TransferLab

appliedAI institute for europe

Simulated data is all you need: Bayesian parameter inference for scientific simulators with SBI

Jan Boelts (Teusen) | EuroSciPy2024 | August 30th, 2024 | Szczecin

A joint initiative

UNTERNEHMER TUM | IPAI

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  - Cognitive Science
  - Computational Neuroscience
  - “Machine Learning for Science”

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Outline

1. **Why** simulators?
2. **Why** Bayesian parameter inference?
3. **How** to do Bayesian inference for simulators?
4. **Demo:** How can you apply SBI to your simulator?

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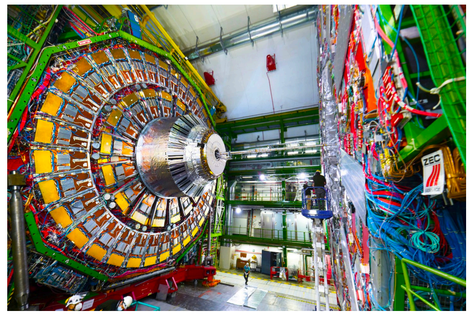
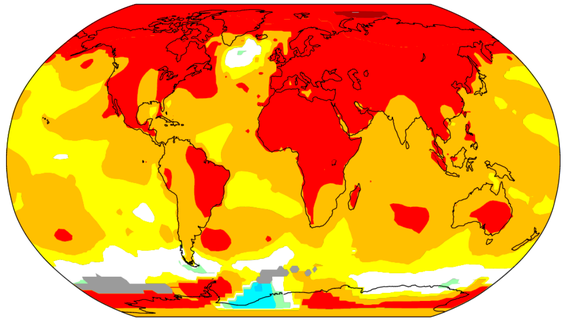
Simulators are used all across science



particle physics

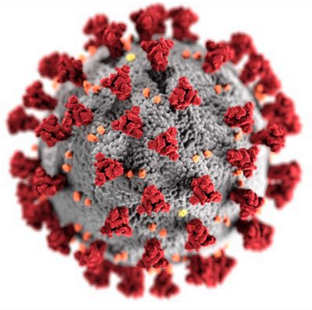
neuroscience



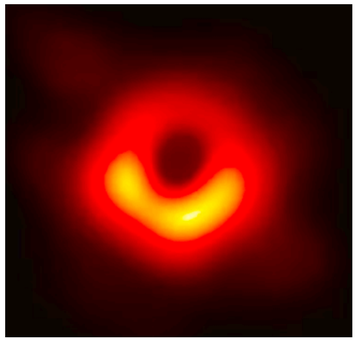
climate science

genomics

epidemiology



astrophysics



CERN; getty images; Wikipedia

What is a simulator?

Simulator: A computer program that takes input parameters θ and returns simulated data x

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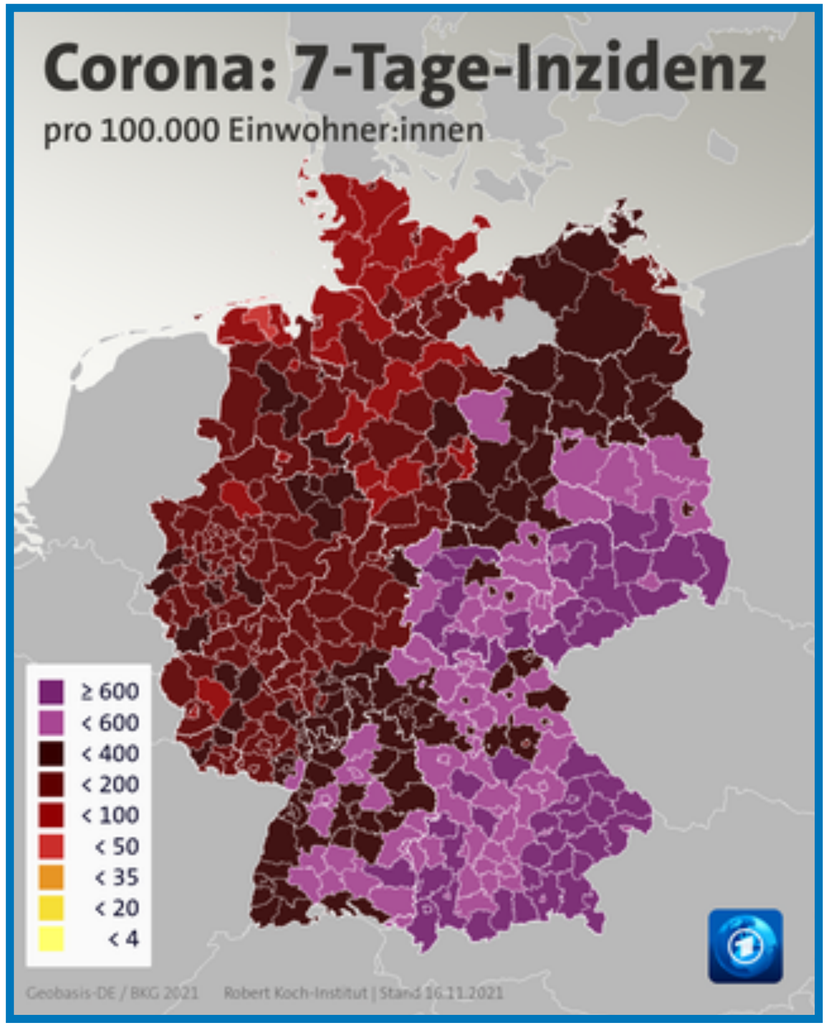
- **no access** to the inner workings (no likelihoods, no gradients)

Example: The SIR Simulator for COVID-19



tagesschau.de, 2021; Dehning et al. 2020, Science

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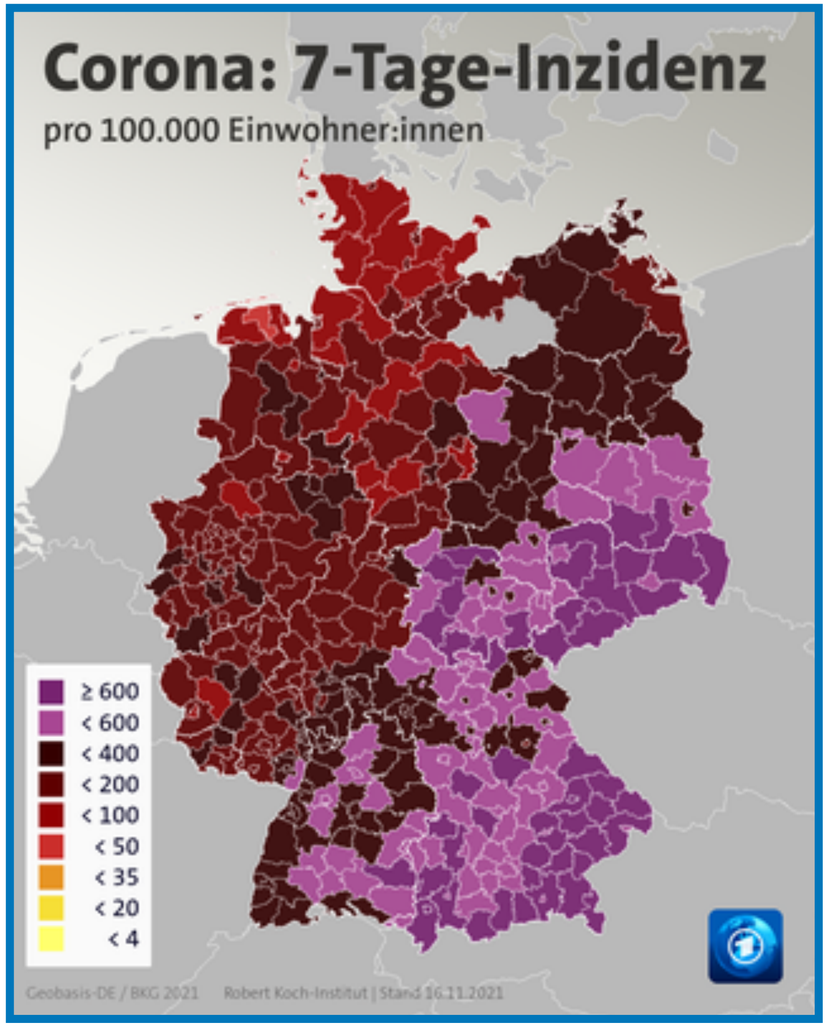

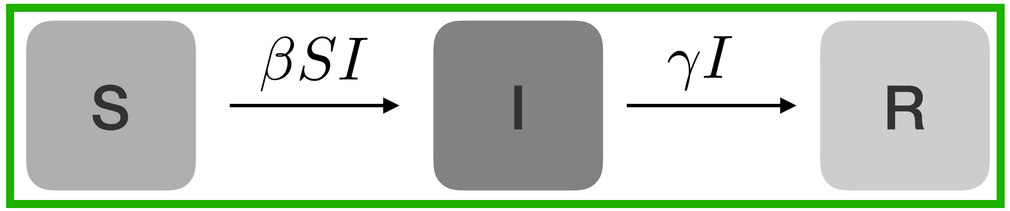

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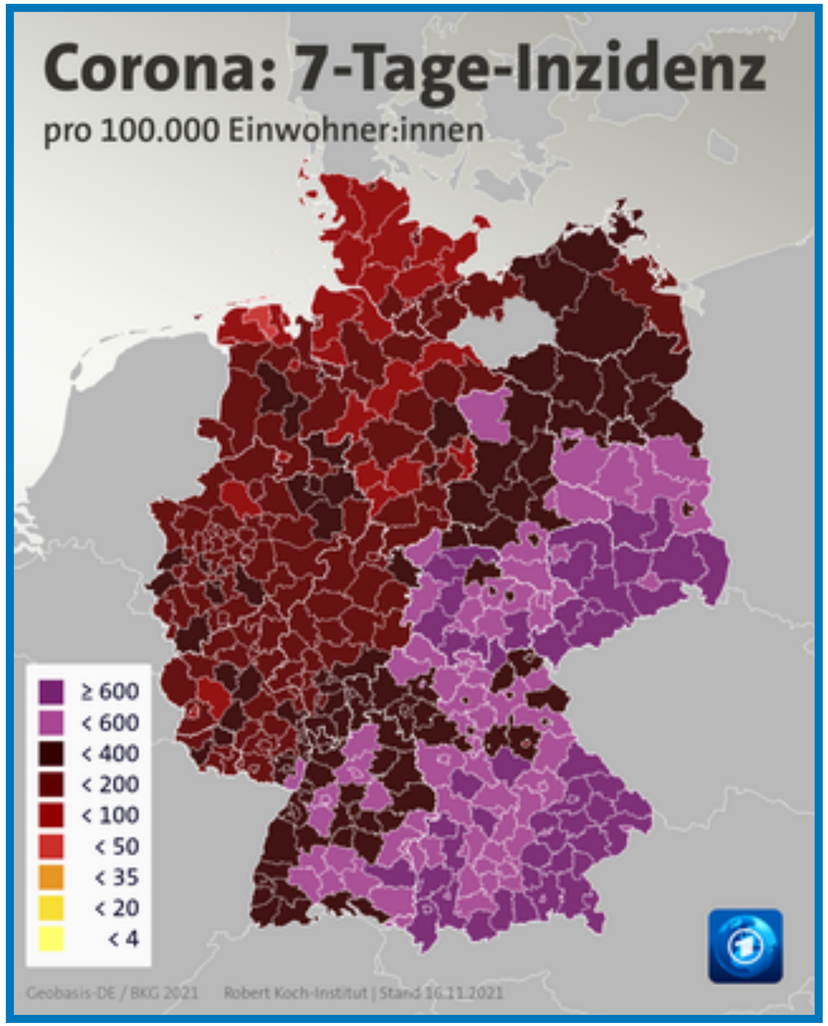

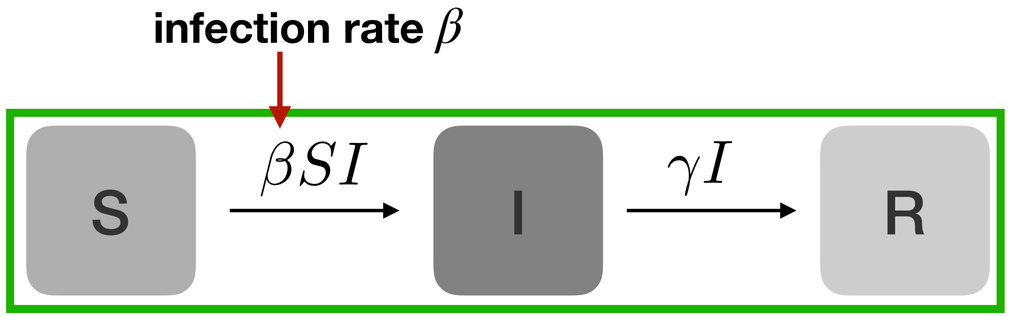

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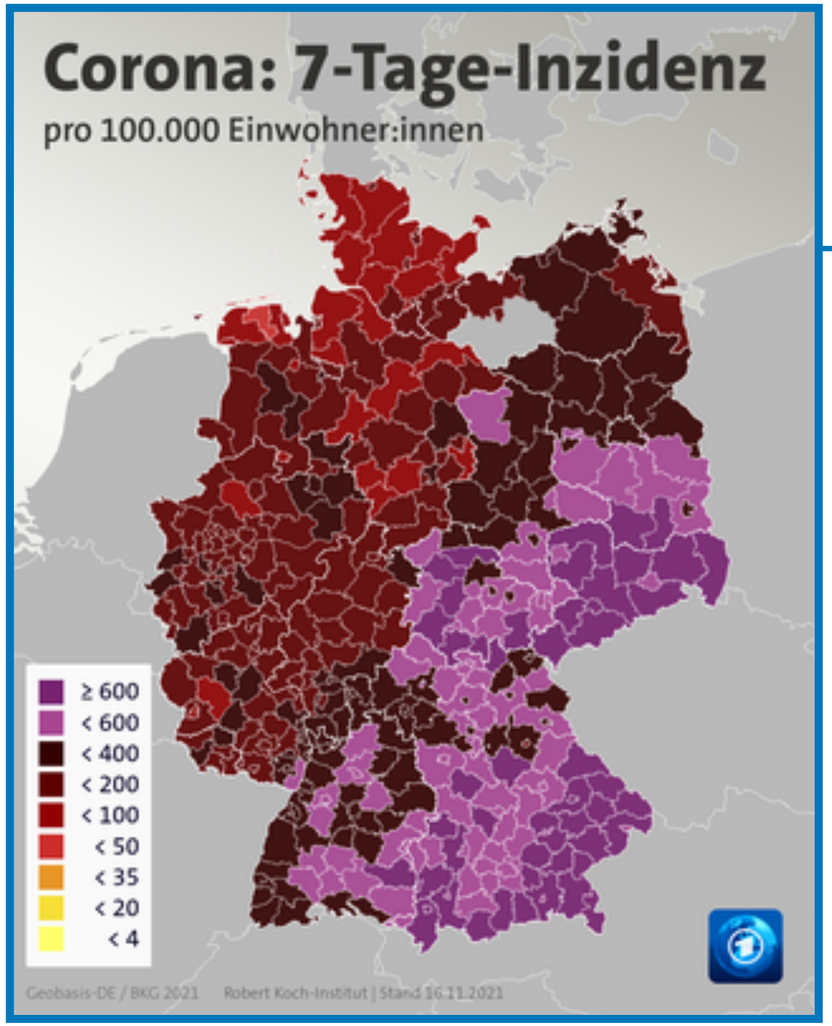

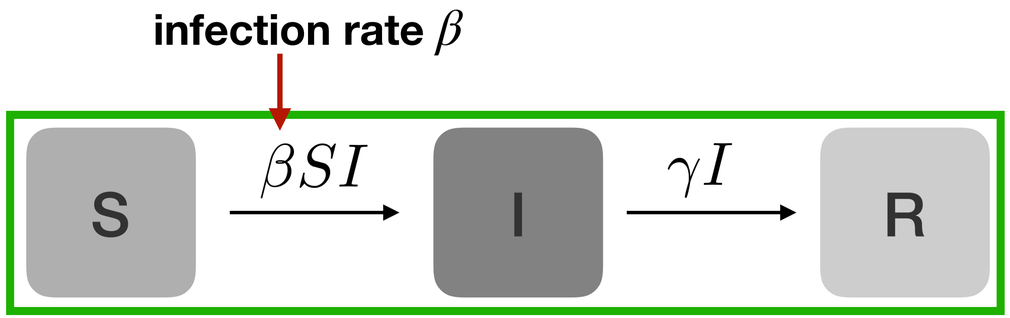

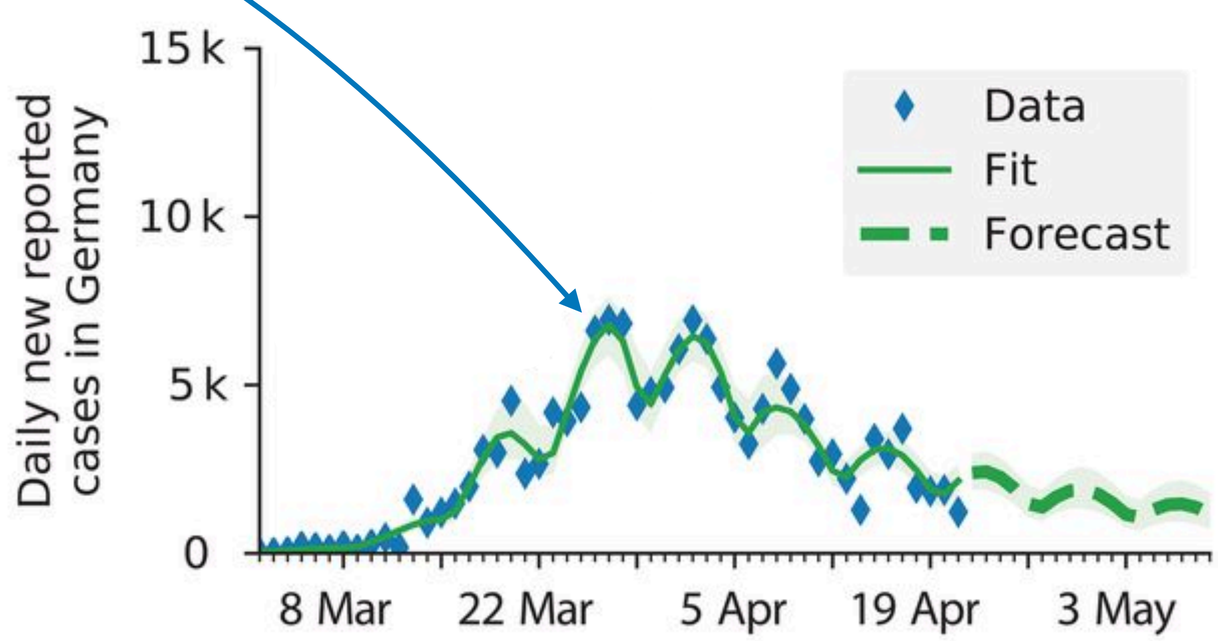

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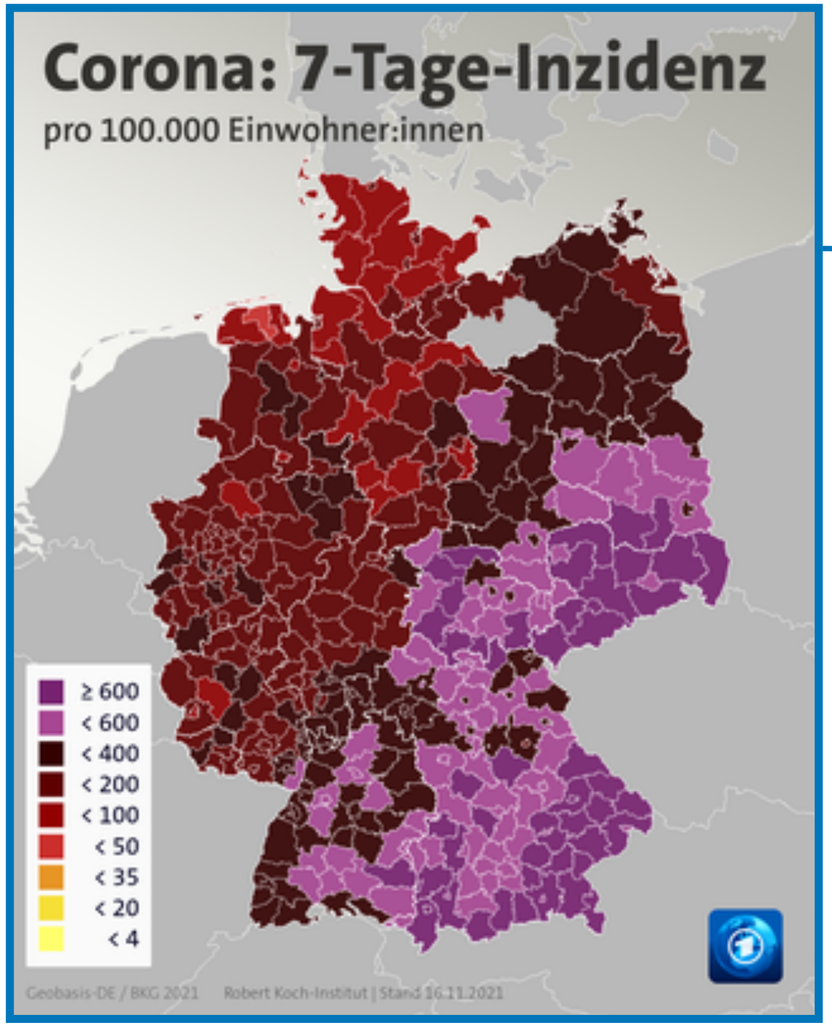

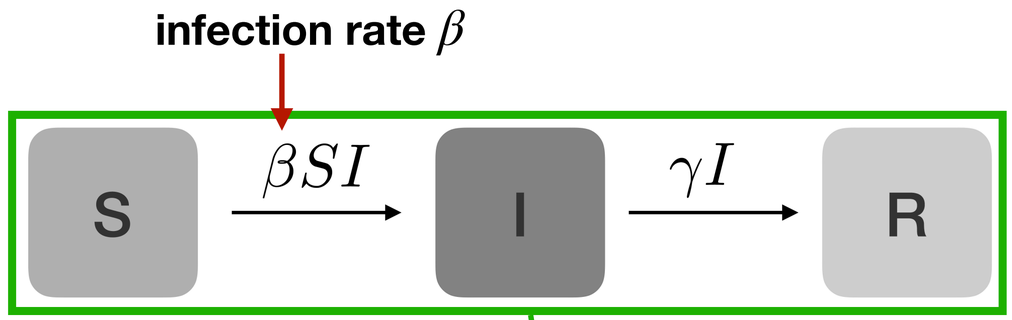

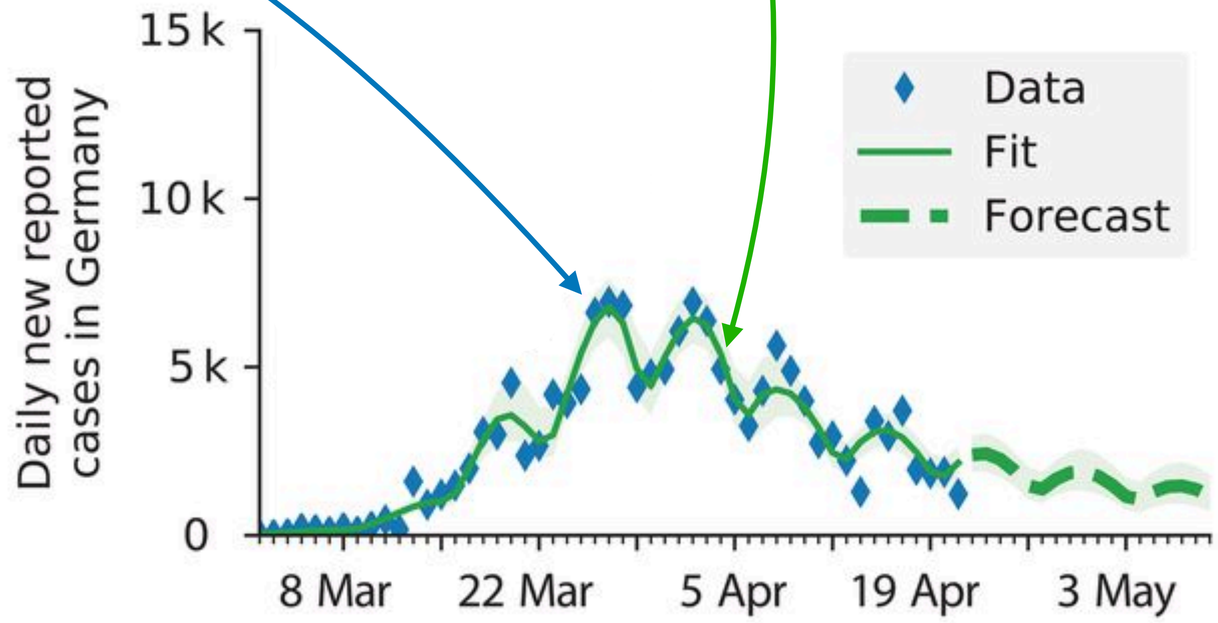

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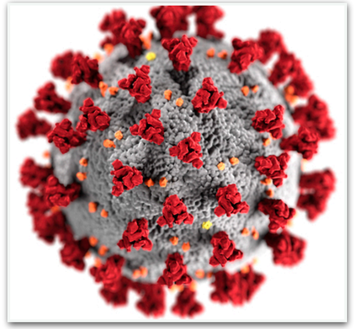
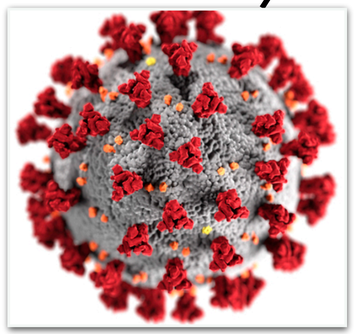
The simulation-based modeling approach

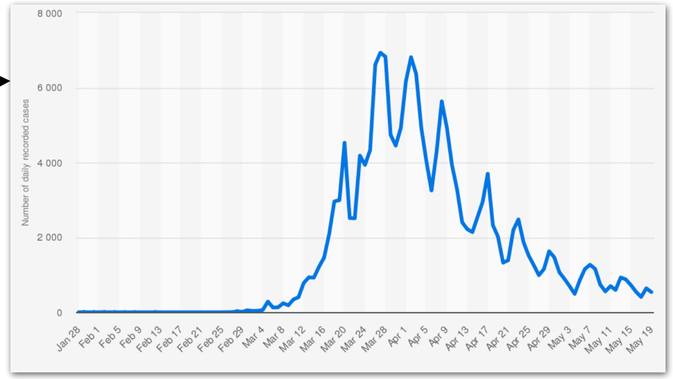


Paul Ehrlich Institut; WHO; Dehning et al. 2020

The simulation-based modeling approach

observe data





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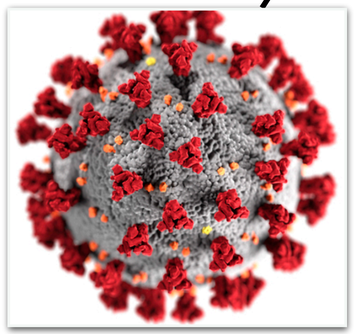
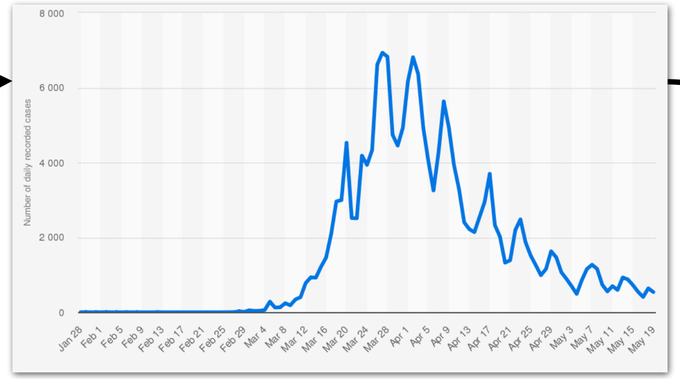
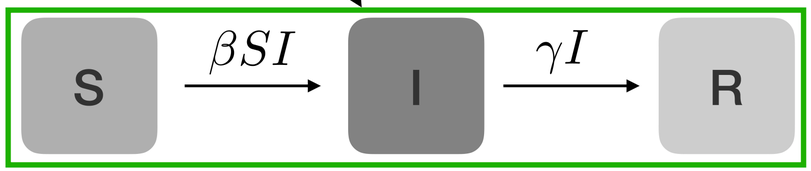




build a model



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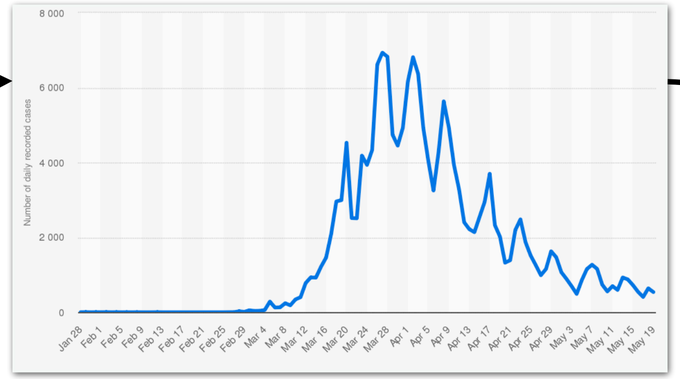

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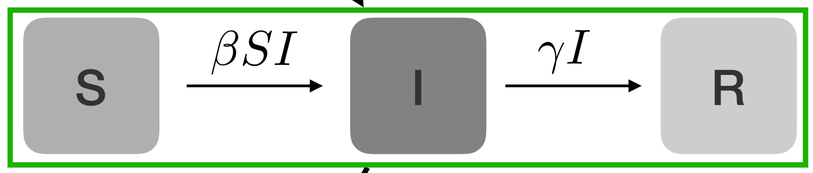
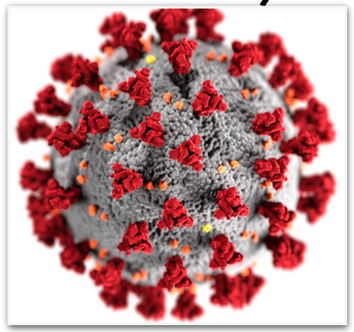
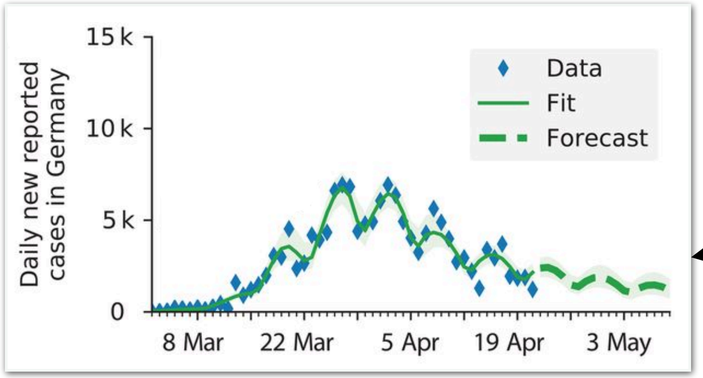




fit model to data



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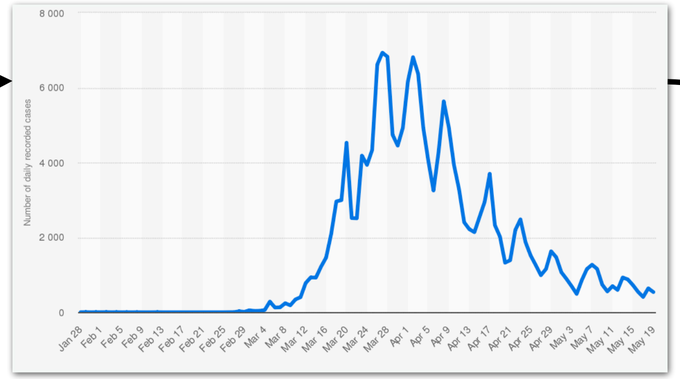

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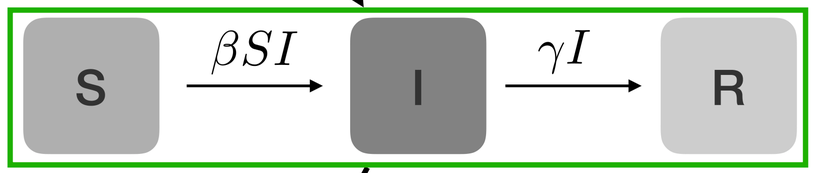

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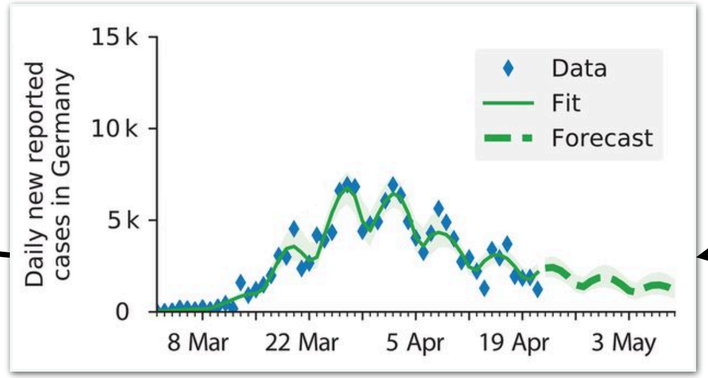
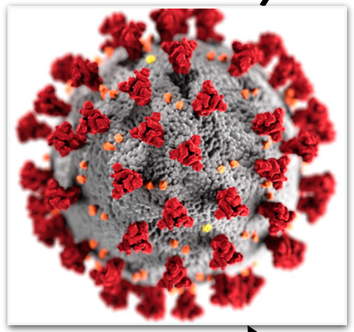


draw conclusions, make predictions



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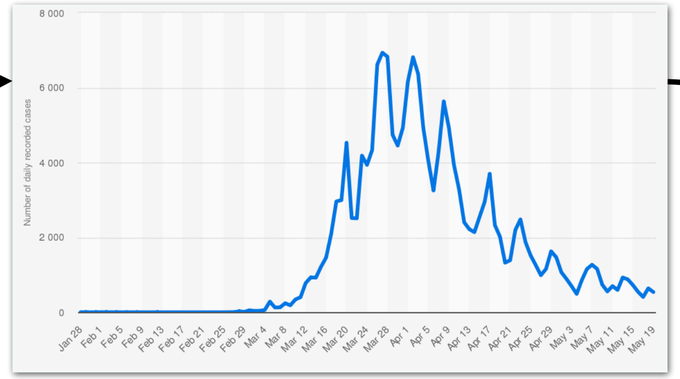

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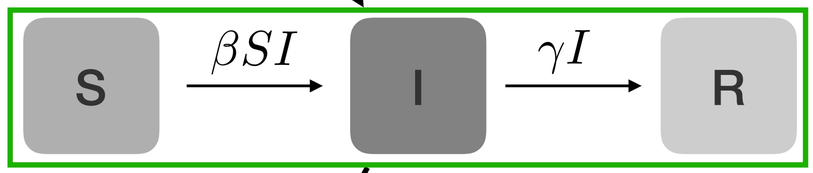

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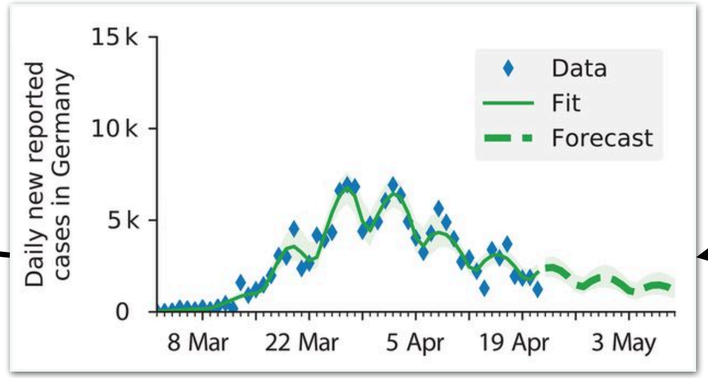

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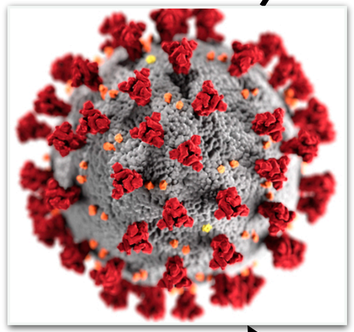

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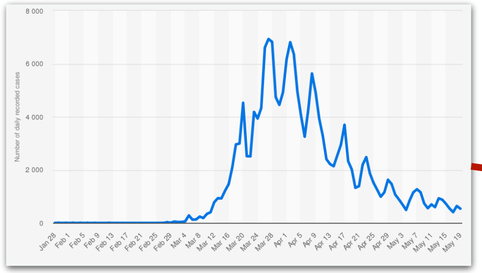
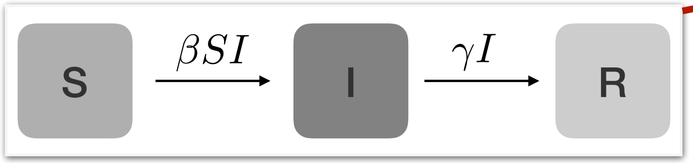
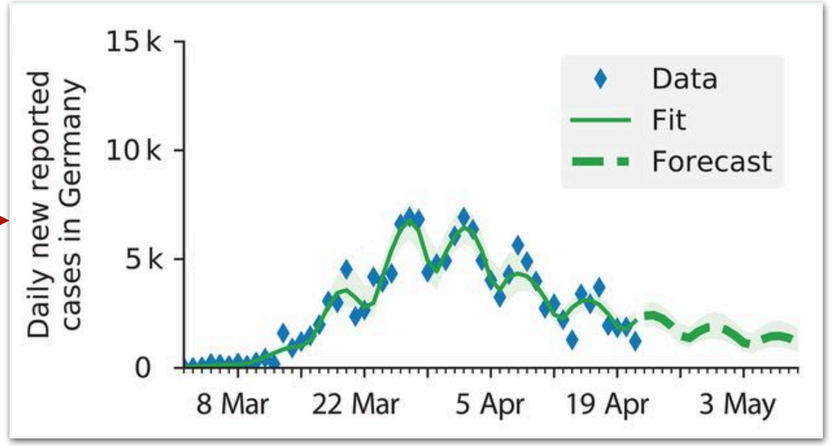
Central challenge: finding model parameters





infection rate β
?
recovery rate γ



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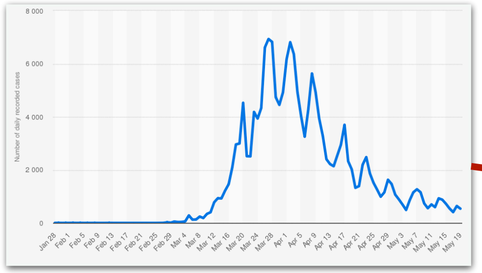

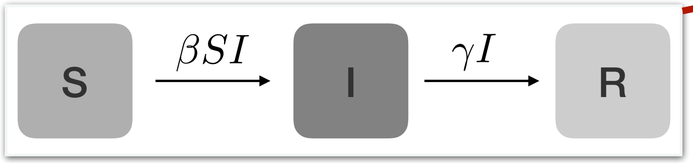

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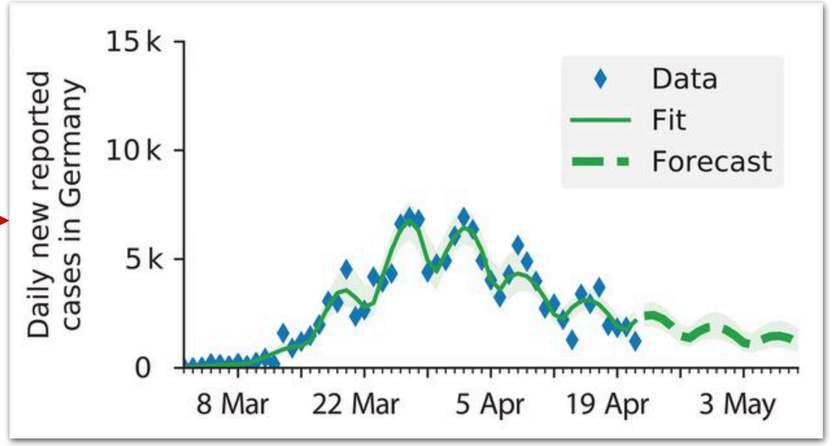
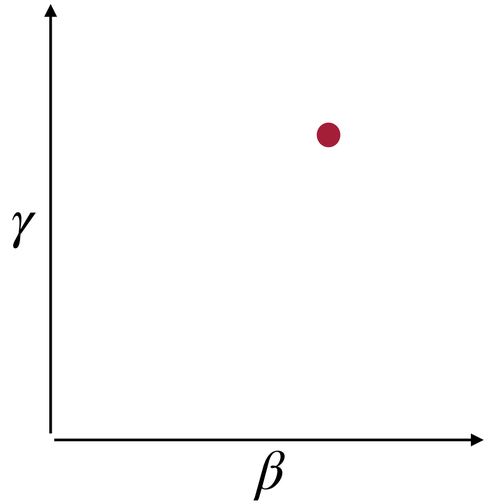


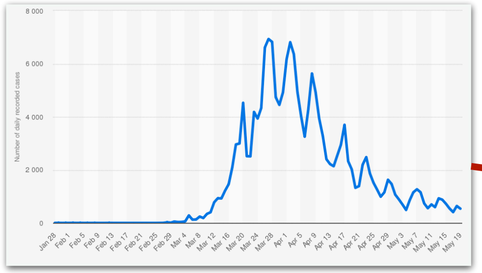
Naive approach

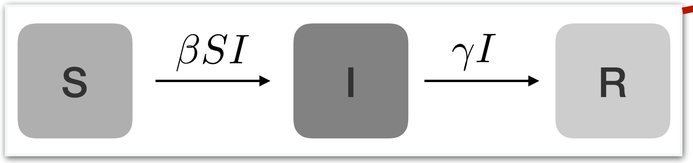
- find single best-fitting parameters
  - hand tuning, grid search
  - optimization, genetic algorithms



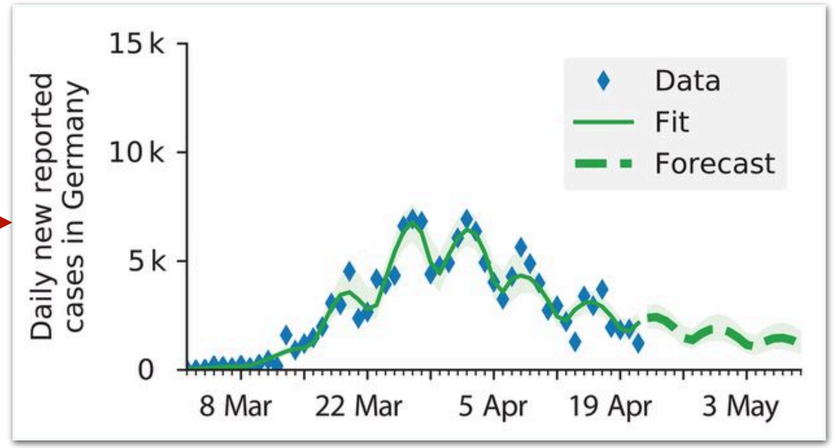
TransferLab

Central challenge: finding model parameters



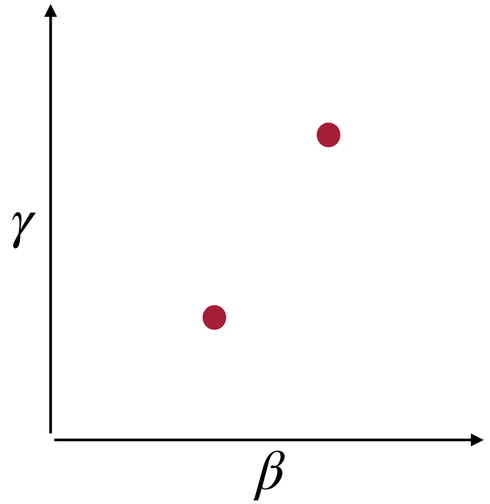


infection rate β
?
recovery rate γ



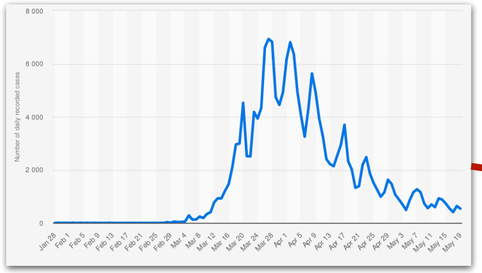
Naive approach

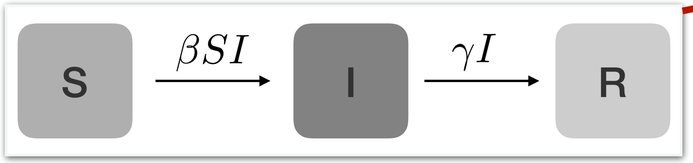
- find single best-fitting parameters
  - hand tuning, grid search
  - optimization, genetic algorithms



TransferLab

Central challenge: finding model parameters





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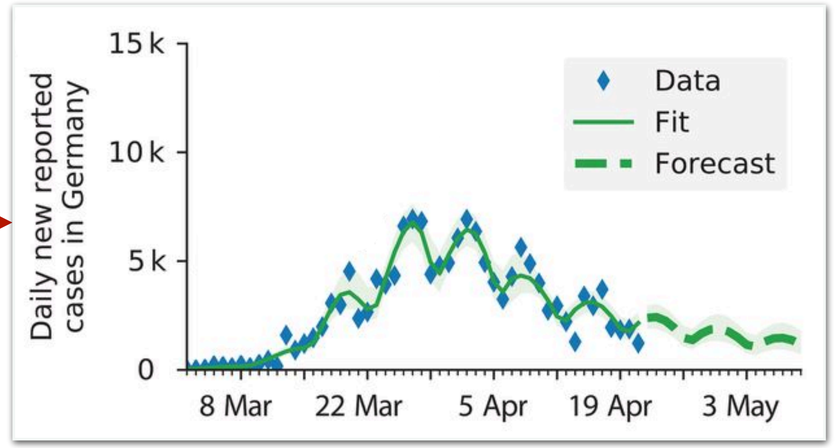

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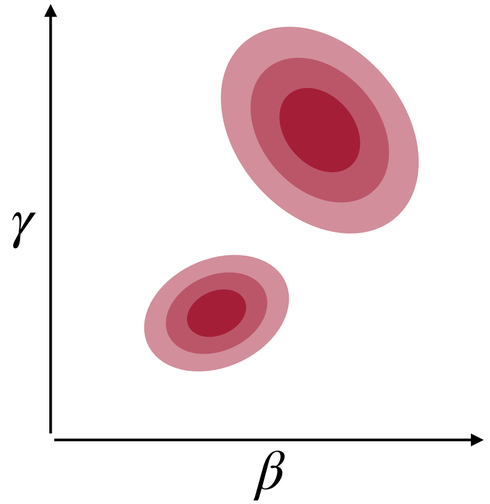
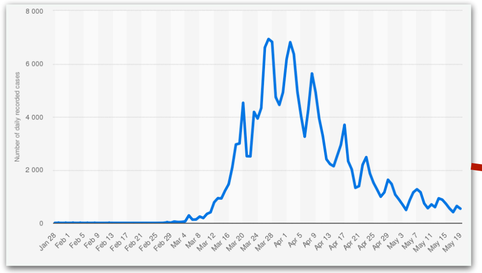
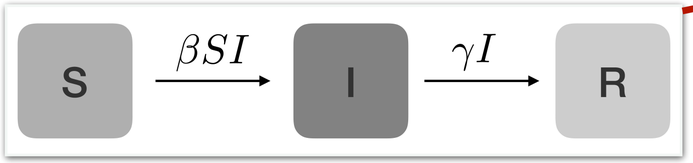


TransferLab

Central challenge: finding model parameters





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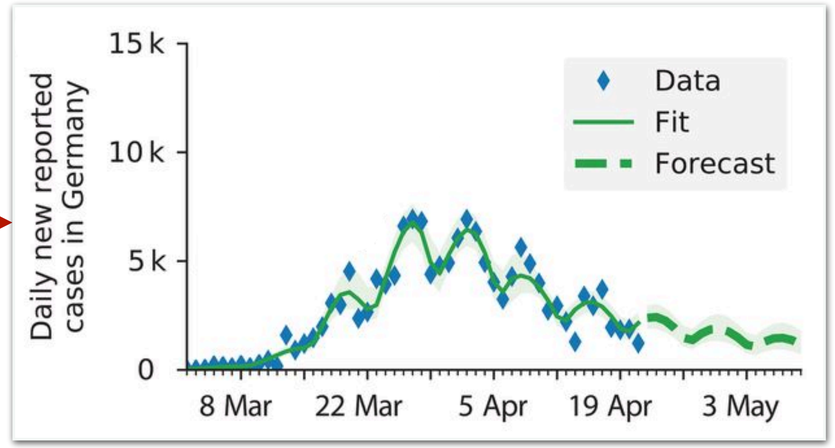

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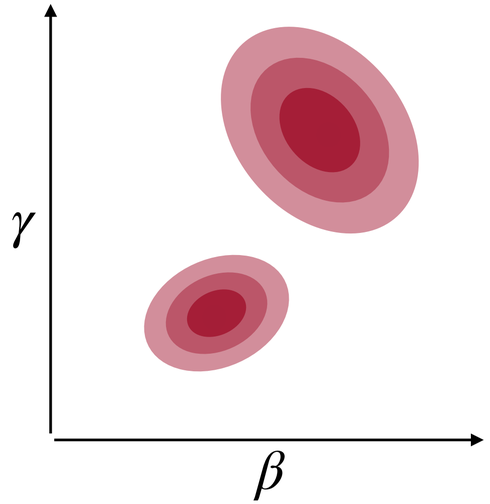


Ideal approach

- find all parameters
- quantify uncertainty
- quantify relations between parameters

TransferLab

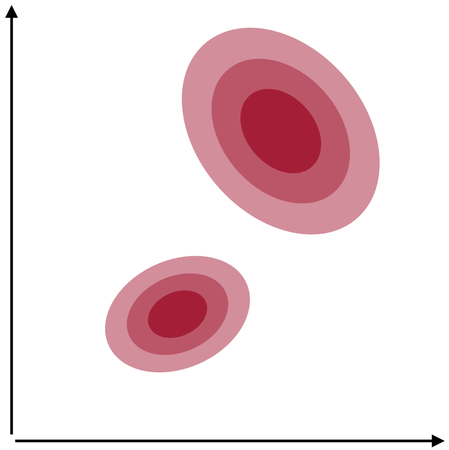
Outline

1. **Why** simulators?
2. **Why** Bayesian parameter inference?
3. **How** to do Bayesian inference for simulators?
4. **How** can you apply SBI to your simulator?

Bayesian parameter inference

Ideal approach

- find all parameters
- quantify uncertainty
- quantify relations between parameters



Laplace, Bayes, 1764

Bayesian parameter inference

Ideal approach

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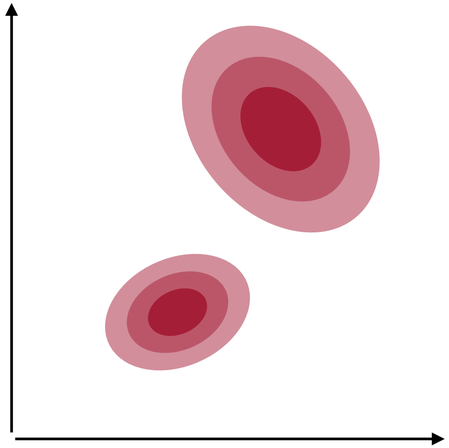
- quantify relations between parameters



- data x and parameters θ are *random variables*

Laplace, Bayes, 1764

Bayesian parameter inference

Ideal approach

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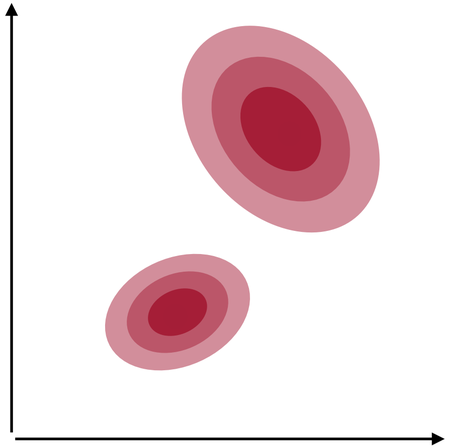

- data x and parameters θ are *random variables*
- **goal**: infer a distribution over parameters $p(\theta \mid x)$

Laplace, Bayes, 1764

Bayesian parameter inference

Ideal approach

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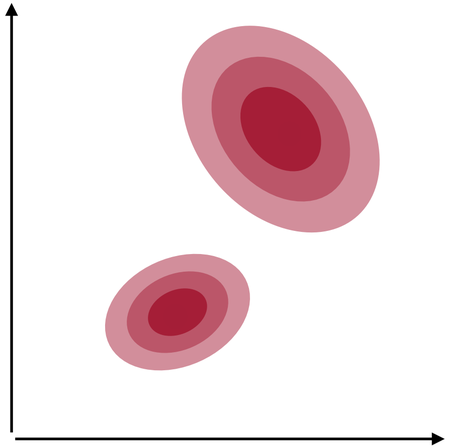


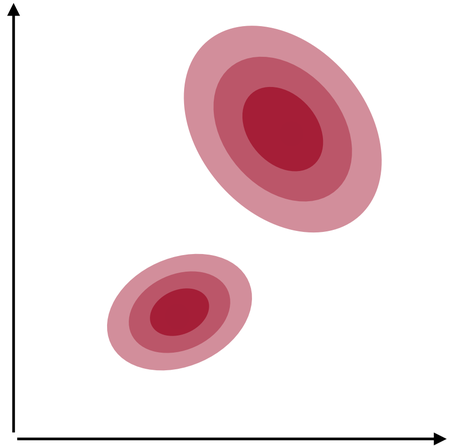
- data x and parameters θ are *random variables*
- **goal**: infer a distribution over parameters $p(\theta \mid x)$
  - characterizes **all** suitable parameters

Laplace, Bayes, 1764

Bayesian parameter inference

Ideal approach

- find all parameters
- quantify uncertainty
- quantify relations between parameters



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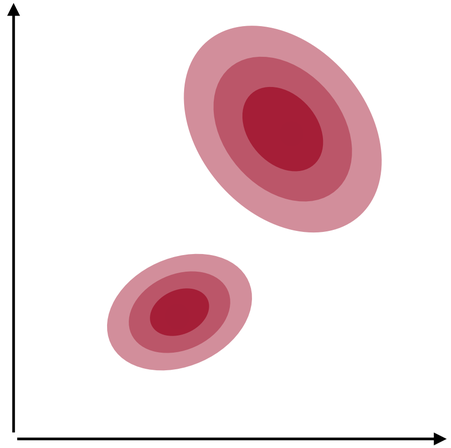

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Bayes' Theorem

$$p(\theta \mid x) \propto p(x \mid \theta)\ p(\theta)$$

Laplace, Bayes, 1764

Bayesian parameter inference

Ideal approach

- find all parameters
- quantify uncertainty
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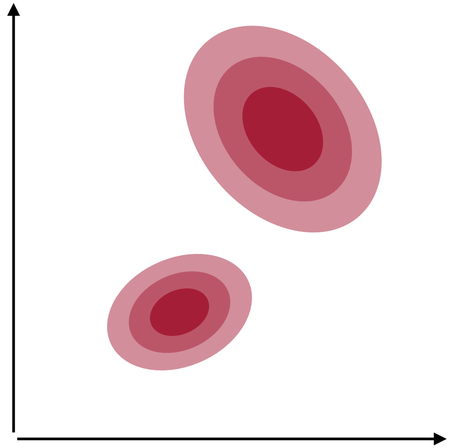


- data x and parameters θ are *random variables*
- **goal**: infer a distribution over parameters $p(\theta \mid x)$
  - characterizes **all** suitable parameters
  - quantifies uncertainty

Bayes' Theorem

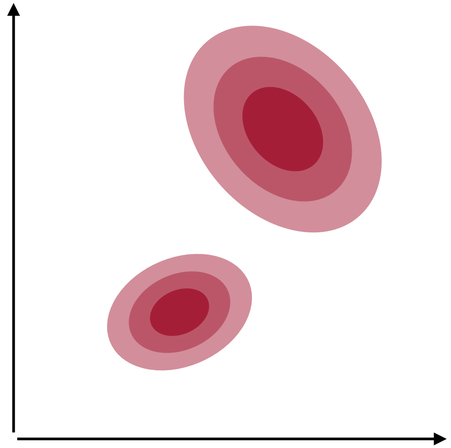
"posterior" → $p(\theta \mid x) \propto p(x \mid \theta)\ p(\theta)$

Laplace, Bayes, 1764

Bayesian parameter inference

Ideal approach

- find all parameters
- quantify uncertainty
- quantify relations between parameters



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Bayes' Theorem

"prior"

"posterior" → $p(\theta \mid x) \propto p(x \mid \theta)\ p(\theta)$

Laplace, Bayes, 1764

Bayesian parameter inference

Ideal approach

- find all parameters
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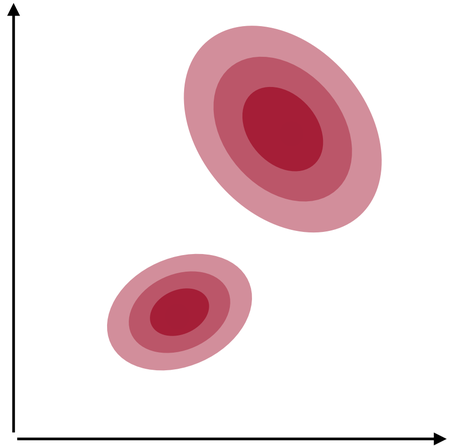

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Bayes' Theorem

"prior"

"posterior" $\rightarrow$ $p(\theta \mid x) \propto p(x \mid \theta)\ p(\theta)$

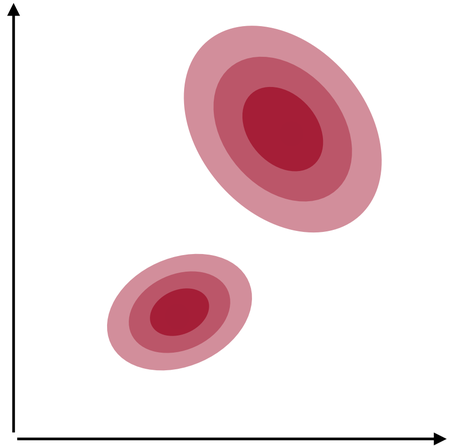
"likelihood"

Laplace, Bayes, 1764

Bayesian parameter inference

Ideal approach

- find all parameters
- quantify uncertainty
- quantify relations between parameters



- data x and parameters θ are *random variables*
- **goal**: infer a distribution over parameters $p(\theta \mid x)$
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  - quantifies uncertainty

Bayes' Theorem

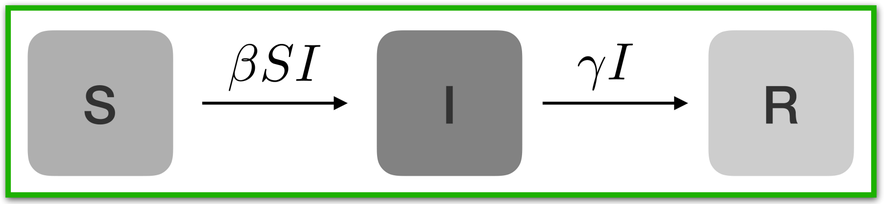
"prior"

"posterior" → $p(\theta \mid x) \propto p(x \mid \theta)\ p(\theta)$

"likelihood" = simulator

Laplace, Bayes, 1764

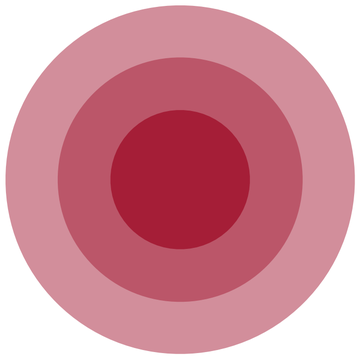
Bayesian parameter inference for simulators



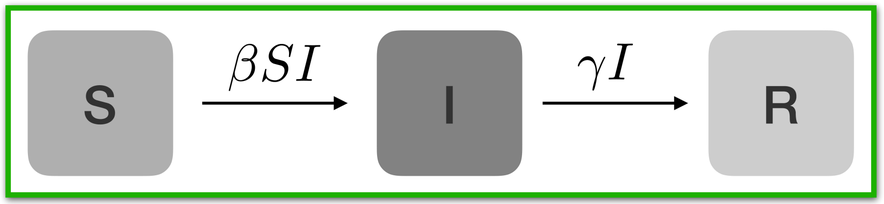
$$p(\theta \mid x) \propto p(x \mid \theta)\, p(\theta)$$

Bayesian parameter inference for simulators

parameters θ



$\theta \sim p(\theta)$



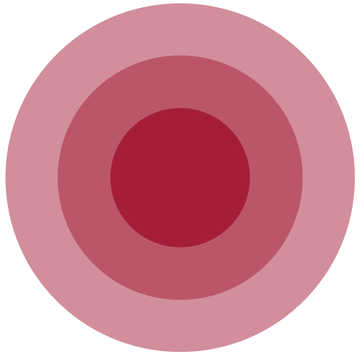
$$p(\theta \mid x) \propto p(x \mid \theta)\, p(\theta)$$

TransferLab

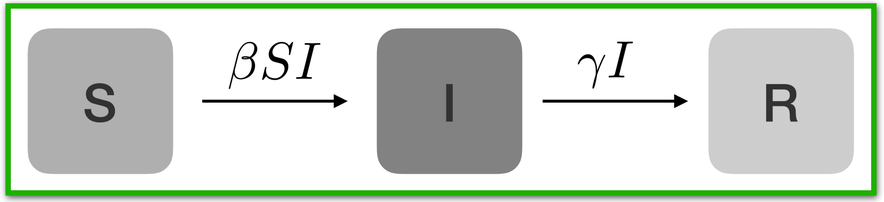
Bayesian parameter inference for simulators

simulation (forward model)

parameters θ

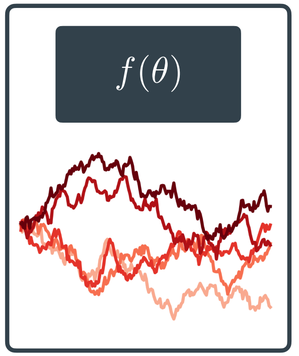


$\theta \sim p(\theta)$



$$p(\theta \mid x) \propto p(x \mid \theta)\, p(\theta)$$

data x

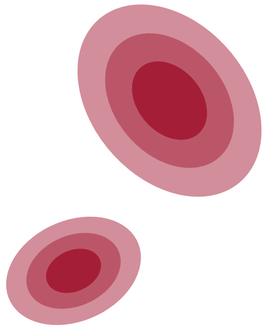


$x \sim p(x \mid \theta)$

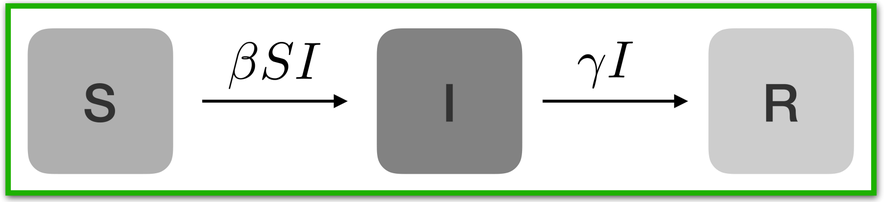
Bayesian parameter inference for simulators

simulation (forward model)

parameters θ



$p(\theta \mid x)$



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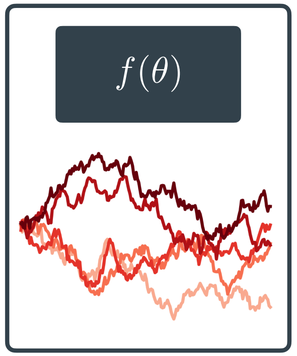
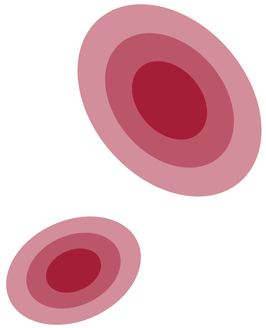


$x \sim p(x \mid \theta)$

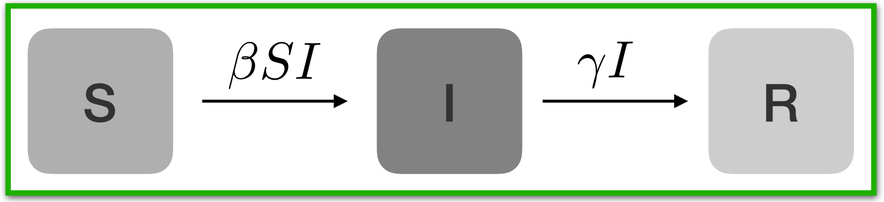
inference (inverse model)

Simulation-based Bayesian inference (SBI)

parameters θ

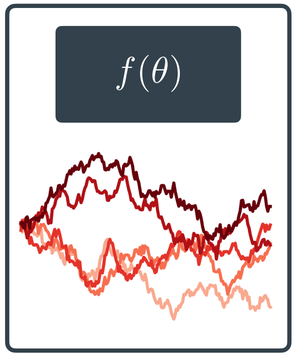


$p(\theta \mid x)$



$$p(\theta \mid x) \propto p(x \mid \theta)\, p(\theta)$$

data x

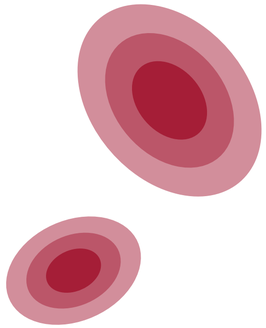


$x \sim p(x \mid \theta)$

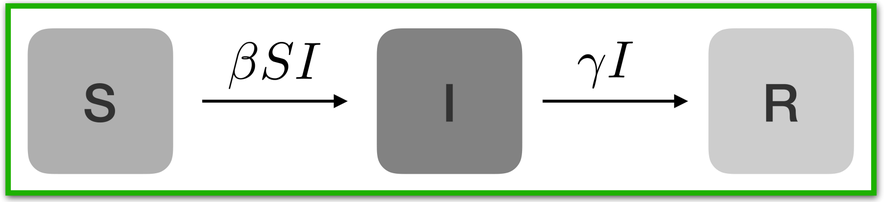
TransferLab

Simulation-based Bayesian inference (SBI)

parameters θ



$p(\theta \mid x)$



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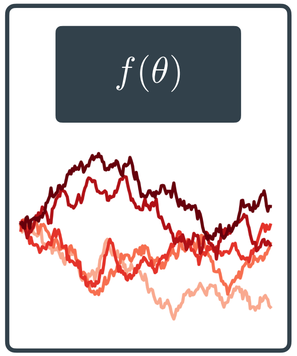
data x

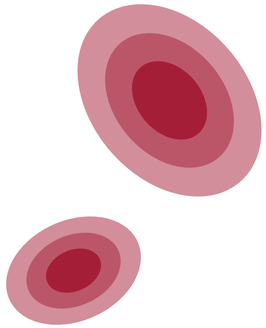


$x \sim p(x \mid \theta)$

TransferLab

Simulation-based Bayesian inference (SBI)

parameters θ



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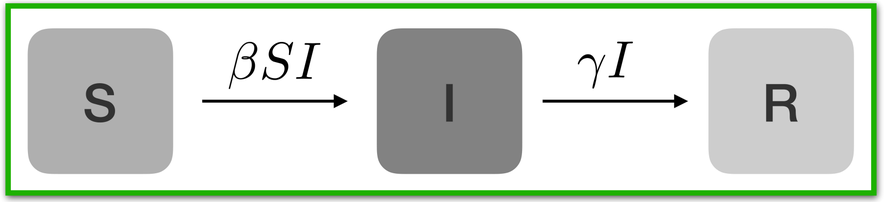

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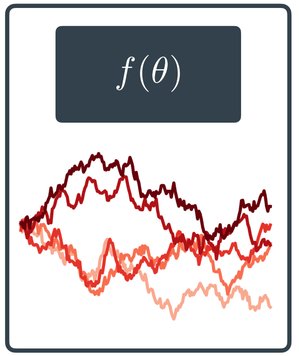


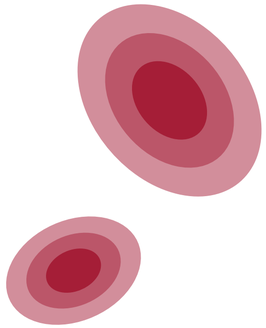
$x \sim p(x \mid \theta)$

TransferLab

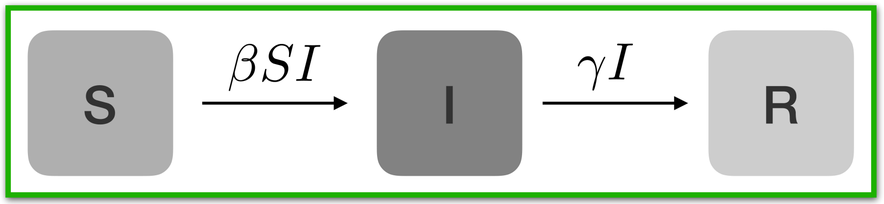
Simulation-based Bayesian inference (SBI)

parameters θ

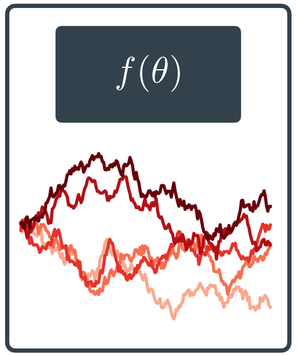
data x



$p(\theta \mid x)$



$$p(\theta \mid x) \propto p(x \mid \theta)\, p(\theta)$$



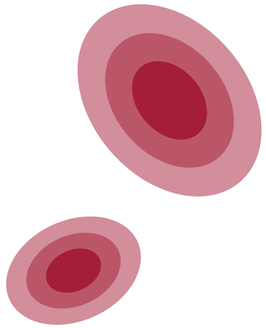
$x \sim p(x \mid \theta)$

No Markov Chain Monte Carlo (MCMC)
No variational inference
No Bayesian optimization

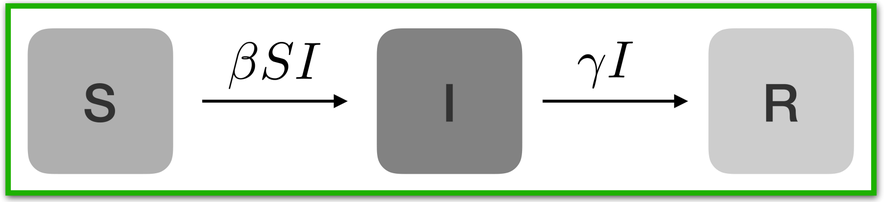
TransferLab

Simulation-based Bayesian inference (SBI)

parameters θ



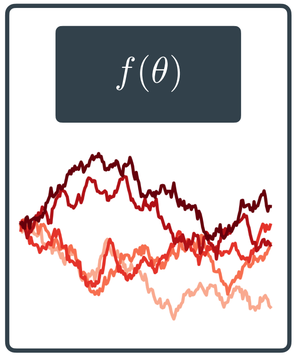
$p(\theta \mid x)$



$$\boxed{p(\theta \mid x)} \propto \boxed{p(x \mid \theta)} p(\theta)$$

use machine learning to perform inference

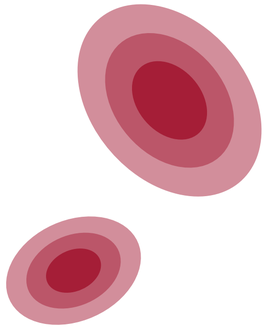
data x



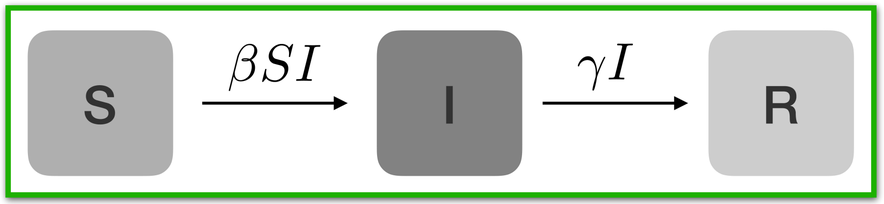
$x \sim p(x \mid \theta)$

Simulation-based Bayesian inference (SBI)

parameters θ

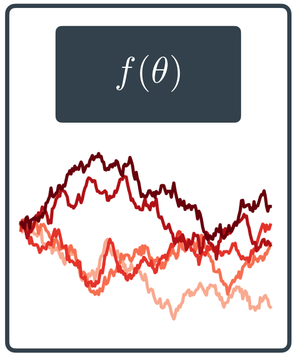


$p(\theta \mid x)$



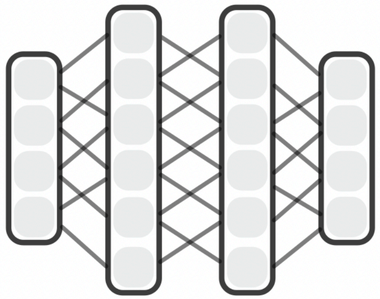
$$p(\theta \mid x) \propto p(x \mid \theta)\, p(\theta)$$

data x



$x \sim p(x \mid \theta)$

use machine learning to perform inference



training data

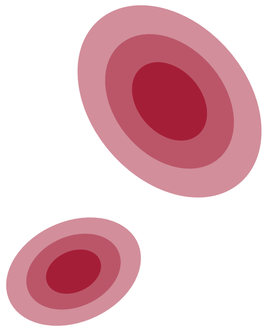
$\{(\theta_1, x_1), (\theta_2, x_2), \ldots\}$

TransferLab

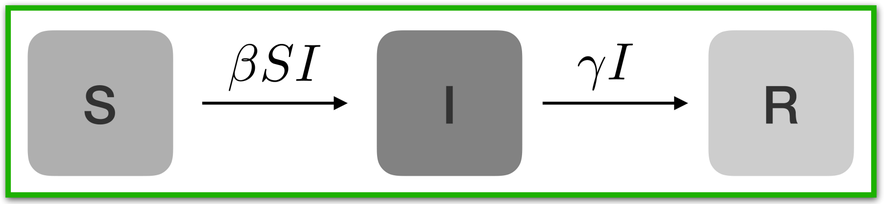
Simulation-based Bayesian inference (SBI)

simulation (forward model)

parameters θ

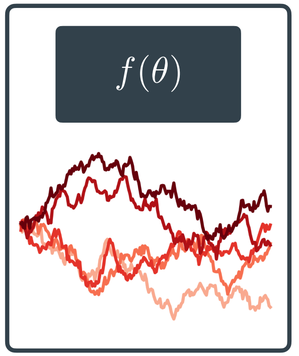


$p(\theta \mid x)$



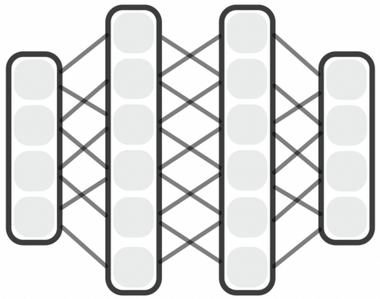
$$p(\theta \mid x) \propto p(x \mid \theta)\, p(\theta)$$

data x



$x \sim p(x \mid \theta)$

use machine learning to perform inference



training data

$\{(\theta_1, x_1), (\theta_2, x_2), \ldots\}$

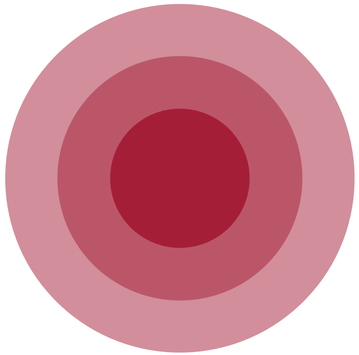
TransferLab

Outline

1. **Why** simulators?
2. **Why** Bayesian parameter inference?
3. **How** to do Bayesian inference for simulators?
4. **How** can you apply SBI to your simulator?

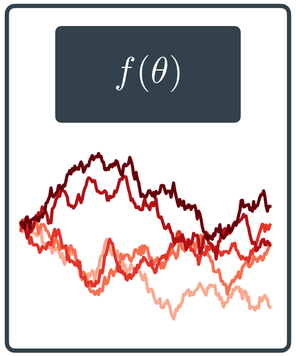
Neural Simulation-Based Inference

prior



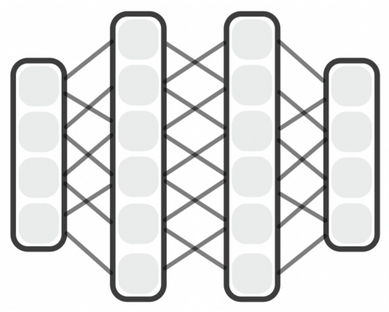
$\theta_i \sim p(\theta)$

simulated data



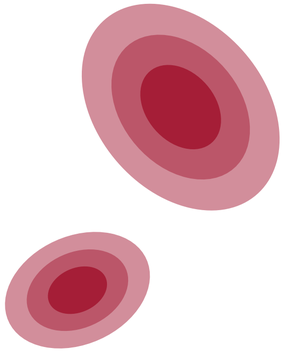
$x_i \sim p(x|\theta_i)$

density estimator



$\underset{\phi}{\operatorname{argmin}}\ \mathcal{L}(\phi)$

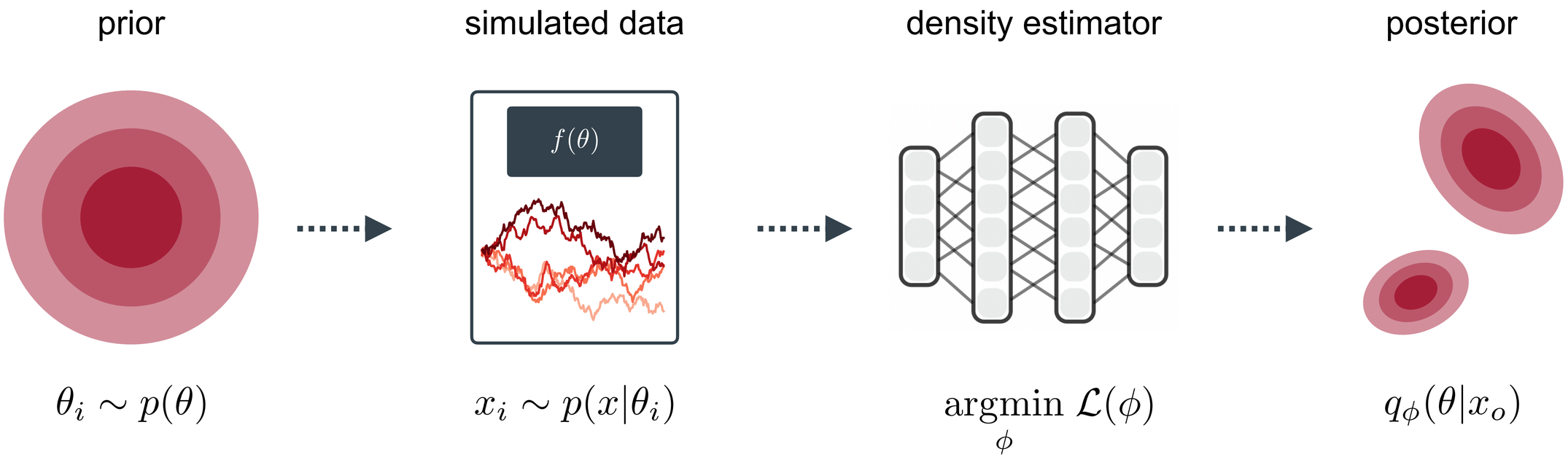
posterior



$q_\phi(\theta|x_o)$

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

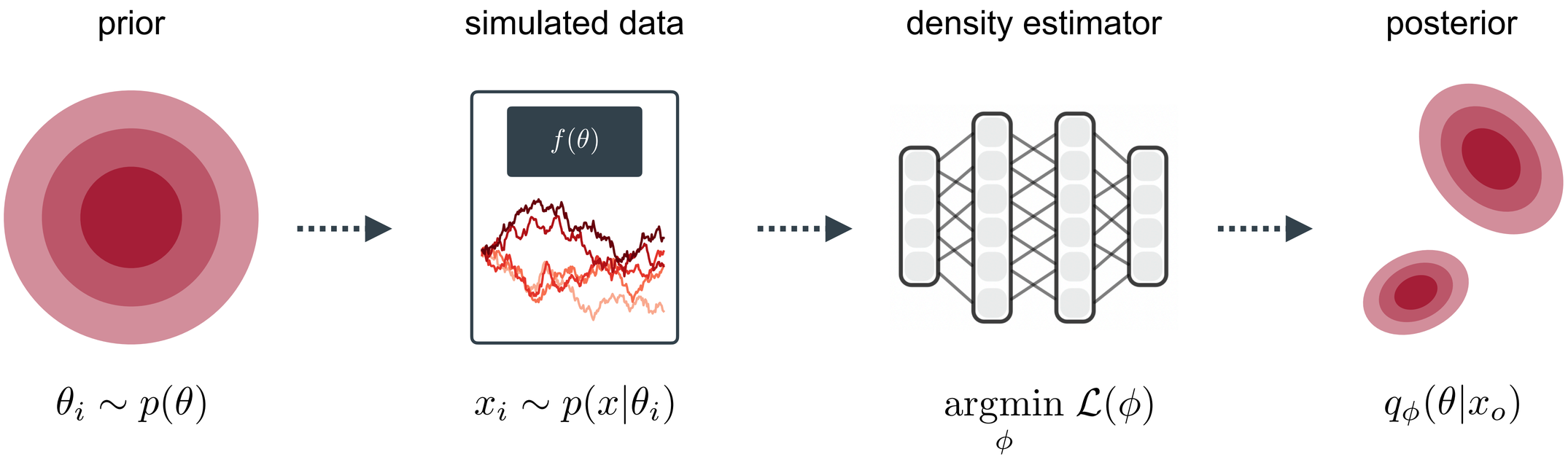
Neural Simulation-Based Inference



1. **Training**: train neural network (NN) with simulated data to learn $q_\phi(\theta \,|\, x)$

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

Neural Simulation-Based Inference



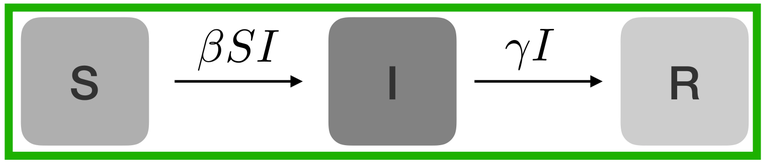
1. **Training**: train neural network (NN) with simulated data to learn $q_\phi(\theta \,|\, x)$

2. **Inference**: plug x_o into NN to obtain $q_\phi(\theta \,|\, x_o)$

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

Neural Simulation-Based Inference

Simulator



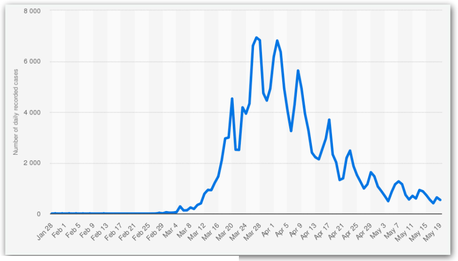
Prior

$$p(\theta) = p(\beta, \gamma)$$

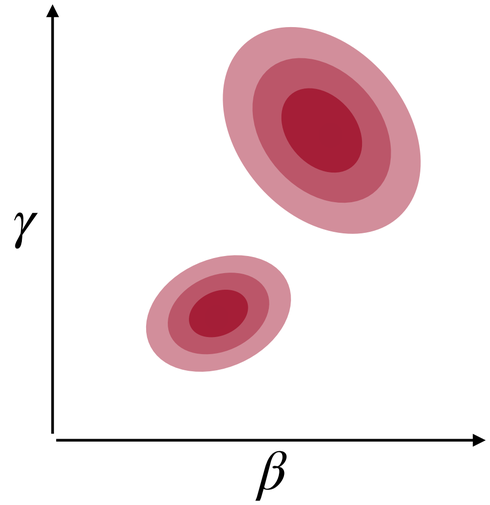
Simulated data

$$\theta_i \sim p(\theta)$$
$$x_i = \textbf{SIR}(\theta_i)$$

Observed data x_o



Conditional Density Estimation

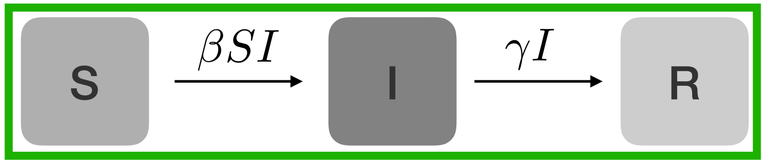


TransferLab

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

Neural Simulation-Based Inference

Simulator



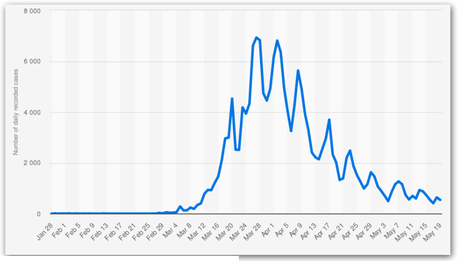
Prior

$$p(\theta) = p(\beta, \gamma)$$

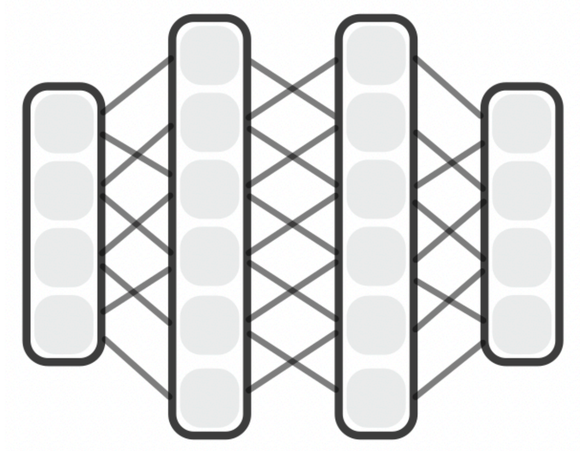
Simulated data

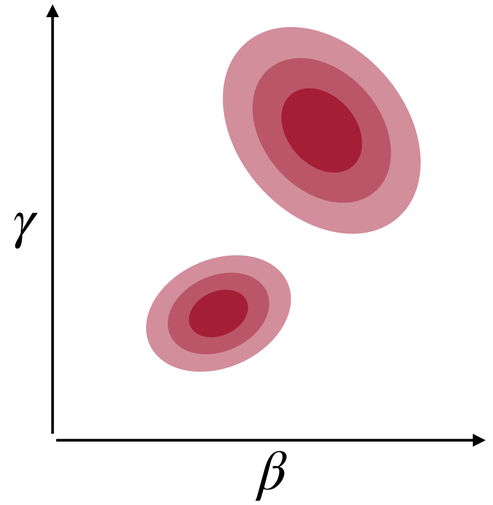
$$\theta_i \sim p(\theta)$$
$$x_i = \textbf{SIR}(\theta_i)$$

Observed data x_o



Conditional Density Estimation



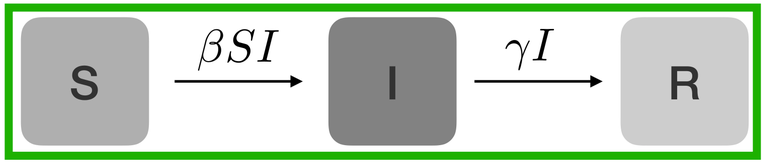


TransferLab

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

Neural Simulation-Based Inference

Simulator



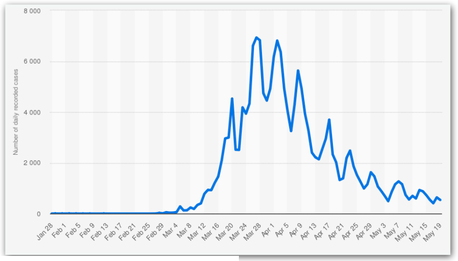
Prior

$$p(\theta) = p(\beta, \gamma)$$

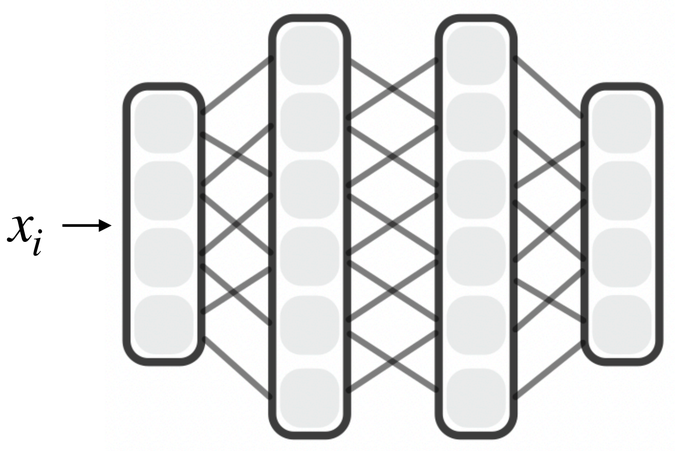
Simulated data

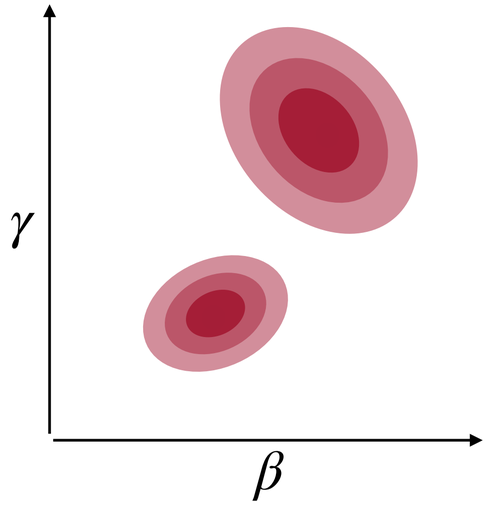
$$\theta_i \sim p(\theta)$$
$$x_i = \textbf{SIR}(\theta_i)$$

Observed data x_o



Conditional Density Estimation



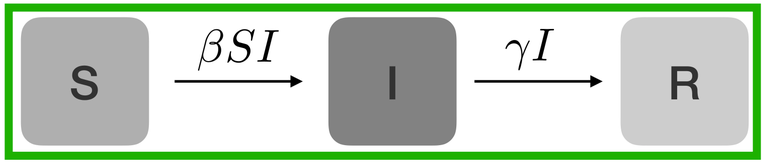


TransferLab

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

Neural Simulation-Based Inference

Simulator



Prior

$$p(\theta) = p(\beta, \gamma)$$

Simulated data

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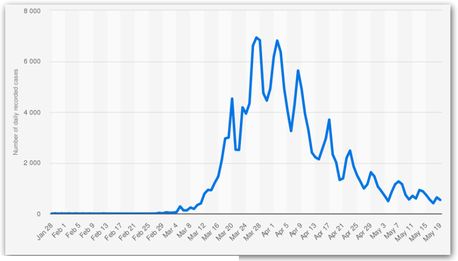
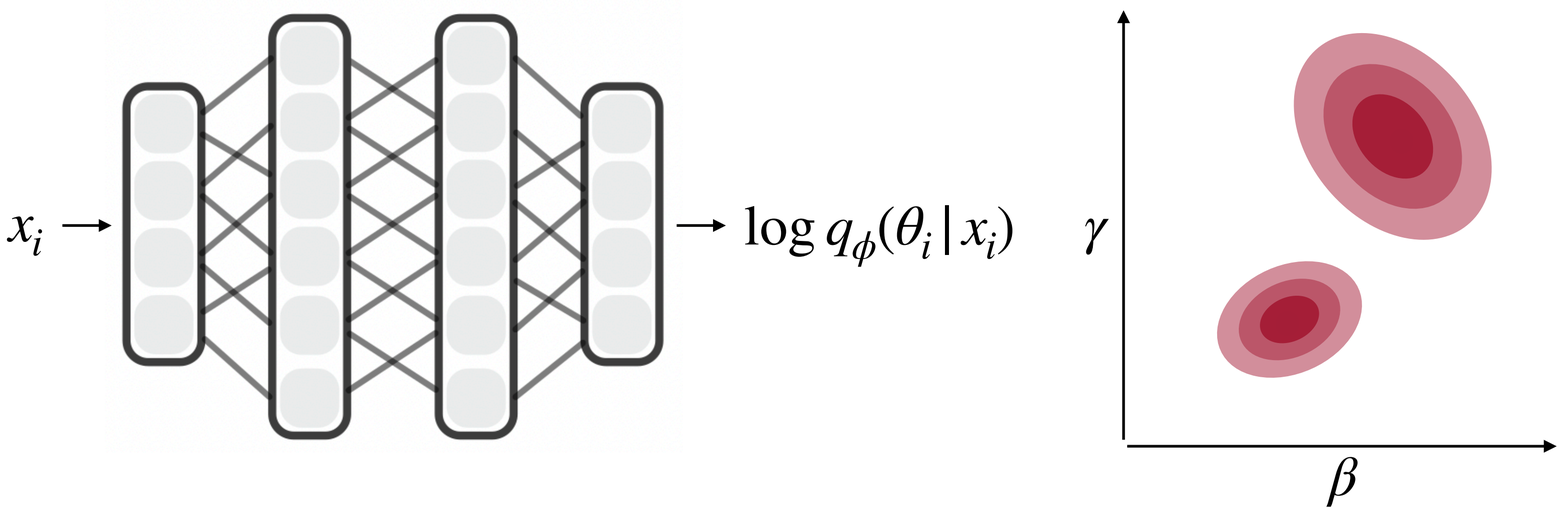
Observed data x_o



Conditional Density Estimation

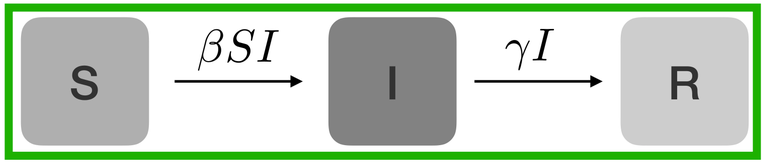


TransferLab

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

Neural Simulation-Based Inference

Simulator



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Simulated data

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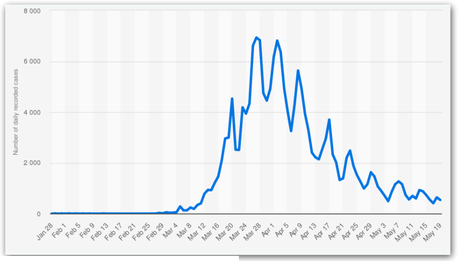
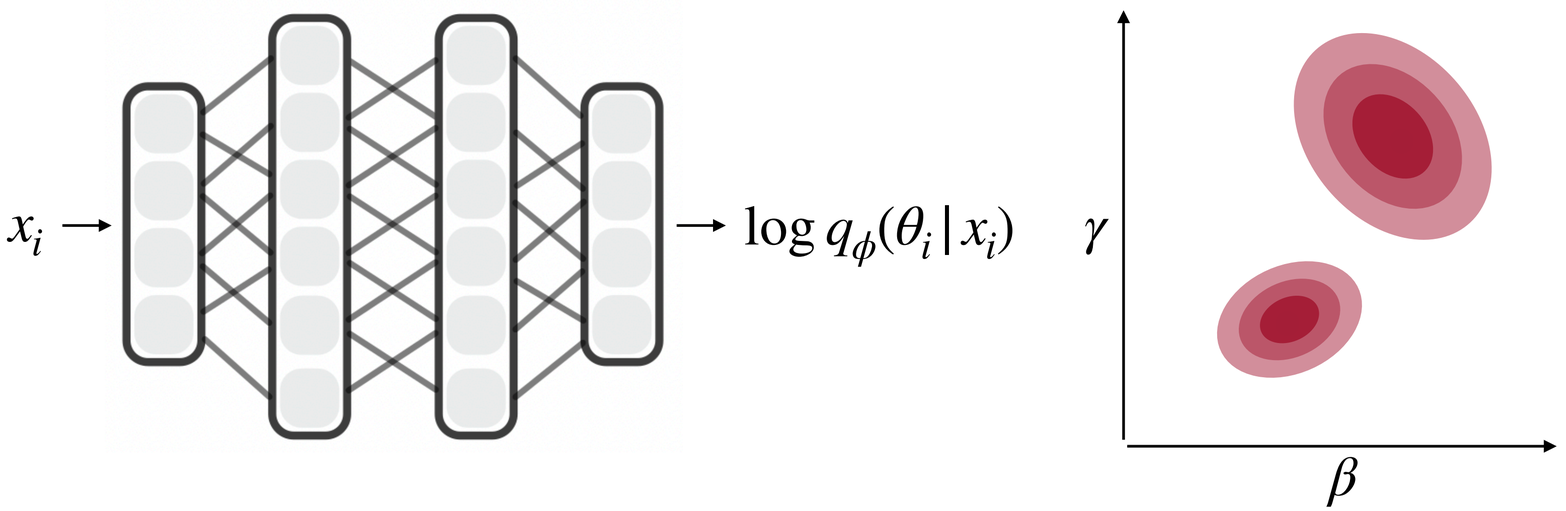
Observed data x_o



Conditional Density Estimation

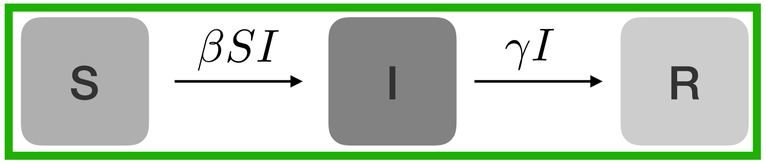


1. Train with simulated data

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

Neural Simulation-Based Inference

Simulator



Prior

$$p(\theta) = p(\beta, \gamma)$$

Simulated data

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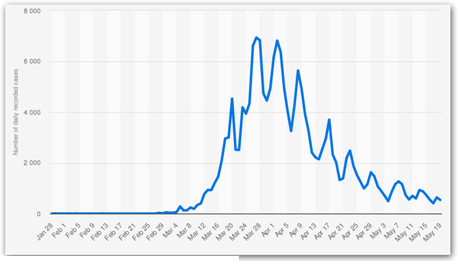
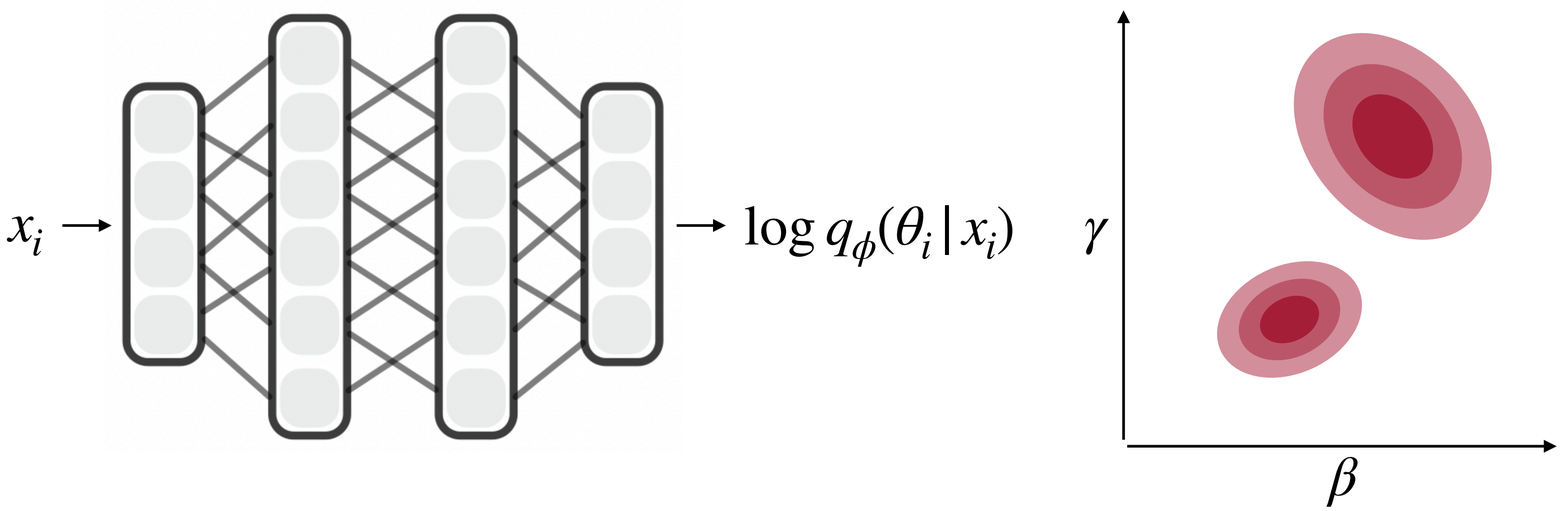
Observed data x_o



Conditional Density Estimation



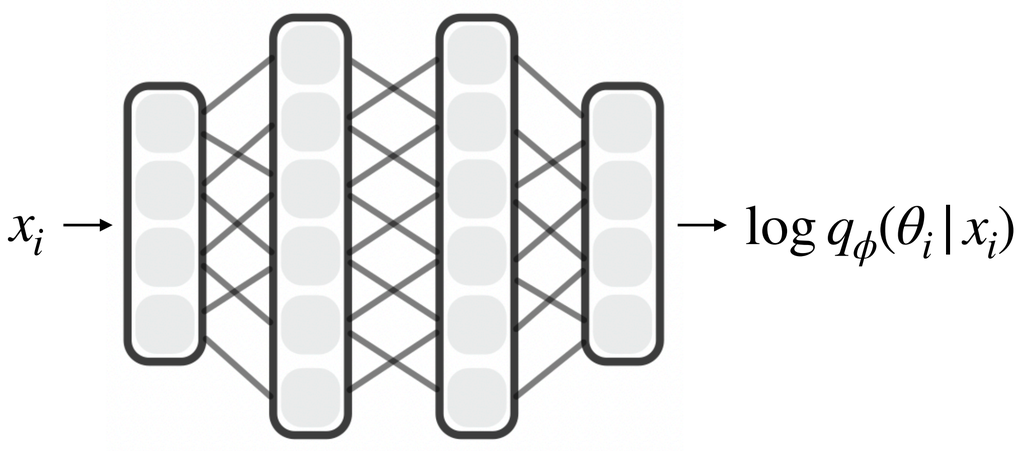
1. Train with simulated data
2. Infer given observed data

TransferLab

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

Conditional density estimation in a nutshell

Conditional Density Estimation

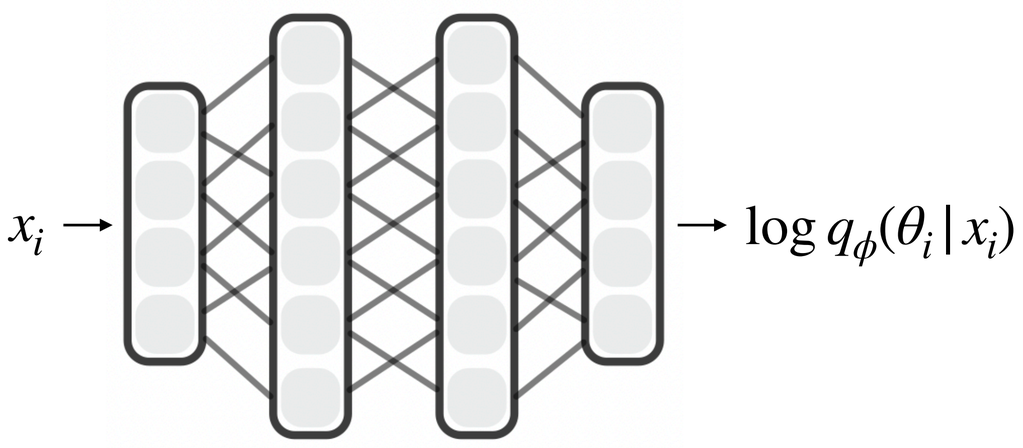


Papamakarios et al. 2016, Greenberg et al. 2019

Conditional density estimation in a nutshell

Conditional Density Estimation

- Assume a parametric model for the posterior, e.g., a Gaussian

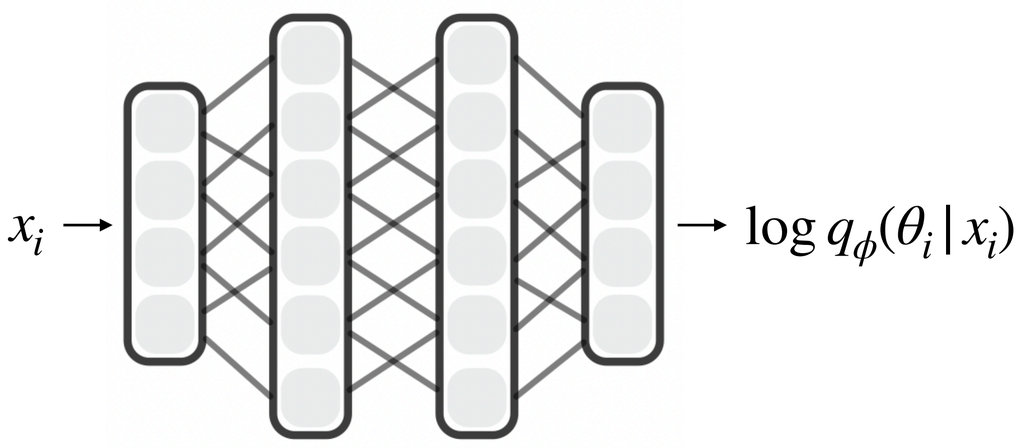


Papamakarios et al. 2016, Greenberg et al. 2019

Conditional density estimation in a nutshell

Conditional Density Estimation

- Assume a parametric model for the posterior, e.g., a Gaussian
- NN predicts Gaussian mean and variance

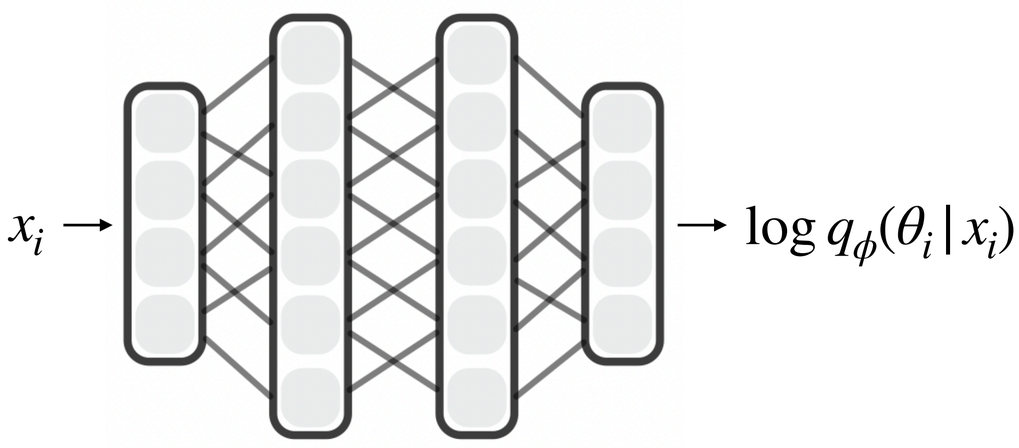


Papamakarios et al. 2016, Greenberg et al. 2019

Conditional density estimation in a nutshell

Conditional Density Estimation

- Assume a parametric model for the posterior, e.g., a Gaussian
- NN predicts Gaussian mean and variance
- Loss signal: **model probability**

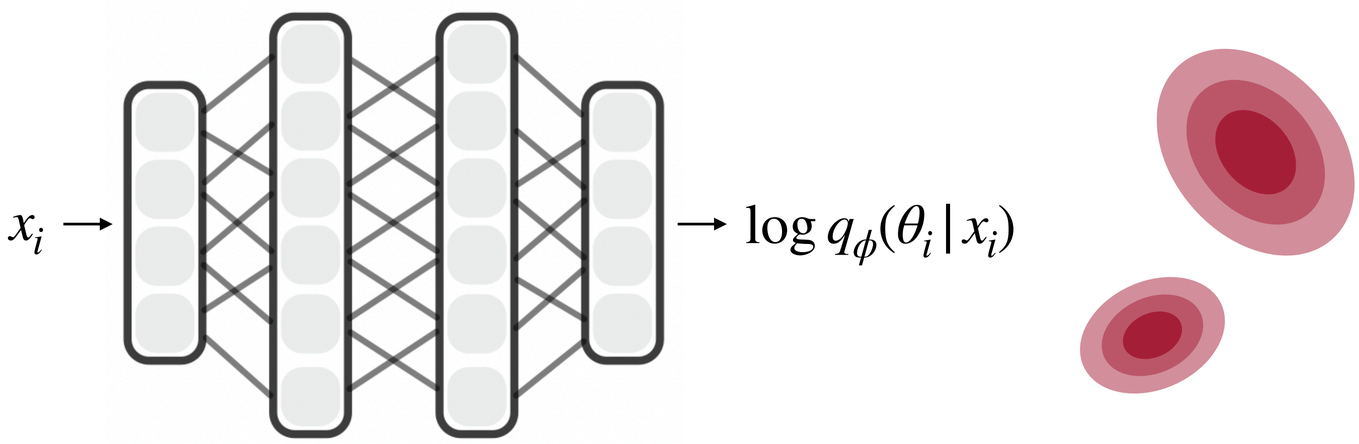


Papamakarios et al. 2016, Greenberg et al. 2019

Conditional density estimation in a nutshell

Conditional Density Estimation

- Assume a parametric model for the posterior, e.g., a Gaussian
- NN predicts Gaussian mean and variance
- Loss signal: **model probability**

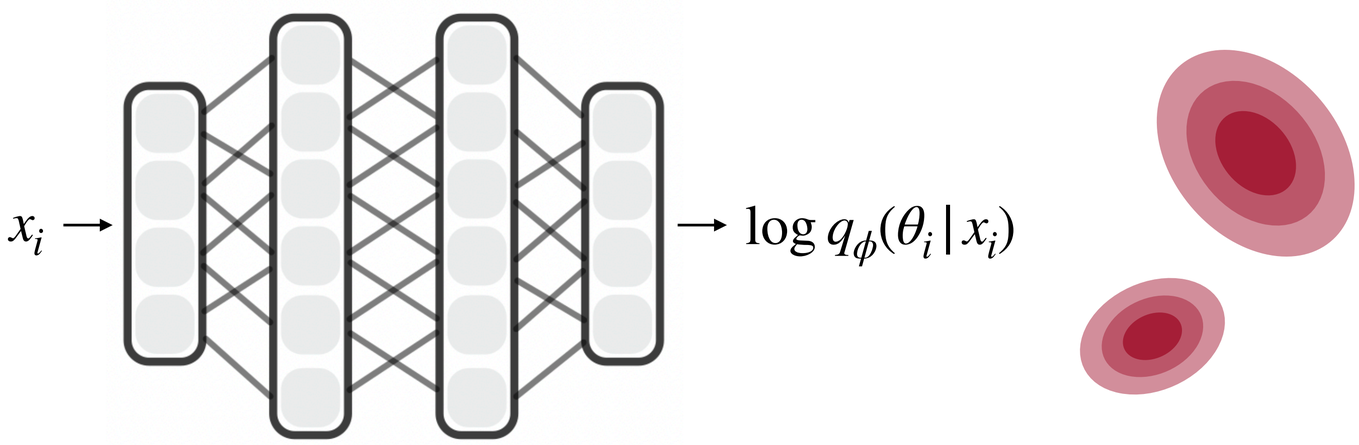


Papamakarios et al. 2016, Greenberg et al. 2019

Conditional density estimation in a nutshell

Conditional Density Estimation

- Assume a parametric model for the posterior, e.g., a Gaussian
- NN predicts Gaussian mean and variance
- Loss signal: **model probability**
- Used in practice:
  - Mixture of Gaussians
  - Normalizing Flows
  - (Flow Matching, Score Matching)



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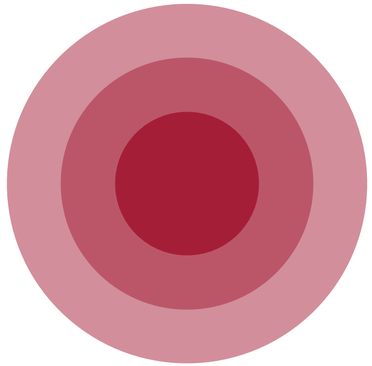
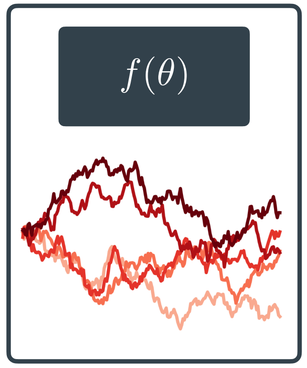
Three main neural SBI approaches

prior



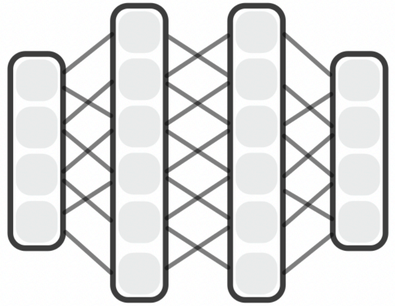
$\theta_i \sim p(\theta)$

simulated data



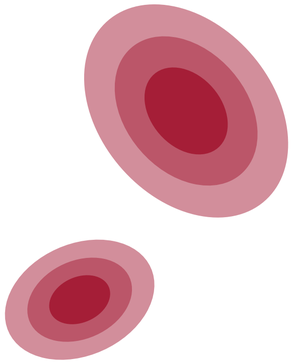
$x_i \sim p(x|\theta_i)$

density estimator



$\underset{\phi}{\text{argmin}}\ \mathcal{L}(\phi)$

posterior

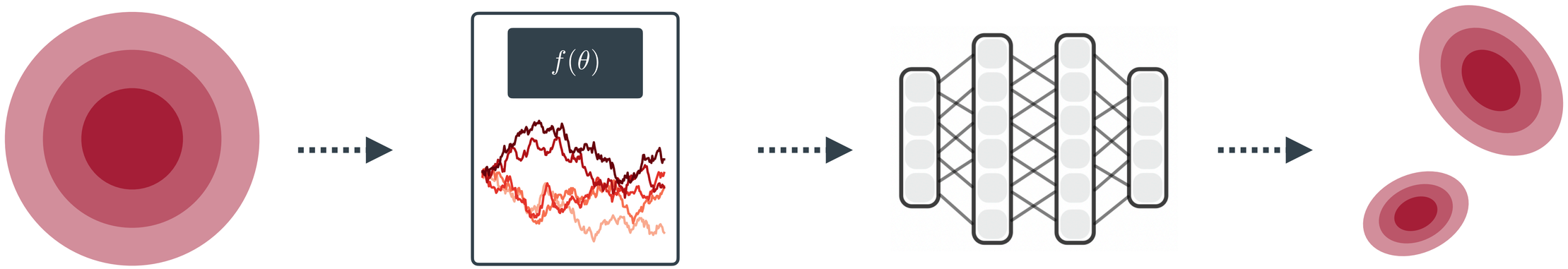


$q_\phi(\theta|x_o)$

Papamakarios et al. 2016, 2018; Hermans et al. 2020

Three main neural SBI approaches

prior | simulated data | density estimator | posterior



$\theta_i \sim p(\theta)$ $\quad x_i \sim p(x|\theta_i)$ $\quad \underset{\phi}{\text{argmin}}\ \mathcal{L}(\phi)$ $\quad q_\phi(\theta|x_o)$

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Papamakarios et al. 2016, 2018; Hermans et al. 2020

Three main neural SBI approaches

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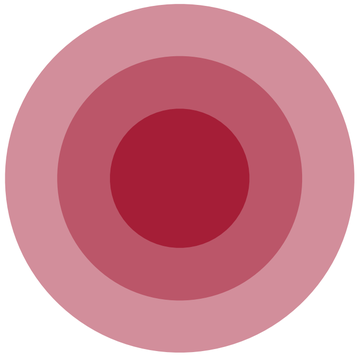
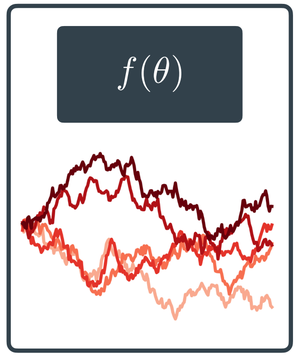


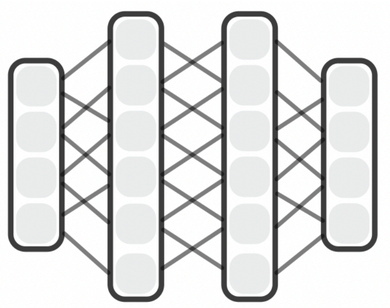
$\theta_i \sim p(\theta)$

simulated data



$\{\theta_i, x_i\}_{i=1}^{N}$

density estimator



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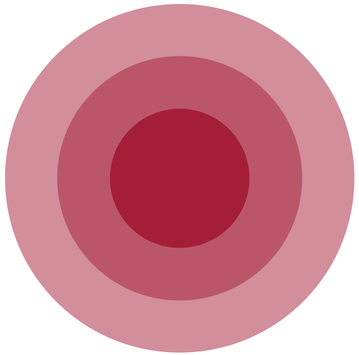

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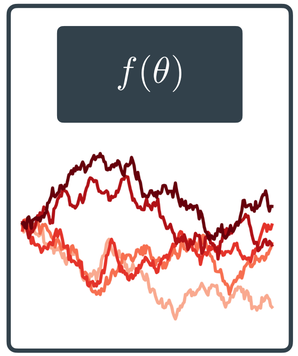

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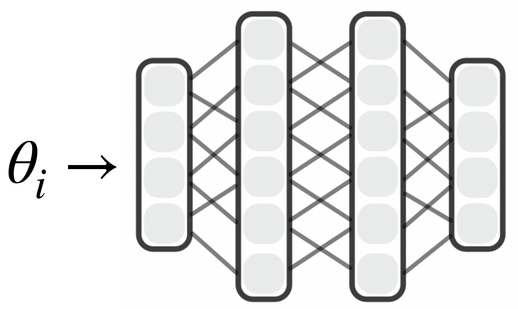

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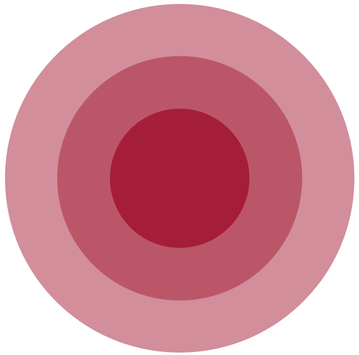

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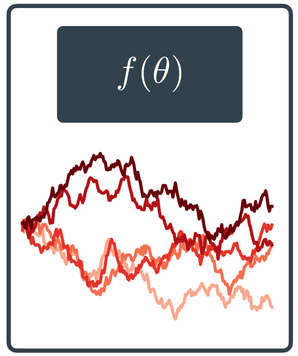

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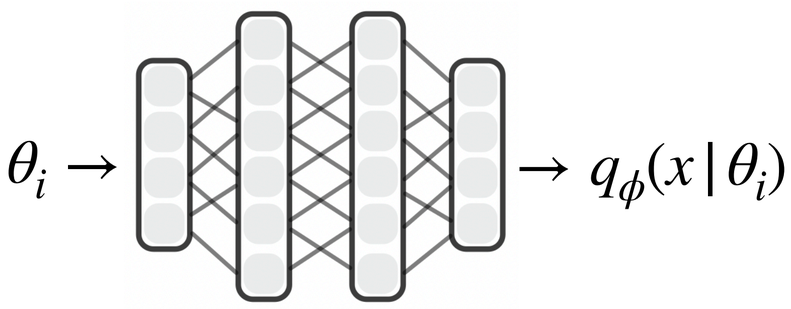

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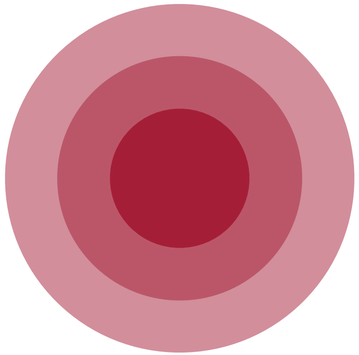

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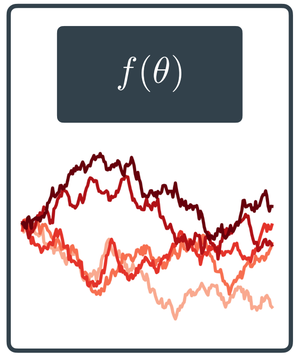

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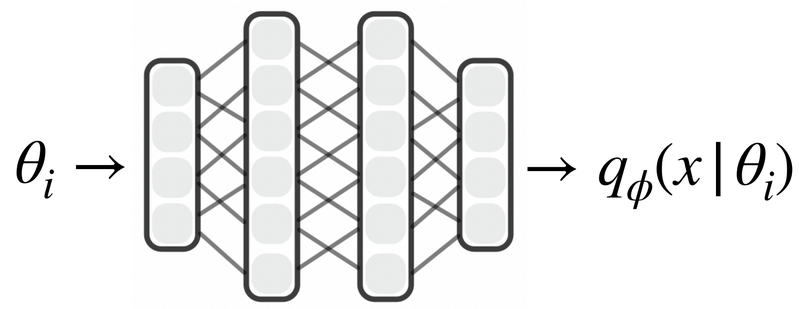

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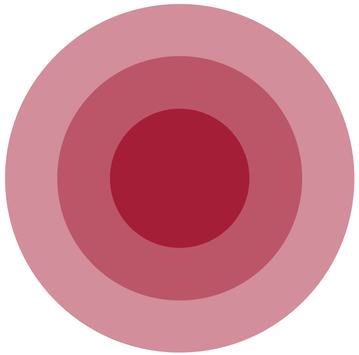

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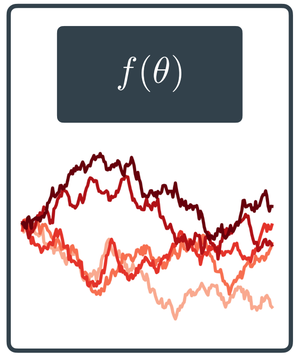

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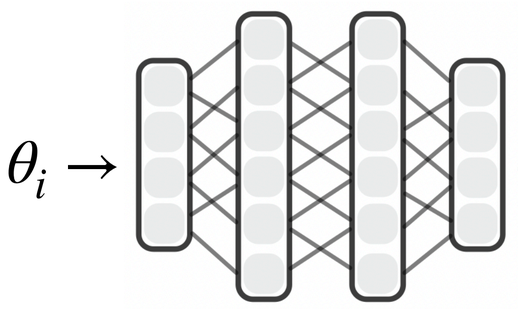
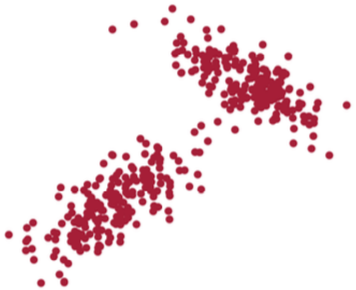


$\underset{\phi}{\operatorname{argmin}} \mathcal{L}(\phi)$

posterior



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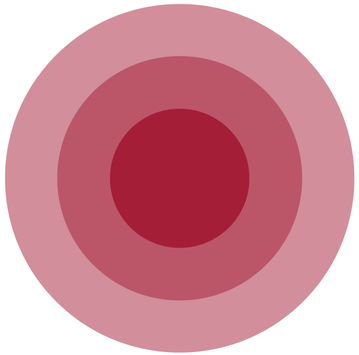

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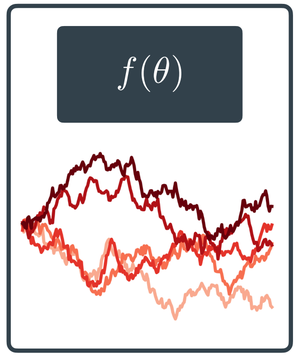

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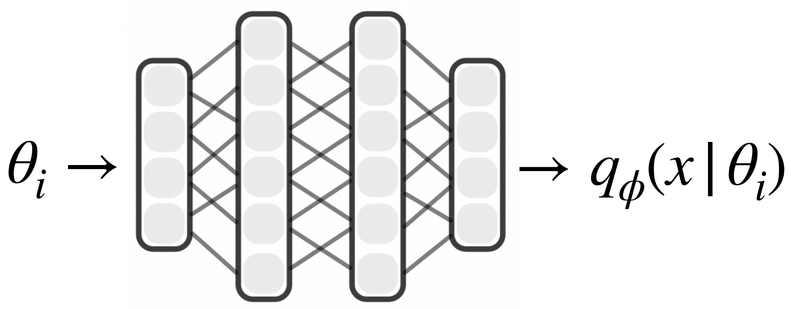

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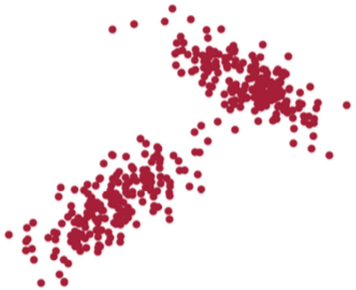

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3. **Neural Ratio Estimation** (NRE): learn the likelihood ratio $r(x \mid \theta)$, run MCMC to sample from $p(\theta \mid x_o)$

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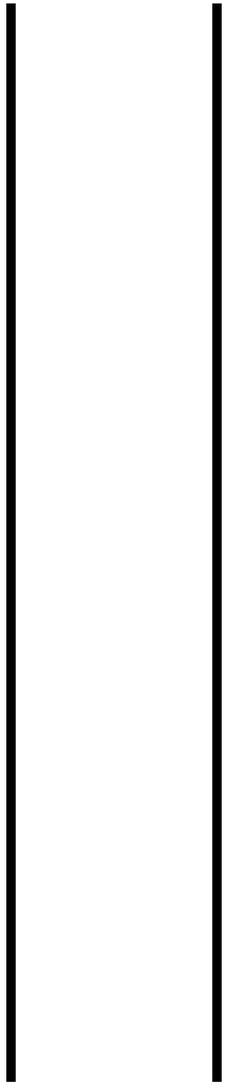
Outline

1. **Why** simulators?
2. **Why** Bayesian parameter inference?
3. **How** to do Bayesian inference for simulators?
4. **How** can you apply SBI to your simulator?

Mind the Gap: Methods and Applicability of SBI



Tejero-Cantero, Boelts*, Deistler*, Lueckmann*, Durkan* et al. 2020*

Mind the Gap: Methods and Applicability of SBI

NPE, NLE, NRE

SNLE, SNPE, SNRE

diffusion models

flow matching

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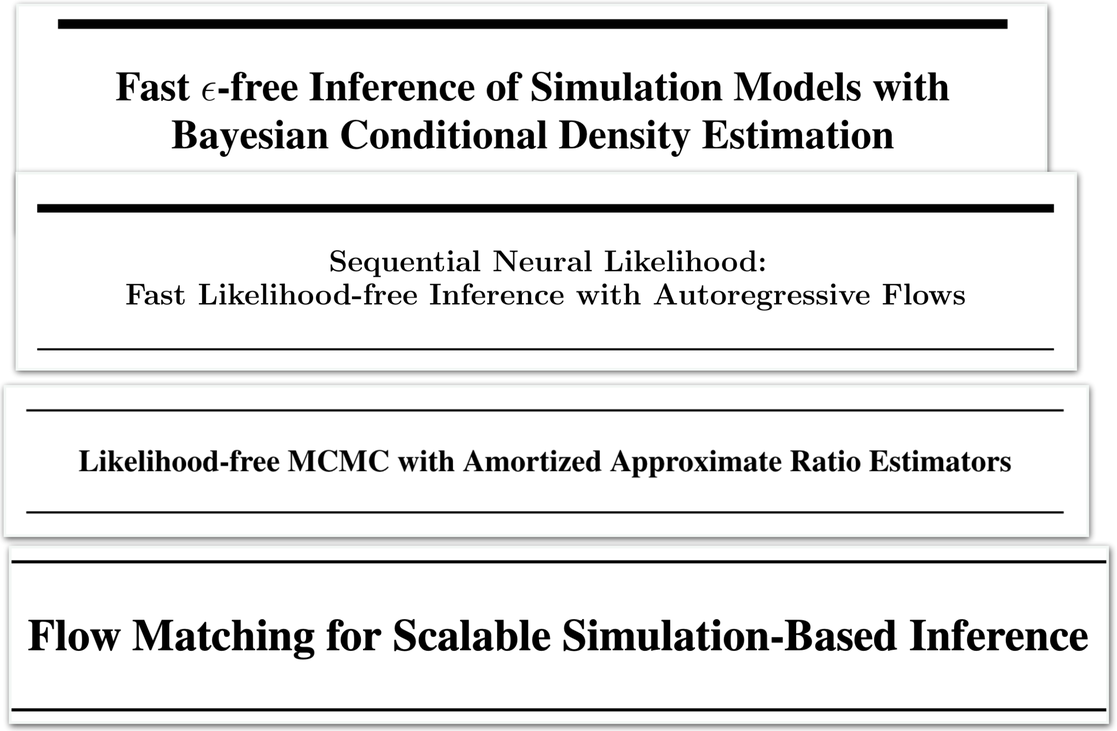

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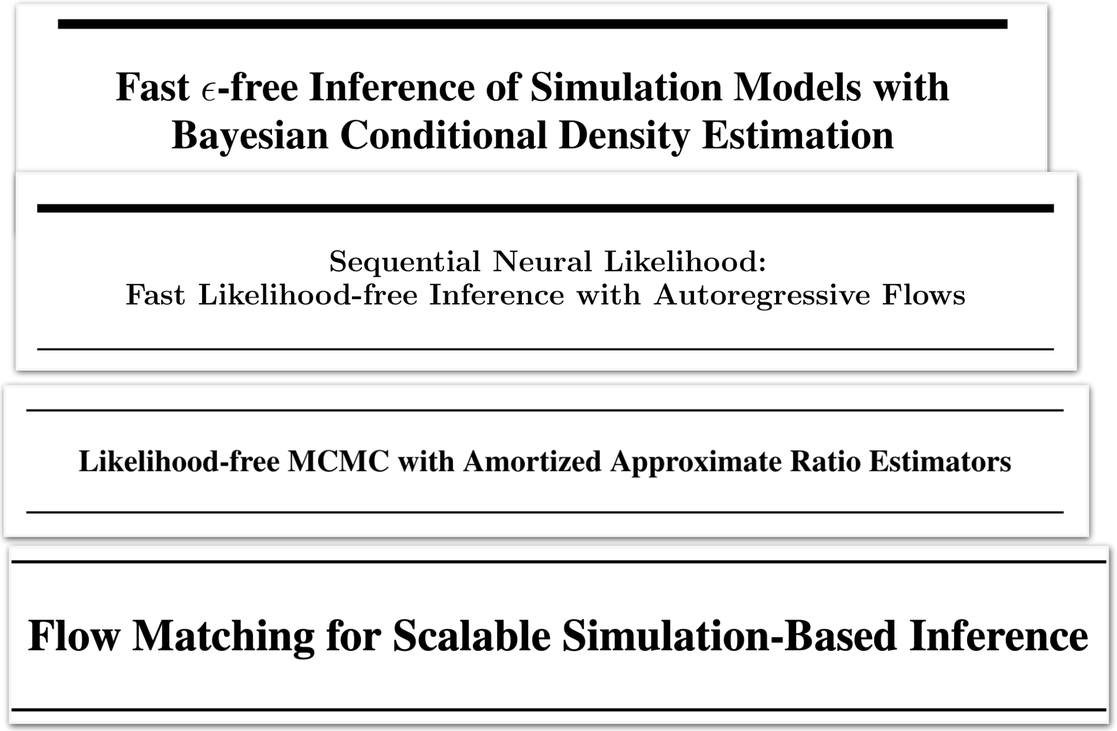

- Which method to use?
- How to use it?
- Is there usable code?
- How does it compare to other methods
- …

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Fast ϵ-free Inference of Simulation Models with Bayesian Conditional Density Estimation

Sequential Neural Likelihood:
Fast Likelihood-free Inference with Autoregressive Flows

Likelihood-free MCMC with Amortized Approximate Ratio Estimators

Flow Matching for Scalable Simulation-Based Inference

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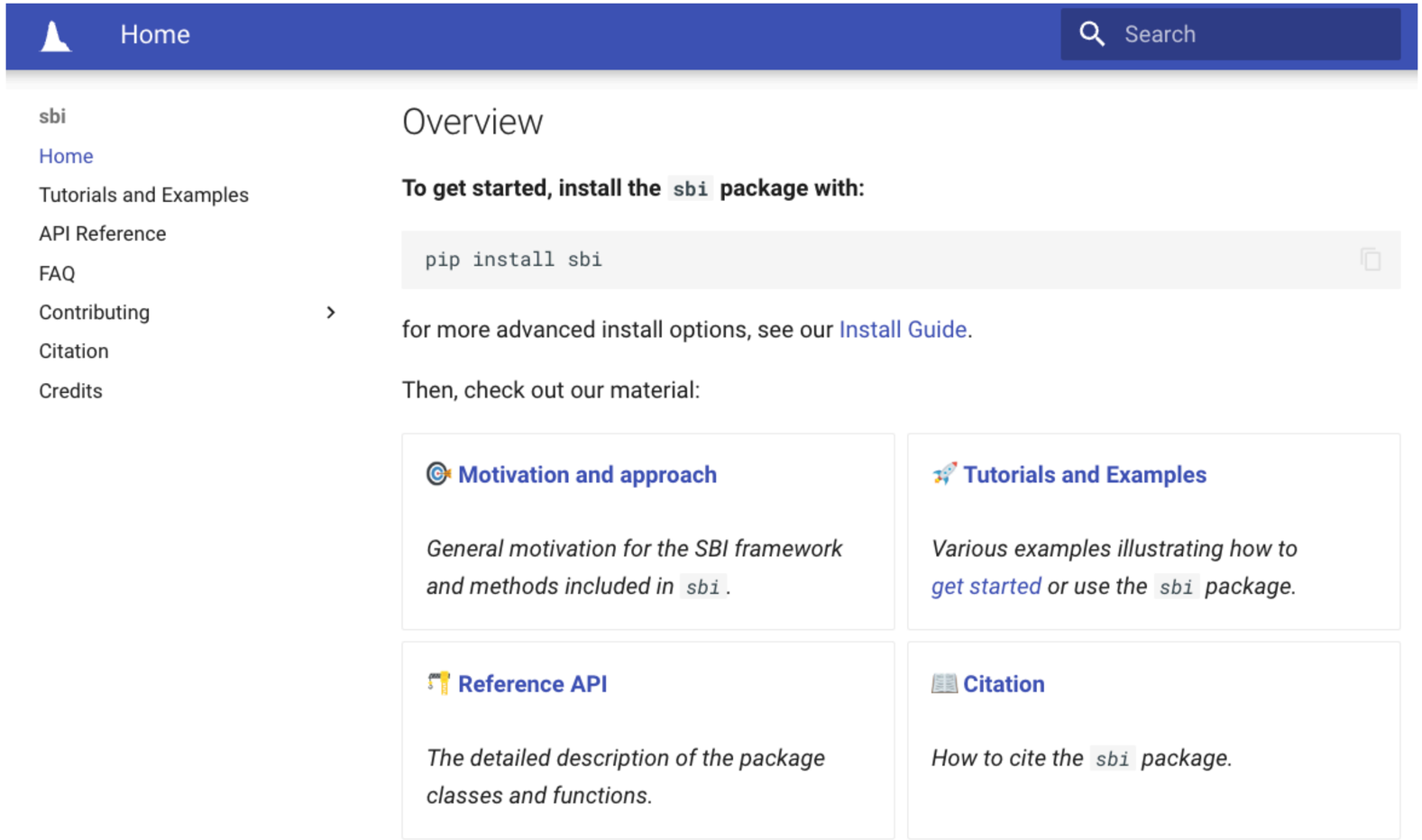
Flow Matching for Scalable Simulation-Based Inference

```python
import torch
from sbi.inference import NPE

# define shifted Gaussian simulator.
def simulator(θ):
  return θ + torch.randn_like(θ)

# draw parameters from Gaussian prior.
θ = torch.randn(1000, 2)
# simulate data
x = simulator(θ)

# choose sbi method and train
inference = NPE()
inference.append_simulations(θ, x).train()

# do inference given observed data
x_o = torch.ones(2)
posterior = inference.build_posterior()
samples = posterior.sample((1000,), x=x_o)
```

TransferLab

Tejero-Cantero, Boelts*, Deistler*, Lueckmann*, Durkan* et al. 2020*

An accessible toolkit for applying SBI



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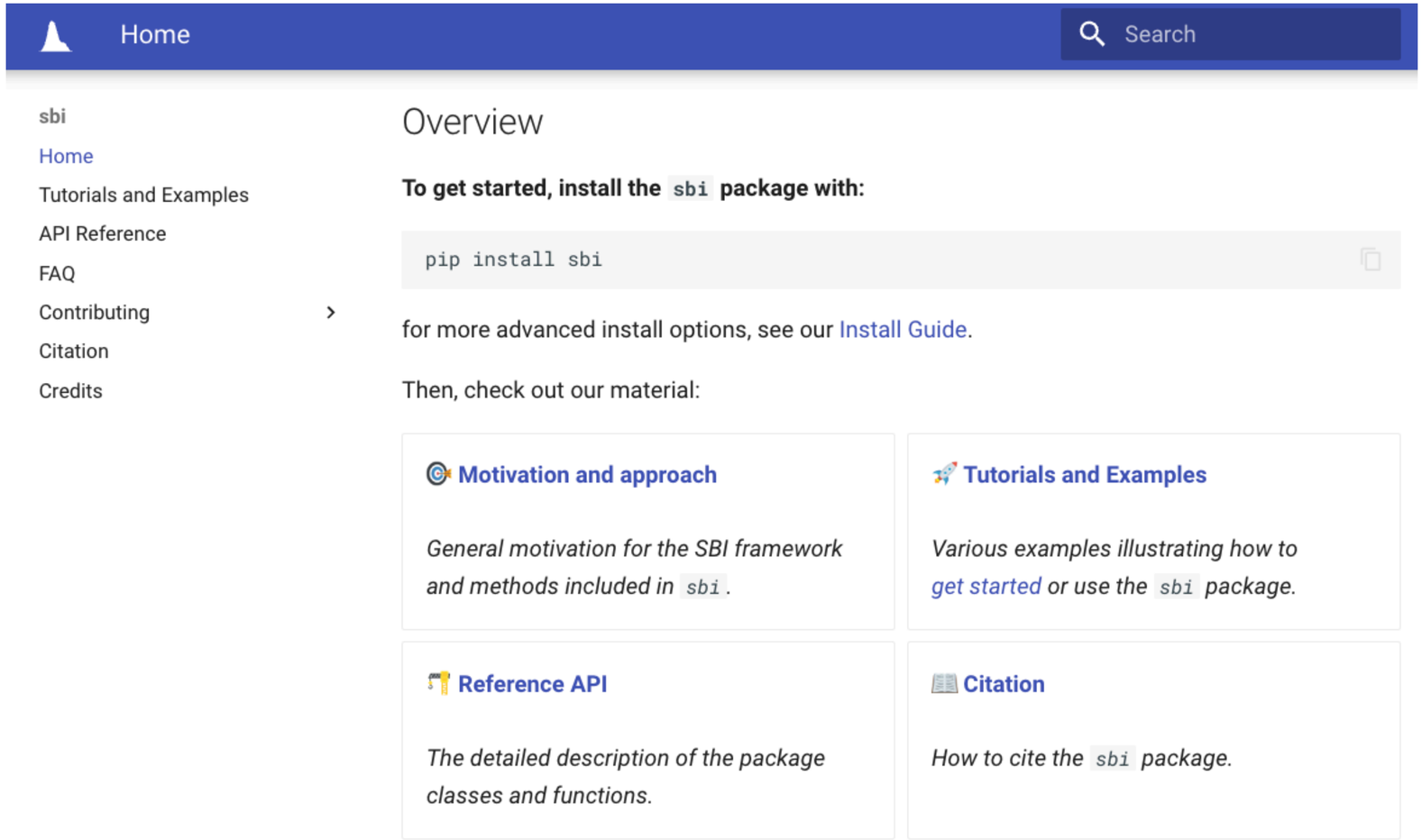

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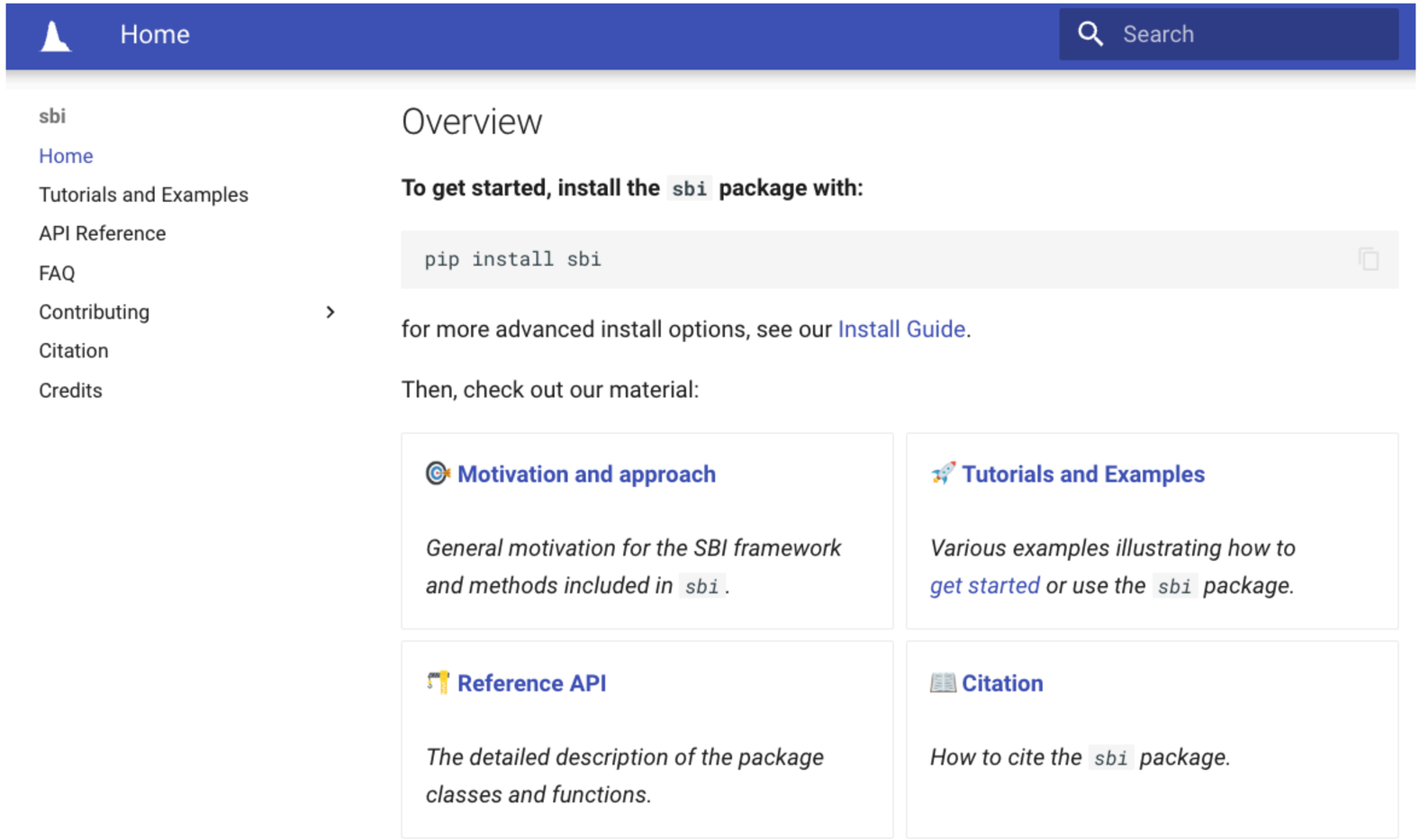
- Thorough documentation
- Tutorials and examples
- Issues, discussions



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Demo: SBI on the SIR model

SBI toolkit has been adopted by the community

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Article

A biophysical account of multiplication by a single neuron

PNAS RESEARCH ARTICLE | NEUROSCIENCE

Energy-efficient network activity from disparate circuit parameters

Michael Deistler[a], Jakob H. Macke[a,b,1,2], and Pedro J. Gonçalves[a,c,1,2]

ELSEVIER

Neural Networks

Volume 163, June 2023, Pages 178-194

Amortized Bayesian inference on generative dynamical network models of epilepsy using deep neural density estimators

Journal of Neural Engineering

PAPER

Fast inference of spinal neuromodulation for motor control using amortized neural networks

Using simulation-based inference to determine the parameters of an integrated hydrologic model: a case study from the upper Colorado River basin

Calibrating Agent-based Models to Microdata with Graph Neural Networks

Farmer[1 2 4] Sebastian M. Schmon[3 5]

THE ASTROPHYSICAL JOURNAL

OPEN ACCESS

Calibrating Cosmological Simulations with Implicit Likelihood Inference Using Galaxy Growth Observables

Bayesian Object Models for Robotic Interaction with Differentiable Probabilistic Programming

Krishna Murthy Jatavallabhula, Miles

Proceedings of The 6th Conference on

Neural simulation-based inference approach for characterizing the Galactic Center γ-ray excess

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Phys. Rev. D **105**, 063017 – Published 23 March 2022

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>50 contributors

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… Farmer [1 2 4] Sebastian M. Schmon [3 5]

THE ASTROPHYSICAL JOURNAL

OPEN ACCESS

Calibrating Cosmological Simulations with Implicit Likelihood Inference Using Galaxy Growth Observables

Bayesian Object Models for Robotic Interaction with Differentiable Probabilistic Programming

Krishna Murthy Jatavallabhula, Miles …

Proceedings of The 6th Conference on …

Neural simulation-based inference approach for characterizing the Galactic Center γ-ray excess

Siddharth Mishra-Sharma and Kyle Cranmer

Phys. Rev. D **105**, 063017 – Published 23 March 2022

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New contributors welcome!

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OPEN CODE = BETTER SCIENCE

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  - **Tomorrow** 9am-11am “New Contributor Sprint”

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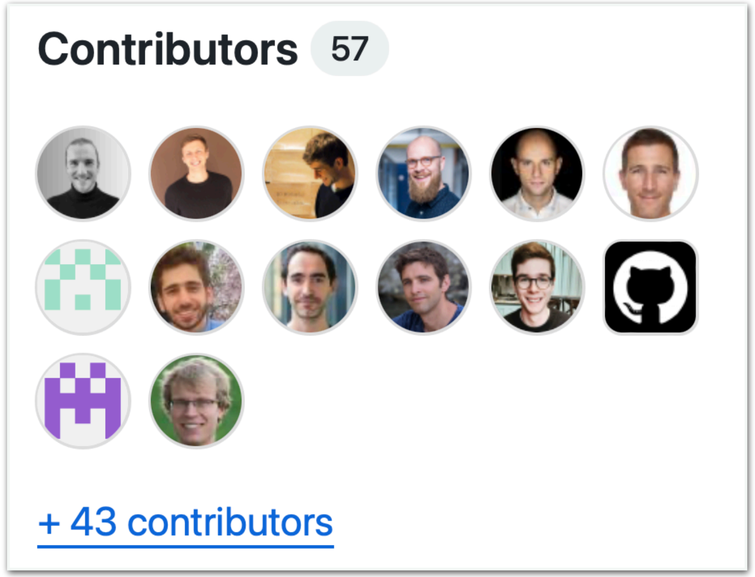
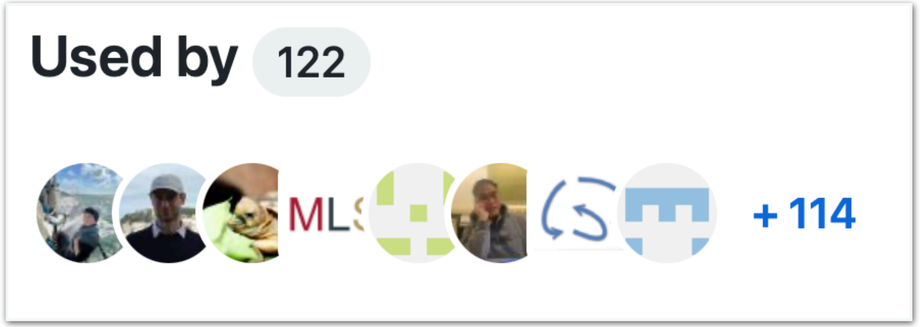
  - Spring 2025: SBI Hackathon & Workshop

Acknowledgments





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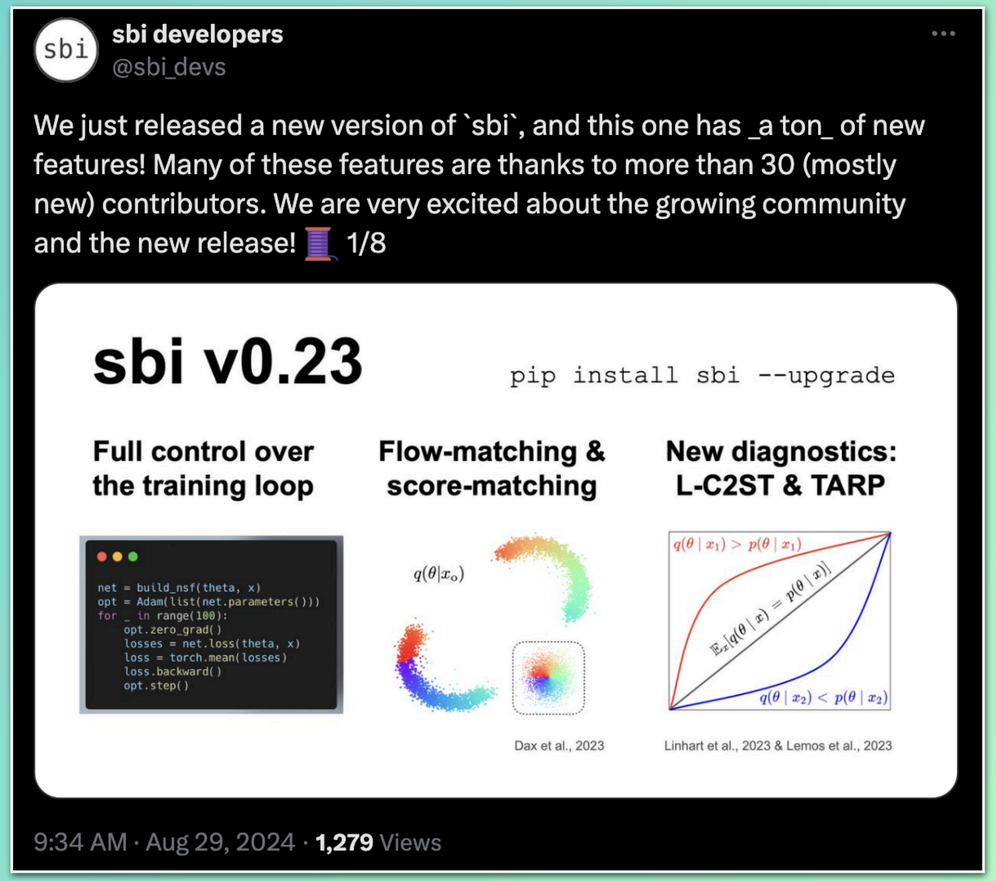
Thank you!

Questions?

Try it out: **pip install sbi**
GitHub: github.com/sbi-dev/sbi

X, Mastodon: @sbi_devs

TransferLab website: transferlab.ai



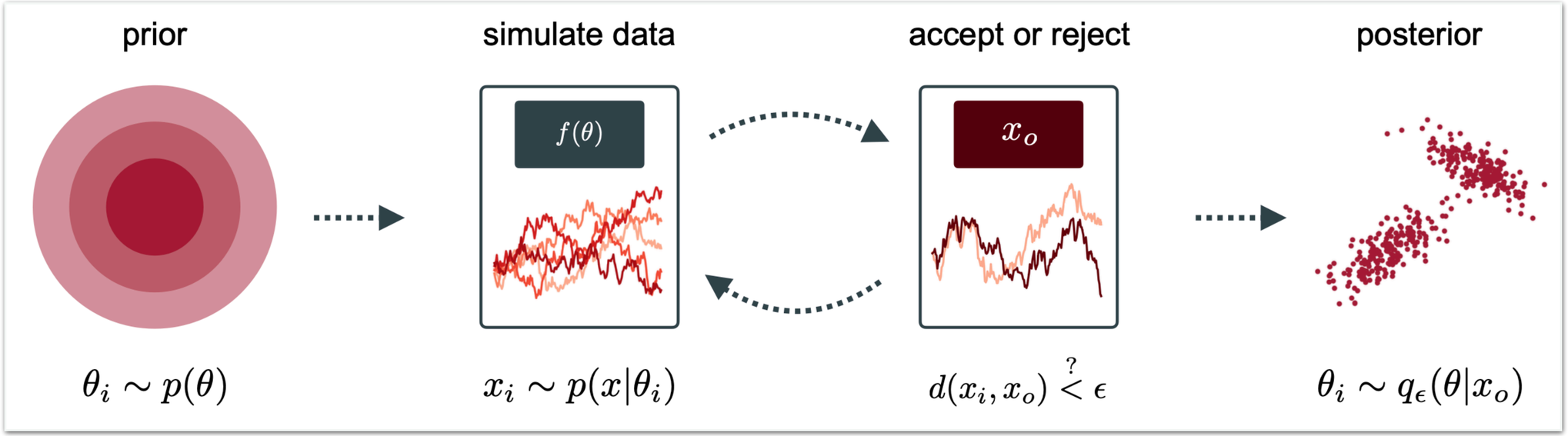
Supplementary slides

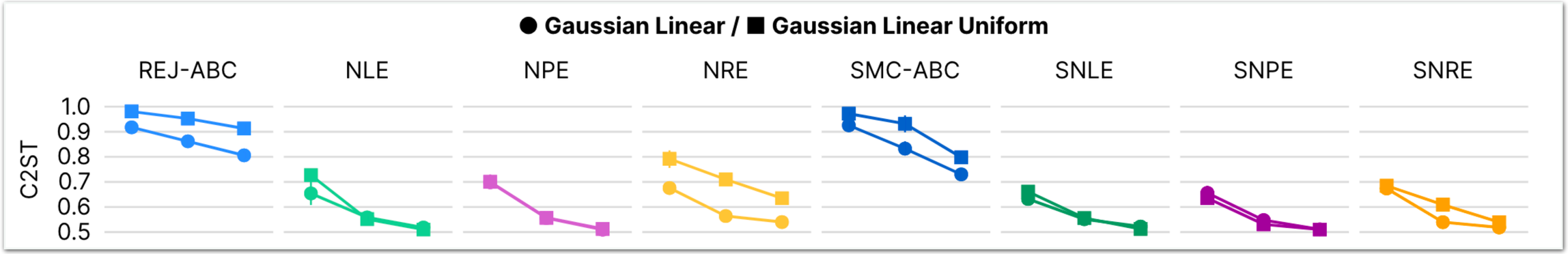
Is SBI for you?

Some heuristics

- Has been applied to simulators with ~10 parameters, ~100 in some cases
- Depends on how much data you can generate: runtime ~sec
- High-dimensional data can be embedded: CNNs, RNNs, transformers etc.
- Different methods for different settings: i.i.d. data, hierarchical models, amortized inference, sequential inference

Approximate Bayesian Computation (ABC)





Diggle et al. 1984; Beaumont et al. 2002; Sisson et al. 2008; Lueckmann et al. 2021

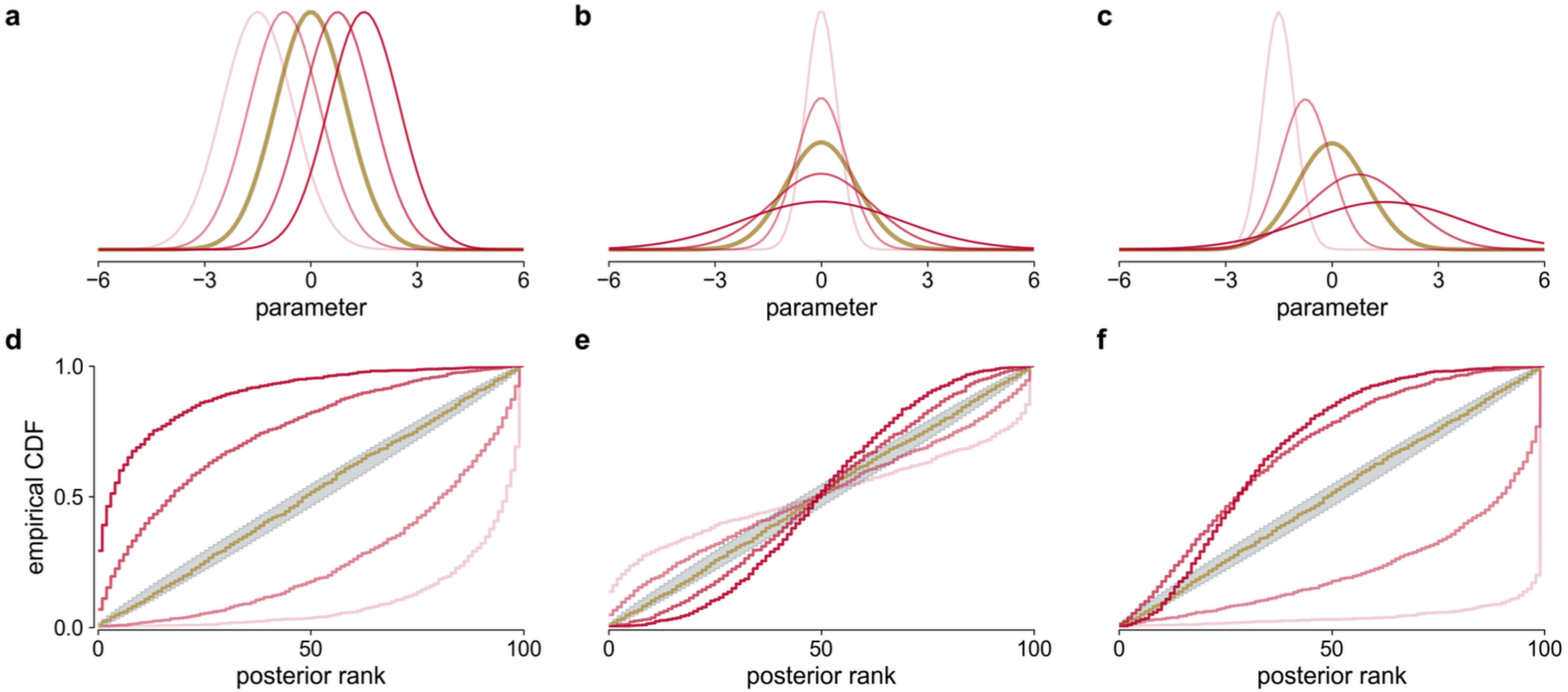
NLE / NPE loss functions

Algorithm 5: Single round Neural Posterior Estimation as in Papamakarios and Murray (2016)

for $j = 1 : N$ **do**
  Sample $\boldsymbol{\theta}_j \sim p(\boldsymbol{\theta})$
  Simulate $\mathbf{x}_j \sim p(\mathbf{x}|\boldsymbol{\theta}_j)$
end
$\boldsymbol{\phi} \leftarrow \arg\min \sum_j^N - \log q_{F(\mathbf{x}_j, \boldsymbol{\phi})}(\boldsymbol{\theta}_j)$
Set $\hat{p}(\boldsymbol{\theta}|\mathbf{x}_o) = q_{F(\mathbf{x}_o, \boldsymbol{\phi})}(\boldsymbol{\theta})$
return Samples from $\hat{p}(\boldsymbol{\theta}|\mathbf{x}_o)$; $q_{F(\mathbf{x}, \boldsymbol{\phi})}(\boldsymbol{\theta})$

Papamakarios & Murray 2016

Simulation-based calibration



$$\theta^* \sim p(\theta)$$
$$x^* \sim p(x|\theta^*)$$

$$\{\theta_1, \ldots \theta_L\} \sim p_i(\theta|x^*)$$

$$r_i = \sum_{j=1}^{L} \mathbb{I}[f(\theta_j) < f(\theta_i^*)] \in [0, L],$$

Talts et al. 2018; figure: Boelts, 2023

Model misspecification in SBI

- **Notation**: $x \sim p(x \mid \theta)$ simulated data; $y \sim p^*(y)$ observed data
- **Problem**: simulator is misspecified
- **Approach**: assume an error model $\tilde{x} \sim p(x \mid y)$, e.g., “spike and slab”

Algorithm 1: Robust neural posterior estimation (RNPE)

for i *in* $1 : N$ **do**
1 Sample $\boldsymbol{\theta}_i \sim p(\boldsymbol{\theta})$
2 Simulate $\boldsymbol{x}_i \sim p(\boldsymbol{x} \mid \boldsymbol{\theta})$
end
3 Train NPE $q(\boldsymbol{\theta} \mid \boldsymbol{x})$ on $\{(\boldsymbol{\theta}_i, \boldsymbol{x}_i)\}_{i=1}^N$
4 Train $q(\boldsymbol{x})$ on $\{\boldsymbol{x}_i\}_{i=1}^N$
5 Sample $\tilde{\boldsymbol{x}}_m \sim \hat{p}(\boldsymbol{x} \mid \boldsymbol{y}_o) \propto p(\boldsymbol{y}_o \mid \boldsymbol{x}) q(\boldsymbol{x}),\ m = 1, \ldots, M$ using MCMC
6 Sample $\tilde{\boldsymbol{\theta}}_m \sim q(\boldsymbol{\theta} \mid \tilde{\boldsymbol{x}}_m),\ m = 1, \ldots, M$
return $\{(\tilde{\boldsymbol{\theta}}_m, \tilde{\boldsymbol{x}}_m)\}_{m=1}^M$, samples drawn approximately from $p(\boldsymbol{\theta}, \boldsymbol{x} \mid \boldsymbol{y}_o)$

Ward et al. 2022