

# Bayesian Inference via Classification

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M.U. Gutmann, R. Dutta, S. Kaski, and J. Corander  
Statistical Inference of Intractable Generative Models via  
Classification, *arXiv:1407.4981*.

J. Lintusaari, M.U. Gutmann, R. Dutta, S. Kaski, and J. Corander  
Fundamentals and Recent Developments in Approximate Bayesian  
Computation, *Systematic Biology*, in press, 2016.

# Take-home message

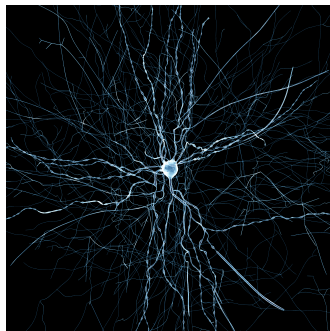
By using classification, we can measure the distance between two data sets and infer the parameters of intractable generative models.

# Problem statement

- ▶ Given:
  - ▶ Observed data  $\mathbf{y}^o$
  - ▶ Intractable generative model, parametrised by  $\theta$
  - ▶ (Possibly) A prior probability density function (pdf) for  $\theta$ ,  $p_\theta$
- ▶ Task: Perform inference about  $\theta$ 
  - ▶ Maximum likelihood estimate
  - ▶ Posterior distribution of  $\theta$

# Generative model

- ▶ Model that specifies a mechanism for generating data  $\mathbf{y}$ 
  - ▶ e.g. stochastic dynamical system
  - ▶ computer model / simulator of some complex biological process
- ▶ Such models are widely used
  - ▶ Evolutionary biology:  
Simulating evolution
  - ▶ Neuroscience:  
Simulating neural circuits
  - ▶ Ecology:  
Simulating species migration
  - ▶ Health science:  
Simulating the spread of an infectious disease



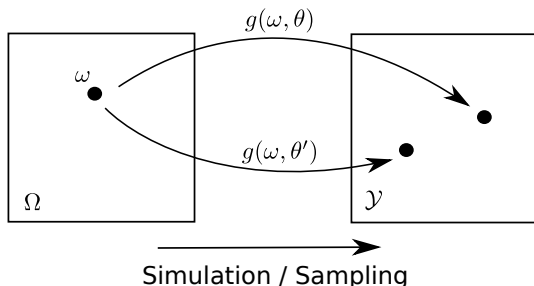
Simulated neural activity in rat somatosensory cortex  
(Figure from <https://bbp.epfl.ch/nmc-portal>)

# Generative model

- ▶ Let  $(\Omega, \mathcal{F}, \mathcal{P})$  be a probability space.
- ▶ A generative model is a collection of (measurable) functions  $g(\cdot, \theta)$  parametrized by  $\theta$ ,

$$\omega \in \Omega \mapsto \mathbf{y} = g(\omega, \theta) \in \mathcal{Y} \quad (1)$$

- ▶ For any fixed  $\theta$ ,  $\mathbf{y} = g(\cdot, \theta)$  is a random variable.



# Intractable generative model

- ▶ Generally impossible to write down the pdf  $p(\mathbf{y}|\boldsymbol{\theta})$  of the generated data.
- ▶ Likelihood function  $L(\boldsymbol{\theta}) = p(\mathbf{y}^o|\boldsymbol{\theta})$  not known well defined, but computation not tractable
- ▶ Exact inference not possible

supplemental

# Approximate inference for generative models

- ▶ Inference is approximate due to approximation of  $p(\mathbf{y}^o|\boldsymbol{\theta})$
- ▶ Rough classification:
  - ▶ Parametric approximation: e.g. synthetic likelihood  
(Wood, Nature, 2010)
  - ▶ Nonparametric approximation: e.g. approximate Bayesian computation  
(Recent review: Gutmann et al, Systematic Biology, 2016)
- ▶ General idea: Identify the values of the parameters  $\boldsymbol{\theta}$  for which simulated data resemble the observed data



# Meta algorithm for approximate Bayesian computation

- ▶ Let  $\mathbf{y}^o$  be the observed data.
- ▶ Iterate many times:
  1. Sample  $\theta$  from a proposal distribution  $q(\theta)$
  2. Sample  $\mathbf{y}|\theta$  according to the model
  3. Compute the distance  $d(\mathbf{y}, \mathbf{y}^o)$  between simulated and observed data
  4. Retain  $\theta$  if  $d(\mathbf{y}, \mathbf{y}^o) \leq \epsilon$
- ▶ Different choices for  $q(\theta)$  give different algorithms
- ▶ Produces samples from the (approximate) posterior when the bandwidth  $\epsilon$  is small.

## Two major difficulties

1. How to handle the computational cost?
2. How to measure the distance  $d$  between simulated and observed data?

# Two major difficulties

## 1. How to handle the computational cost?

→ Use Bayesian optimization

M.U. Gutmann and J. Corander

Bayesian optimization for likelihood-free inference of simulator-based statistical models

*Journal of Machine Learning Research*, 17(125): 1–47, 2016

## 2. How to measure the distance $d$ between simulated and observed data?

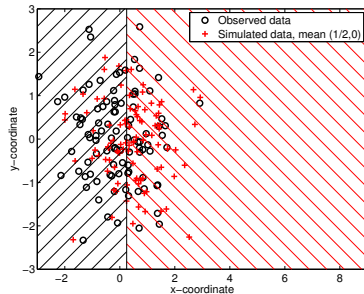
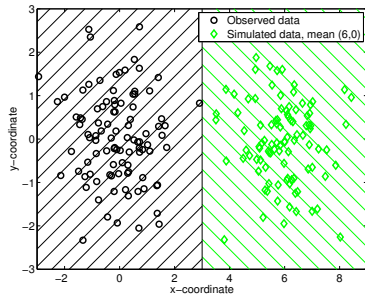
→ Use classification

M.U. Gutmann, R. Dutta, S. Kaski, and J. Corander

Statistical Inference of Intractable Generative Models via Classification, *arXiv:1407.4981*

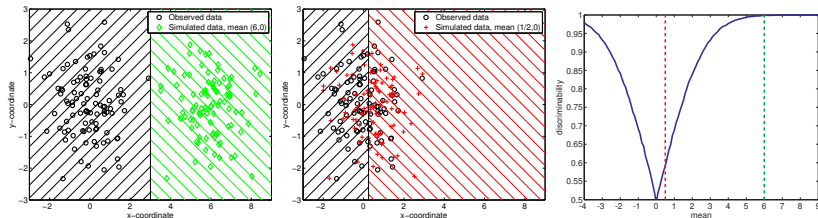
# Using classification to measure the distance

Correctly classifying data into two categories is usually easier if the two data sets were generated with very different values of  $\theta$  (left) than with similar values (right).



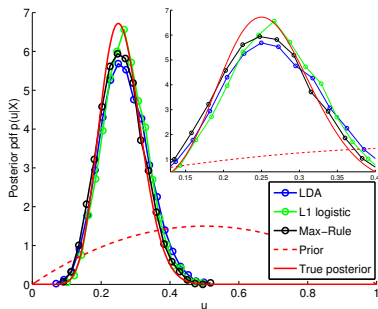
# Using classification to measure the distance

- ▶ Classification accuracy (discriminability) serves as distance measure.
- ▶ Value of  $1/2$ : close; Value of 1: far
- ▶ Complete arsenal of classification methods becomes available to inference.

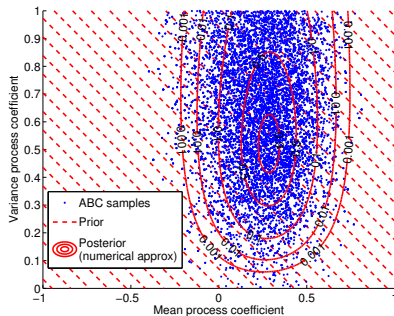


# Using the distance for posterior inference

- ▶ Approximate Bayesian computation (ABC) with classification accuracy as distance measure
- ▶ Results for toy models:



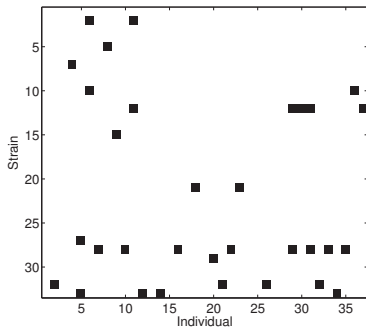
(a) binary data (Bernoulli)



(b) time series (ARCH)

# Application to epidemiology of infectious diseases

- ▶ Data: Colonization states of sampled attendees of 29 child day care centres (DCCs).
- ▶ DCC example: Each square indicates an attendee colonized with a strain of the bacterium *Streptococcus pneumoniae*.



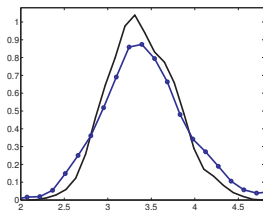
# Application to epidemiology of infectious diseases

- ▶ Generative model: latent continuous-time Markov chain for the transmission dynamics in a DCC and an observation model (Numminen et, Biometrics, 2013).
- ▶ The model has three parameters:
  - ▶  $\beta$ : rate of infections within a DCC
  - ▶  $\Lambda$ : rate of infections outside a DCC
  - ▶  $\theta$ : possibility to be infected with multiple strains
- ▶ Likelihood is intractable (data at a single time point are available only).

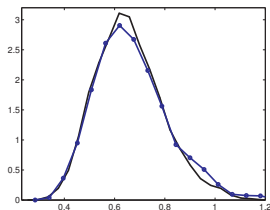


# Application to epidemiology of infectious diseases

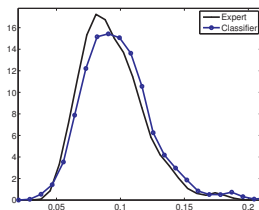
- ▶ Our classification-based distance measure does not use domain/expert knowledge.
- ▶ Performs as well as a distance measure based on domain knowledge (Numminen et, Biometrics, 2013).



(c) Posterior pdf for  $\beta$



(d) Posterior pdf for  $\Lambda$



(e) Posterior pdf for  $\theta$

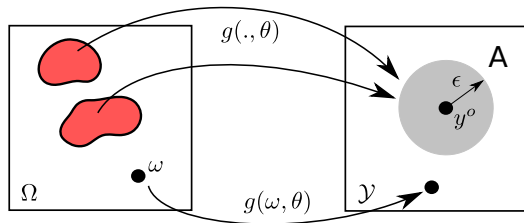
# Summary

- ▶ Topic: Inference for generative models where the likelihood function is intractable
- ▶ Inference principle: Find parameter values for which the distance between simulated and observed data is small
- ▶ Showed that, by using classification, we can
  - ▶ measure the distance between two data sets, and
  - ▶ infer the parameters of intractable generative models.
- ▶ More (results, math, related work, ...) in the reference paper!

# Likelihood function is implicitly defined

$$\Pr(y \in A \mid \theta) = \mathcal{P}(\{\omega : g(\omega, \theta) \in A\})$$

Parameter value  $\theta$



Parameter value  $\theta'$

