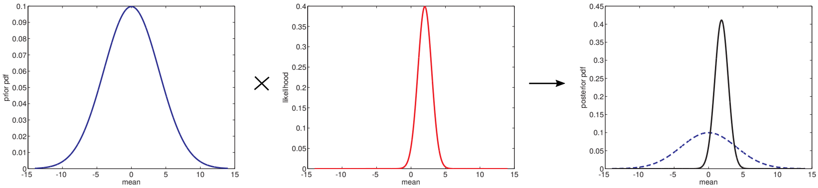
Allows us to learn from data by updating probabilities

Model specification

- Textbook: model $\equiv$ family of probability density functions
- Probability density functions (pdfs) $p(x|\theta)$ satisfy

$$\underbrace{p(x|\theta) \geq 0}_{\text{non-negativity}} \qquad \underbrace{\int p(x|\theta)\mathrm{d}x = 1}_{\text{normalization}}$$

- Likelihood function $L(\theta) = p(x^o|\theta)$
- Closed form solutions are possible



prior $\times$ likelihood $\rightarrow$ posterior

Models with intractable likelihoods

- Not all models are specified as family of pdfs $p(x|\theta)$.
- I worked on
  1. Simulator-based models
  2. Unnormalised models
- The models are rather different, common point:

  Multiple integrals needed to be computed to represent the models in terms of pdfs $p(x|\theta)$.
- Solving the integrals exactly is computationally impossible. (curse of dimensionality)

  $\Rightarrow$ No model pdfs $p(x|\theta)$
  $\Rightarrow$ No likelihood function $L(\theta) = p(x^o|\theta)$
  $\Rightarrow$ No exact inference

General research question

How to efficiently perform (Bayesian) inference when the likelihood function is too expensive too compute?

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Efficiency $\equiv$ good trade-off between speed and accuracy.

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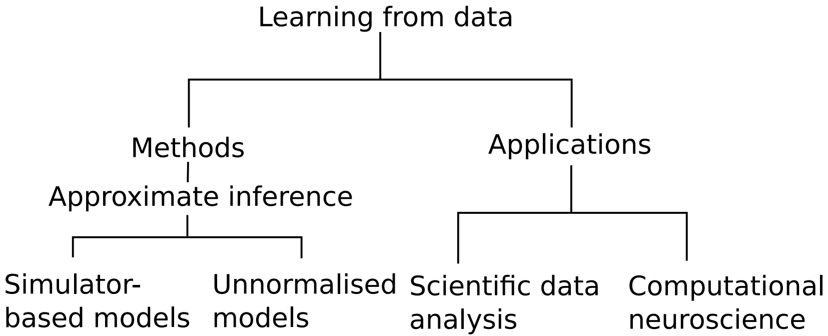


Unnormalised models

- Used for modelling
  - images (Markov random fields)
  - social networks (exponential random graphs)
  - ferro-magnetism (Ising model)
  - ...
- Specified via a non-negative function $q(x|\theta) \propto p(x|\theta)$,

$$\int \cdots \int q(x|\theta) dx = Z(\theta) \neq 1 \qquad p(x|\theta) = \frac{q(x|\theta)}{Z(\theta)}$$

- Advantage: Specifying unnormalised models is often easier than specifying normalized models
- Disadvantage: Integral defining $Z(\theta)$ can generally not be computed. Likelihood function is intractable.

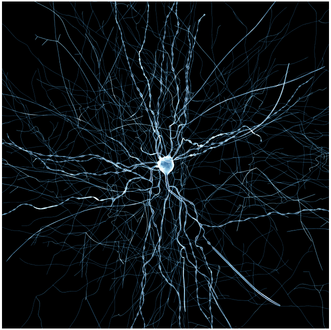
Simulator-based models

- Models which specify a mechanism for generating data
  - e.g. stochastic dynamical systems
  - computer models / simulators of some complex physical process
- Occur in multiple and diverse scientific fields.
- Different communities use different names:
  - Generative (latent-variable) models
  - Implicit models
  - Stochastic simulation models
  - Probabilistic programs

Simulator-based models are widely used

Examples:

- Evolutionary biology:
  Simulating evolution
- Neuroscience:
  Simulating neural circuits
- Ecology:
  Simulating species migration
- Health science:
  Simulating the spread of an infectious disease
- Physics:
  Simulating quantum systems (?)



Simulated neural activity in rat somatosensory cortex
(Figure from `https://bbp.epfl.ch/nmc-portal`)

Pros and Cons

- Advantage: detailed and realistic modelling
- Disadvantage: likelihood function is generally intractable due to unobserved variables.
- To compute $p(x|\theta)$ one has to take into account all possible states of the unobserved variables

$$p(x|\theta) = \int \cdots \int p(x, z|\theta) dz$$

- This is generally computationally impossible.

Program

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Efficient inference for simulator-based models

The likelihood function

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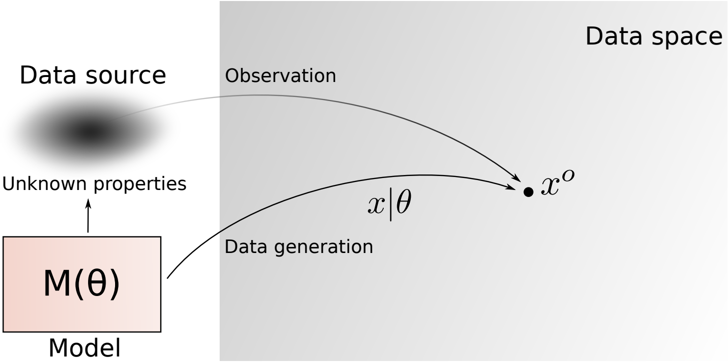
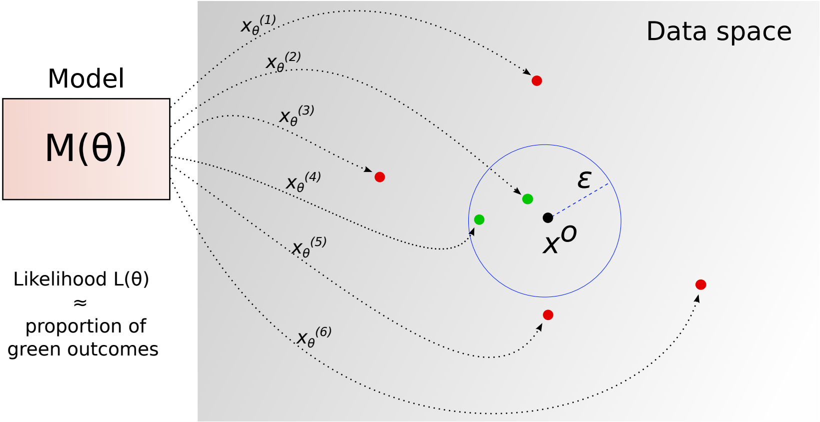


Three foundational issues

1. How should we assess whether $x_\theta \equiv x^o$?
2. How should we compute the probability of the event $x_\theta \equiv x^o$?
3. For which values of θ should we compute it?

Traditional approach

Likelihood: Probability to generate data like x^o if hypothesis θ holds



$$L(\theta) \approx \frac{1}{N} \sum_{i=1}^{N} \mathbb{1} \left(d(x_\theta^{(i)}, x^o) \leq \epsilon \right)$$

Traditional approach

1. How should we assess whether $x_\theta \equiv x^o$?
   $\Rightarrow$ Check whether $||T(x_\theta) - T(x^o)|| \leq \epsilon$
2. How should we compute the probability of the event $x_\theta \equiv x^o$?
   $\Rightarrow$ By counting
3. For which values of θ should we compute it?
   $\Rightarrow$ Sample from the prior

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- Corresponds to a traditional version of a method called approximate Bayesian computation.
- Trade-off between computational cost and accuracy of the inference may be poor.

Some of my work

1. How should we assess whether $x_\theta \equiv x^o$?
   $\Rightarrow$ Use classification (Gutmann et al, 2014, 2017)

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   $\Rightarrow$ Use density ratio estimation (Dutta et al, 2016, arXiv:1611.10242)

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3. For which values of θ should we compute it?
   $\Rightarrow$ Use Bayesian optimisation (Gutmann and Corander, 2013-2016)

Example: Bacterial infections in child care centres

- Comparison of the Bayesian optimisation approach with a standard population Monte Carlo ABC approach.
- Roughly equal results using 1000 times fewer simulations.

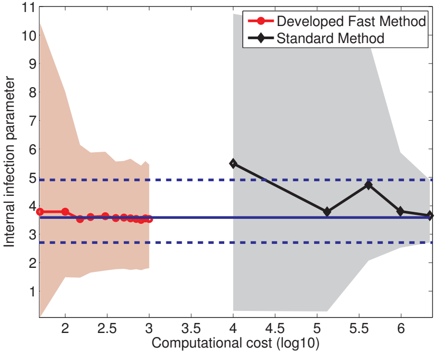
4.5 days with 200 cores

↓

90 minutes with seven cores

Posterior means: solid lines,

credibility intervals: shaded areas or dashed lines.



(Gutmann and Corander, 2016)

Summary

- Learning from data
  - Methods
    - Approximate inference
      - Simulator-based models
        - Importance
        - Difficulty of performing inference
        - Solutions using classification, density ratio estimation, and Bayesian optimimisation
      - Unnormalised models
  - Applications
    - Scientific data analysis
    - Computational neuroscience