

# Simulation-Based Estimation

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## Introduction

Stochastic simulations try to mimic stochastic phenomena observed in nature.

The natural phenomenon is modeled by a probability distribution  $Q$ . We observe what Nature draws from  $Q$ . Independently replicated observations constitute a sample  $\vec{y} = \{y_1, \dots, y_m\}$ .

Analogously, a stochastic simulation is a pseudorandom mechanism for drawing observations from a specified probability distribution. Simulation usually requires specifying the values of various parameters, so we write  $P_\theta$  to denote simulation with parameter values  $\theta$ . Running the simulation with these values means drawing observations from  $P_\theta$ . Independently replicated observations constitute a sample  $\vec{x} = \{x_1, \dots, x_n\}$ .

## Parameter Estimation

Suppose that we've observed an *actual sample*  $\vec{y}$ , drawn by Nature from  $Q$ .

Problem: Guess what parameter value causes  $P_\theta$  to behave most like  $Q$ .

Strategy: Draw simulated samples from different  $P_\theta$ . Choose the value(s) for which the simulated samples most closely resemble the actual sample.

Key questions:

1. How do we measure how closely two samples resemble each other?

(For simplicity, assume that we're observing real numbers, e.g. time from first tumor detected to second tumor detected.)

2. How do we systematically choose different  $P_\theta$  from which to sample?

## Comparing $Q$ and $P(\theta)$

1. Partition  $(-\infty, \infty)$  into  $b$  bins:  $B_1, \dots, B_b$ .

2. Let

$$q_k = Q(B_k)$$

and

$$p_k(\theta) = P_\theta(B_k).$$

3. Let

$$\Delta(Q, P_\theta) = m \sum_{k=1}^b \frac{[q_k - p_k(\theta)]^2}{p_k(\theta)}.$$

4. Choose  $\theta$  to minimize  $\Delta(Q, P_\theta)$ .

Unfortunately,  $Q$  is unknown—we only know  $\vec{y}$ , the sample drawn from  $Q$ .

## Comparing $\vec{y} \sim Q$ and $P(\theta)$

1. Partition  $(-\infty, \infty)$  into  $b$  bins:  $B_1, \dots, B_b$ .

2. Let

$$\hat{q}_k = \# \{y_j \in B_k\} / m$$

and

$$p_k(\theta) = P_\theta(B_k).$$

3. Let

$$f(\theta) = \Delta(\hat{Q}, P_\theta) = m \sum_{k=1}^b \frac{[\hat{q}_k - p_k(\theta)]^2}{p_k(\theta)}.$$

4. Choose  $\hat{\theta}$  to minimize  $f(\theta)$ .

Unfortunately, most stochastic simulations are too complicated for us to determine  $p_k(\theta)$ . Instead, we must sample  $P_\theta$  in order to estimate  $p_k(\theta)$ .

## Comparing $\vec{y} \sim Q$ and $\vec{x} \sim P(\theta)$

1. Partition  $(-\infty, \infty)$  into  $b$  bins:  $B_1, \dots, B_b$ .

2. Let

$$\hat{q}_k = \# \{y_j \in B_k\} / m$$

and

$$\hat{p}_k(\theta) = \# \{x_i \in B_k\} / n.$$

3. Let

$$\hat{f}_n(\theta) = \Delta(\hat{Q}, \hat{P}_\theta) = m \sum_{k=1}^b \frac{[\hat{q}_k - \hat{p}_k(\theta)]^2}{\hat{p}_k(\theta)}.$$

4. Choose  $\hat{\theta}$  to minimize  $f(\theta)$ , using  $\hat{f}_n(\theta)$  to estimate  $f(\theta)$ .

Notice that function evaluation is uncertain—drawing different samples from  $P_\theta$  will produce different  $\hat{f}_n(\theta)$ .

However,  $\hat{f}_n(\theta) \xrightarrow{P} f(\theta)$  as  $n \rightarrow \infty$ .

## Example

Bin	$Q$	$\theta_1$	$\theta_2$	$\theta_3$	$\theta_4$	$\theta_5$	$\theta_6$
$(-\infty, 2)$	5	67	64	27	36	12	13
$(2, 3)$	6	19	16	26	20	22	23
$(3, 4)$	4	6	11	23	21	18	20
$(4, 5)$	2	4	5	10	12	21	19
$(5, \infty)$	3	4	4	14	11	27	25

$\theta$	$\hat{f}_n(\theta)$
$\theta_1$	20.92
$\theta_2$	15.73
$\theta_3$	0.25
$\theta_4$	2.04
$\theta_5$	5.66
$\theta_6$	4.29

## Answer

$$\theta_1 = \theta_2 = 2$$

$$\theta_3 = \theta_4 = 3$$

$$\theta_5 = \theta_6 = 4$$

$$Q = P_\pi$$



## Next: Stochastic Optimization

We want to minimize  $f$ .

Function evaluation is uncertain: because we can't compute  $f(\theta)$ , we must estimate  $f(\theta)$  by sampling  $P_\theta$  and computing  $\hat{f}_n(\theta)$ .

Question: How do we minimize when function evaluation is uncertain?

## Papers to be Presented

1. What is  $P_\theta$ , the stochastic simulation?
2. How are samples compared?
3. How is the comparison criterion optimized?