

# Quantile estimation under monotonicity constraint

MASCOTNUM

Saint Etienne - 08/04/2015

Vincent Moutoussamy - EDF R&D - MRI

Nicolas Bousquet, Bertrand Iooss - EDF R&D - MRI

Fabrice Gamboa, Thierry Klein - Université Paul Sabatier

## Context

- Consider  $g : \mathcal{R}^d \rightarrow \mathcal{R}$

## Context

- Consider  $g : \mathcal{R}^d \rightarrow \mathcal{R}$
- Consider an input  $\mathbf{X}$  as a random vector

## Context

- Consider  $g : \mathcal{R}^d \rightarrow \mathcal{R}$
- Consider an input  $\mathbf{X}$  as a random vector  $\Rightarrow g(\mathbf{X})$  is a random variable

## Context

- Consider  $g : \mathcal{R}^d \rightarrow \mathcal{R}$
- Consider an input  $\mathbf{X}$  as a random vector  $\Rightarrow g(\mathbf{X})$  is a random variable
- An undesirable event is described as  $\{g(\mathbf{X}) \leq q\}$

## Context

- Consider  $g : \mathbf{R}^d \rightarrow \mathbf{R}$
- Consider an input  $\mathbf{X}$  as a random vector  $\Rightarrow g(\mathbf{X})$  is a random variable
- An undesirable event is described as  $\{g(\mathbf{X}) \leq q\}$
- Denote  $F(t) = \mathbb{P}(g(\mathbf{x}) \leq t)$ , the  $p$ -quantile is defined by

$$q = \inf\{t \in \mathbf{R} : F(t) > p\}.$$

## Context

- Consider  $g : \mathbf{R}^d \rightarrow \mathbf{R}$
- Consider an input  $\mathbf{X}$  as a random vector  $\Rightarrow g(\mathbf{X})$  is a random variable
- An undesirable event is described as  $\{g(\mathbf{X}) \leq q\}$
- Denote  $F(t) = \mathbb{P}(g(\mathbf{x}) \leq t)$ , the  $p$ -quantile is defined by

$$q = \inf\{t \in \mathbf{R} : F(t) > p\}.$$

- Knowing the behaviour of the component, a **monotonic** hypothesis is studied
- The monotonicity gives **sure bounds** of  $q$ .

# Context

- Without loss of generality, assume
  - $g : [0, 1]^d \rightarrow \mathcal{R}$  is a **globally increasing** function:  $\mathbf{u}, \mathbf{v} \in [0, 1]^d$  such that  $\mathbf{u} \preceq \mathbf{v}$  then  $g(\mathbf{u}) \leq g(\mathbf{v})$
  - $\mathbf{X}$  is **uniformly distributed** on  $[0, 1]^d$
- An **adaptive** method is provided to estimate a quantile: estimate  $q$  by

$$\hat{q} = \inf\{t \in \mathcal{R} : \hat{F}(t) > p\}.$$

with  $\hat{F}$  an estimator of  $F$ .



# Materials

## Definition

Let  $A \subset [0, 1]^d$ . Define

$$\mathbb{U}^-(A) = \bigcup_{\mathbf{x} \in A} \{\mathbf{u} \in [0, 1]^d : \mathbf{u} \preceq \mathbf{x}\},$$

$$\mathbb{U}^+(A) = \bigcup_{\mathbf{x} \in A} \{\mathbf{u} \in [0, 1]^d : \mathbf{u} \succeq \mathbf{x}\}.$$

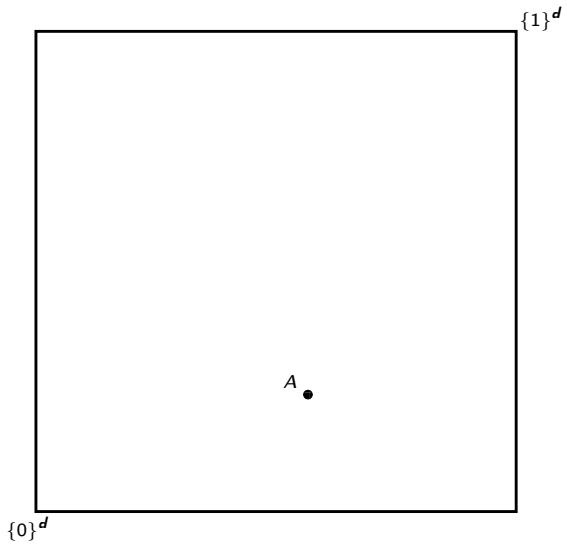
## Definition

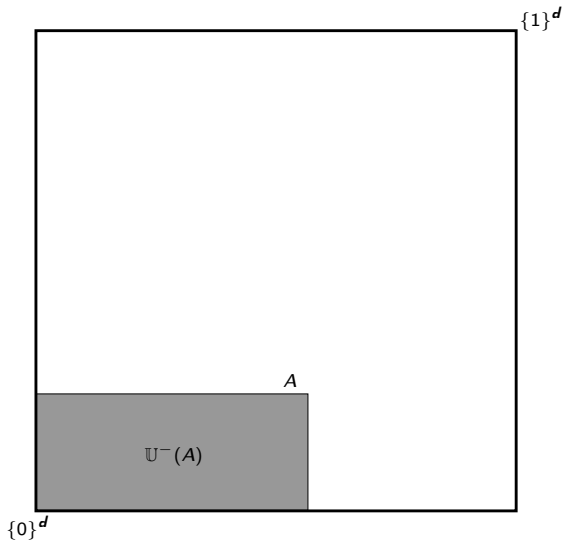
Let  $\alpha \in ]0, 1[$  assume that  $S$  is a  $(d - 1)$ -dimensional surface such that

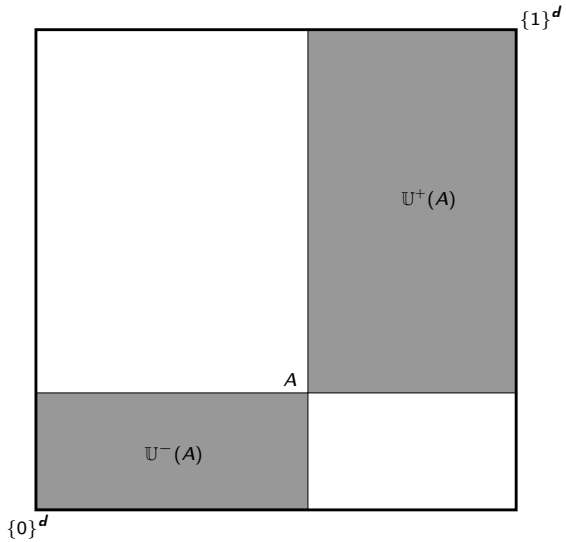
- (i) for all  $\mathbf{u}, \mathbf{v} \in S$ ,  $\mathbf{u}$  is not strictly dominated by  $\mathbf{v}$
- (ii)  $\mu(\mathbb{U}^-(S)) = \alpha$ ,

then  $S$  is said to be  $\alpha$ -monotonic.

*Remark: the set  $\{\mathbf{x} \in [0, 1]^d, g(\mathbf{x}) = q\}$  is  $F(q)$ -monotonic.*







## Main result

### Proposition

Let  $S_p$  be a  $p$ -monotonic surface. Then

$$\min_{\mathbf{x} \in S_p} g(\mathbf{x}) \leq q \leq \max_{\mathbf{x} \in S_p} g(\mathbf{x}).$$

- A  $p$ -monotonic surface is difficult to build in practice. The condition can be relaxed:

## Main result

### Proposition

Let  $S_p$  be a  $p$ -monotonic surface. Then

$$\min_{\mathbf{x} \in S_p} g(\mathbf{x}) \leq q \leq \max_{\mathbf{x} \in S_p} g(\mathbf{x}).$$

- A  $p$ -monotonic surface is difficult to build in practice. The condition can be relaxed:

### Proposition

Let  $p^- \in [0, p]$  and  $p^+ \in [p, 1]$ , and let  $S_{p^-}$ ,  $S_{p^+}$  be respectively a  $(p^-)$ -monotonic surface and a  $(p^+)$ -monotonic surface. Then

$$\min_{\mathbf{x} \in S_{p^-}} g(\mathbf{x}) \leq q \leq \max_{\mathbf{x} \in S_{p^+}} g(\mathbf{x}).$$

# Initialisation

- Let  $\mathbf{x} = (x_1, \dots, x_d) \in [0, 1]^d$ . Since the frontier of  $\mathbb{U}^-(\mathbf{x})$  is monotonic

$$\mu(\mathbb{U}^-(\mathbf{x})) = x_1 \cdots x_d \geq p \Rightarrow q \leq g(\mathbf{x})$$

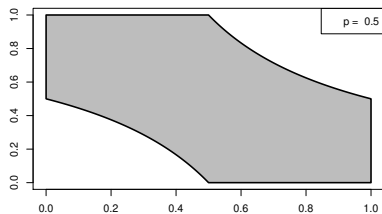
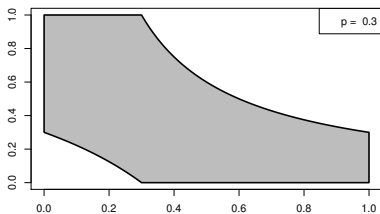
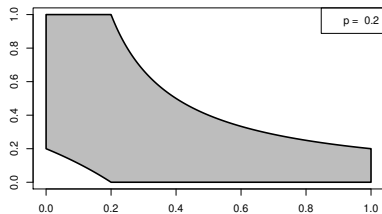
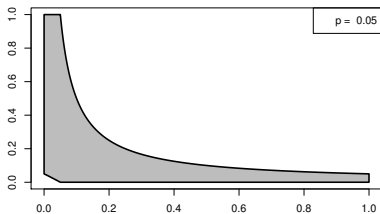
## Proposition

Let

$$\mathbb{W}^-(p) = \left\{ \mathbf{x} = (x_1, \dots, x_d) \in [0, 1]^d : \prod_{i=1}^d (1 - x_i) \geq 1 - p \right\}$$
$$\mathbb{W}^+(p) = \left\{ \mathbf{x} = (x_1, \dots, x_d) \in [0, 1]^d : \prod_{i=1}^d x_i \geq p \right\}.$$

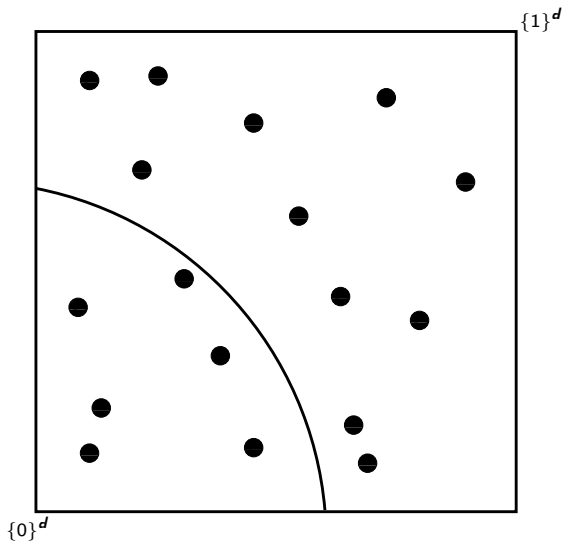
Then for all  $(\mathbf{u}, \mathbf{v}) \in \mathbb{W}^-(p) \times \mathbb{W}^+(p)$ ,  $g(\mathbf{u}) \leq q \leq g(\mathbf{v})$ .

- In gray:  $\mathbb{W}(p) = [0, 1]^d \setminus (\mathbb{W}^-(p) \cup \mathbb{W}^+(p))$

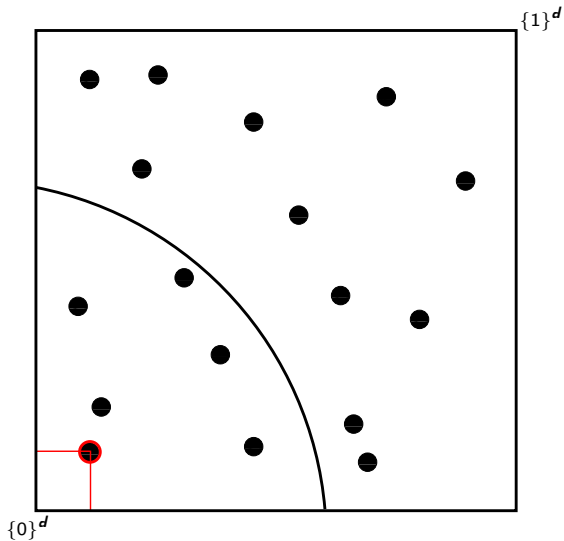




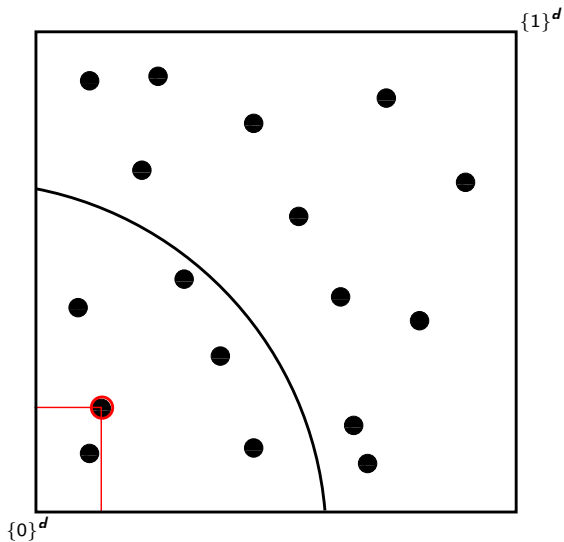
# Bounding a quantile from a sample



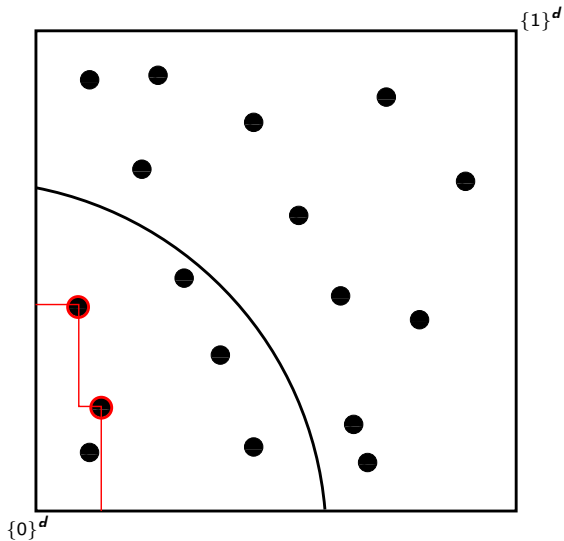
# Bounding a quantile from a sample



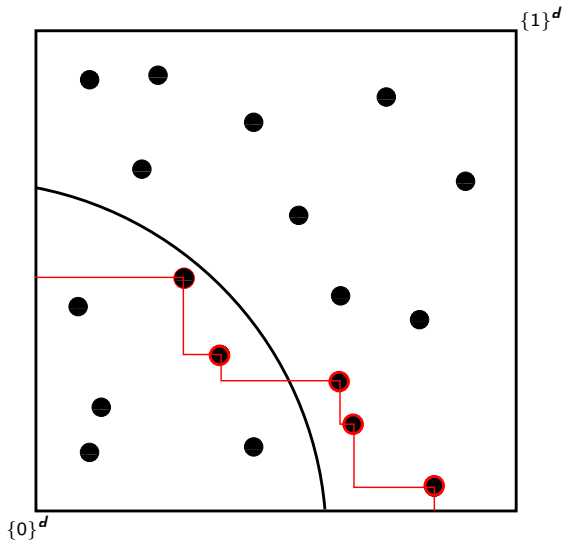
# Bounding a quantile from a sample



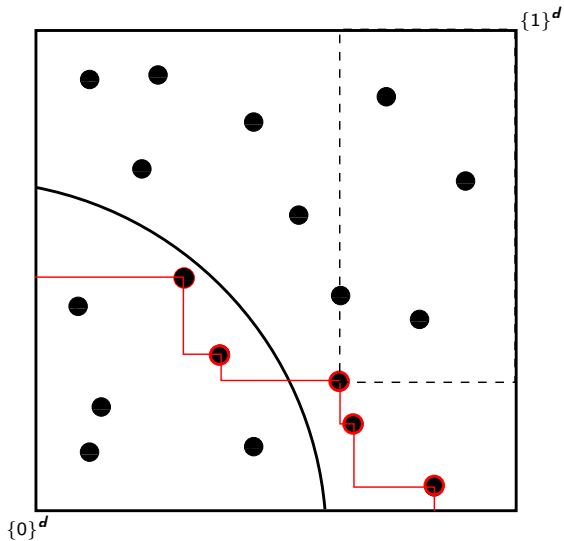
# Bounding a quantile from a sample



# Bounding a quantile from a sample



# Bounding a quantile from a sample



# Probability estimation

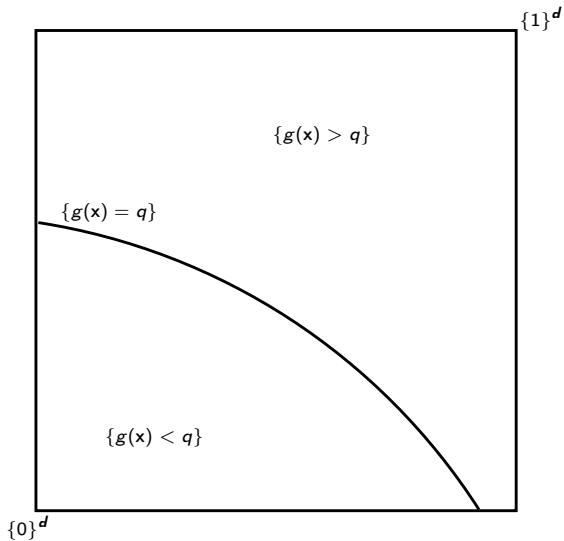
- Aim: estimate  $q$  by

$$\hat{q} = \inf\{t \in \mathbf{R} : \hat{F}(t) > p\}$$

with  $\hat{F}$  an estimator of  $F$

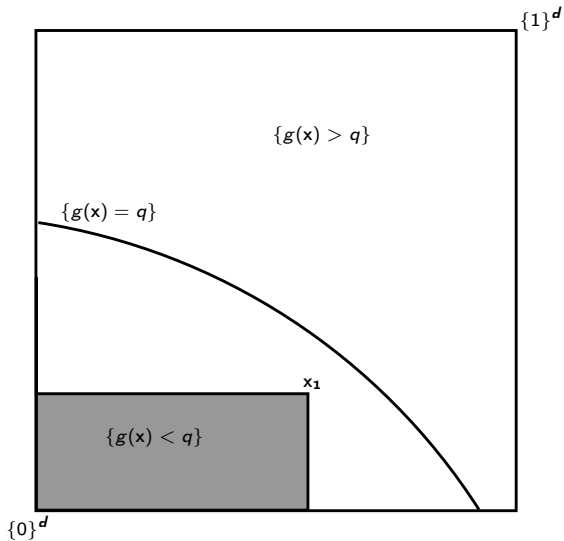
- Taking account of the deterministic bounds, an unbiased estimator  $\hat{F}$  is inspired by Bousquet (2012)

# Probability estimation

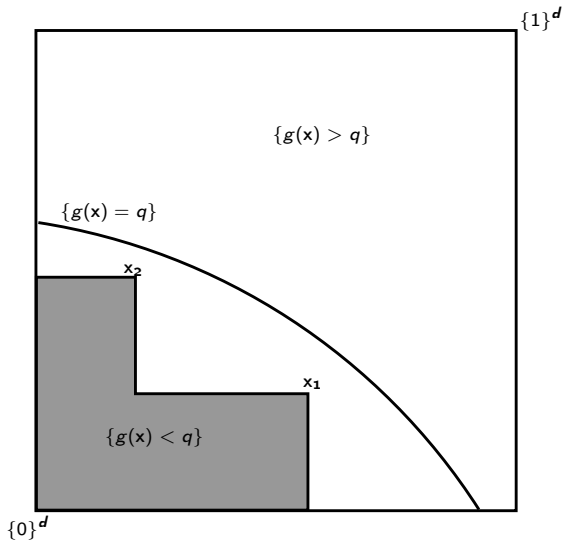




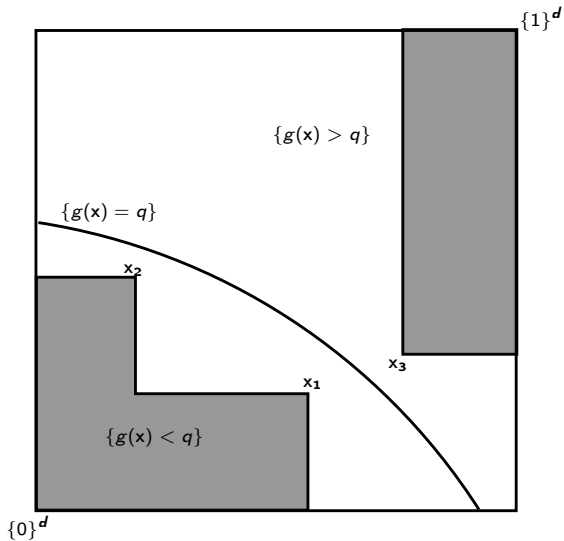
# Probability estimation



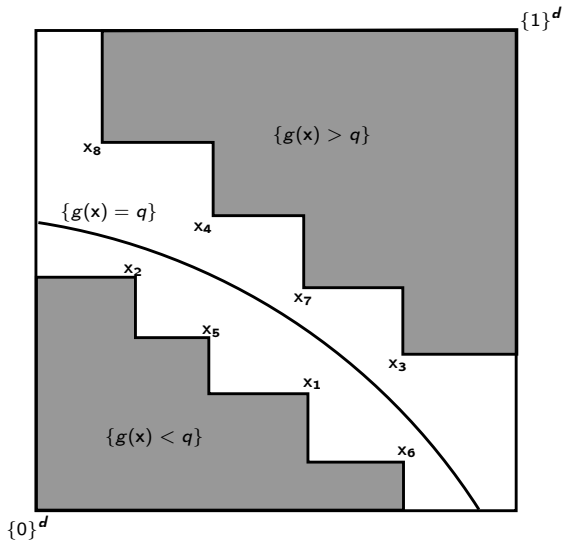
# Probability estimation



# Probability estimation



# Probability estimation



## Probability estimation

- Denote  $\mathbb{U}_{k-1}$  the set where the sign of  $g(\cdot) - q$  is unknown
- Let  $\mathbf{X}_k$  be uniformly distributed on  $\mathbb{U}_{k-1}$ , then

$$p_{k-1}^- + (p_{k-1}^+ - p_{k-1}^-) \mathbb{1}_{\{g(\mathbf{X}_k) \leq q\}}$$

is an unbiased estimator of  $F(q)$ .

*Indeed,  $\mathbb{1}_{\{g(\mathbf{X}_k) \leq q\}} \sim \text{Bernoulli} \left( \frac{F(q) - p_{k-1}^-}{p_{k-1}^+ - p_{k-1}^-} \right)$*

## Probability estimation

- Denote  $\mathbb{U}_{k-1}$  the set where the sign of  $g(\cdot) - q$  is unknown
- Let  $\mathbf{X}_k$  be uniformly distributed on  $\mathbb{U}_{k-1}$ , then

$$p_{k-1}^- + (p_{k-1}^+ - p_{k-1}^-) \mathbb{1}_{\{g(\mathbf{X}_k) \leq q\}}$$

is an unbiased estimator of  $F(q)$ .

*Indeed,  $\mathbb{1}_{\{g(\mathbf{X}_k) \leq q\}} \sim \text{Bernoulli} \left( \frac{F(q) - p_{k-1}^-}{p_{k-1}^+ - p_{k-1}^-} \right)$*

- Let  $(\mathbf{X}_k)_{k \geq 1}$  be a sequence of random vector such that for all  $k \geq 1$ ,  $\mathbf{X}_k$  is uniformly distributed on  $\mathbb{U}_{k-1}$ , then

$$F_n(q) = \frac{1}{n} \sum_{k=1}^n p_{k-1}^- + (p_{k-1}^+ - p_{k-1}^-) \mathbb{1}_{\{g(\mathbf{X}_k) \leq q\}}$$

is also an unbiased estimator of  $F(q)$ .

## Application to quantile estimation

- At step 1, denote :
  - $\mathbb{U}_0 = \mathbb{W}(p)$
  - $g(\mathbf{x}^-) = \mathbf{q}_0^- \leq \mathbf{q} \leq \mathbf{q}_0^+ = g(\mathbf{x}^+)$ , with

$$\mathbf{x}^- = (1 - (1 - p)^{1/d}, \dots, 1 - (1 - p)^{1/d}) \in \mathbb{W}^-(p) \subset [0, 1]^d,$$

$$\mathbf{x}^+ = (p^{1/d}, \dots, p^{1/d}) \in \mathbb{W}^+(p) \subset [0, 1]^d,$$

Remark: without more information on  $g$ ,  $\mathbf{x}^-$ ,  $\mathbf{x}^+$  are chosen arbitrary.

- $p_0^- = \mu(\mathbb{W}^-(p))$ ,  $p_0^+ = 1 - \mu(\mathbb{W}^+(p))$ .

## Application to quantile estimation

- At step 1, denote :
  - $\mathbb{U}_0 = \mathbb{W}(p)$
  - $g(\mathbf{x}^-) = \mathbf{q}_0^- \leq \mathbf{q} \leq \mathbf{q}_0^+ = g(\mathbf{x}^+)$ , with

$$\mathbf{x}^- = (1 - (1 - p)^{1/d}, \dots, 1 - (1 - p)^{1/d}) \in \mathbb{W}^-(p) \subset [0, 1]^d,$$

$$\mathbf{x}^+ = (p^{1/d}, \dots, p^{1/d}) \in \mathbb{W}^+(p) \subset [0, 1]^d,$$

Remark: without more information on  $g$ ,  $\mathbf{x}^-$ ,  $\mathbf{x}^+$  are chosen arbitrary.

- $p_0^- = \mu(\mathbb{W}^-(p))$ ,  $p_0^+ = 1 - \mu(\mathbb{W}^+(p))$ .
- Let  $\mathbf{X}_1$  be uniformly distributed on  $\mathbb{U}_0$ , then

$$\hat{F}_1(q) = p_0^- + (p_0^+ - p_0^-) \mathbb{1}_{\{g(\mathbf{x}_0) \leq q\}}$$

is an unbiased estimator of  $F(q)$ .

- $q$  is estimated by

$$\hat{q}_1 = \inf\{t \in [q_0^-, q_0^+] : \hat{F}_1(t) > p\}$$



## Application to quantile estimation

- At step  $n$ , from  $\mathbf{X}_1, \dots, \mathbf{X}_{n-1}$ :
  - two bounds  $q_{n-1}^- \leq q \leq q_{n-1}^+$  has been obtained
  - the non-dominated set  $\mathbb{U}_{n-1}$  has been updated
- Let  $\mathbf{X}_n$  be uniformly distributed on  $\mathbb{U}_{n-1}$ , then

$$\hat{F}_n(q) = \frac{1}{n} \sum_{k=1}^n p_{k-1}^- + (p_{k-1}^+ - p_{k-1}^-) \mathbb{1}_{\{g(\mathbf{x}_k) \leq q\}}$$

is an unbiased estimator of  $F(q)$ .

- $q$  is estimated by

$$\hat{q}_n = \inf \{t \in [q_{n-1}^-, q_{n-1}^+] : \hat{F}_n(t) > p\}$$

# Numerical applications

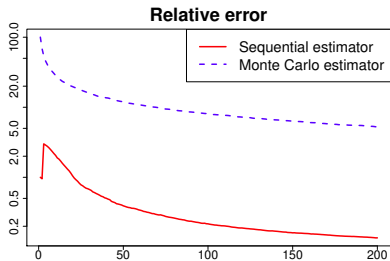
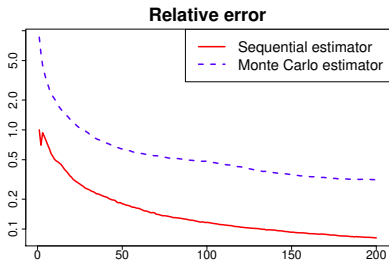
- Consider an analytical example.
- Let  $\mathbf{X} = (X_1, \dots, X_d)$  be a random vector where  $X_i \sim \Gamma(i + 1, 1)$ . Denoting

$$g(\mathbf{X}) = X_1 / \sum_{i=1}^d X_i \sim \text{Beta}(2, (d + 1)(d + 2)/2 - 3),$$

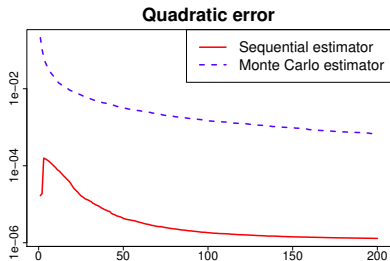
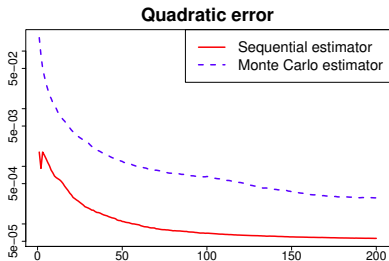
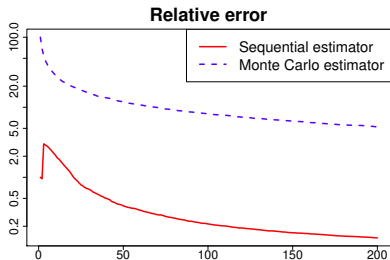
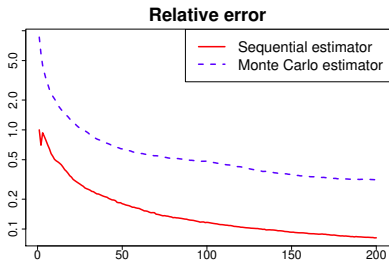
and  $q_{d,p}$  the  $p$ -quantile of  $g(\mathbf{X})$ .

- The method is compared with a standard Monte Carlo Method for different couple  $(d, p)$  with  $n = 200$  evaluations available of  $g$
- The comparison is conducted on four different criterion:
  - the quadratic error  $\mathbb{E}[(q_n - q_{d,p})^2]$
  - the relative error  $\mathbb{E}[|q_n - q_{d,p}|/q_{d,p}]$
  - the bias  $\mathbb{E}[q_n - q_{d,p}]$
  - the length of the confidence interval at 95%

$d = 2$

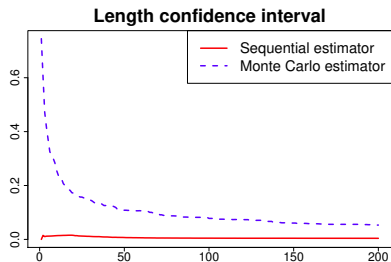
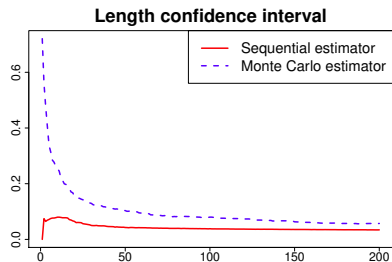
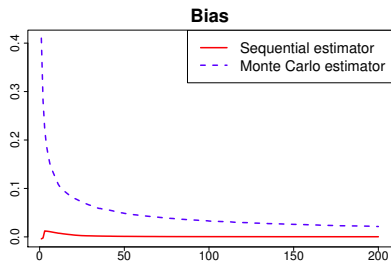
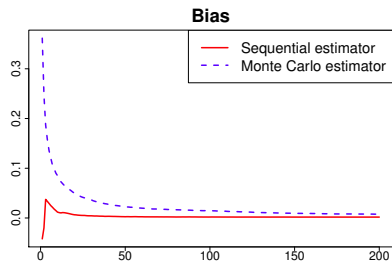


$d = 2$



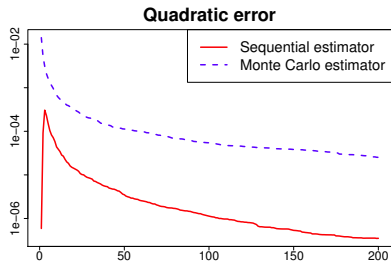
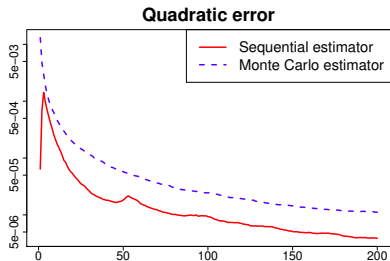
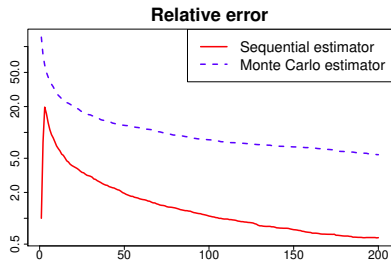
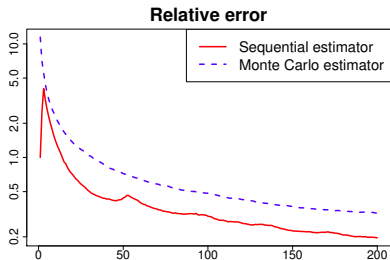
Left:  $p = 10^{-2}$ . Right:  $p = 10^{-4}$

$d = 2$



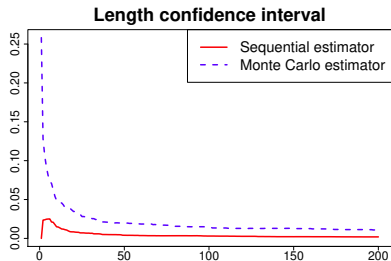
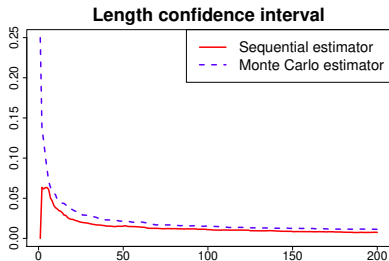
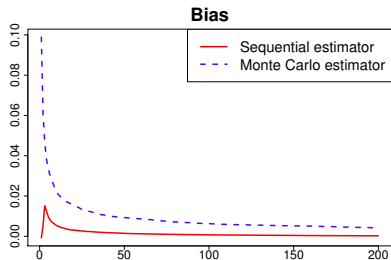
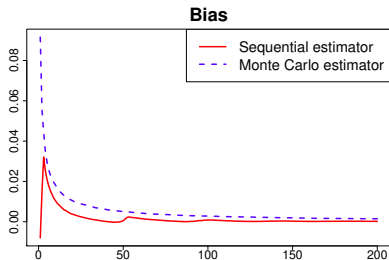
Left:  $p = 10^{-2}$ . Right:  $p = 10^{-4}$

$d = 5$



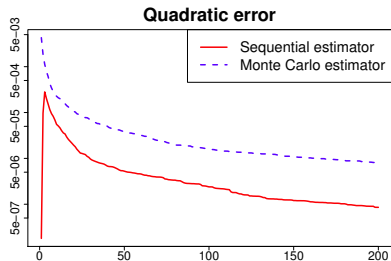
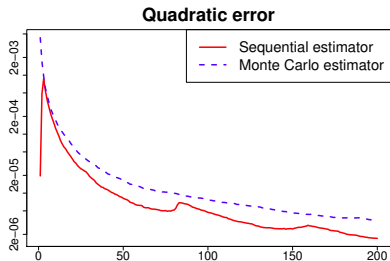
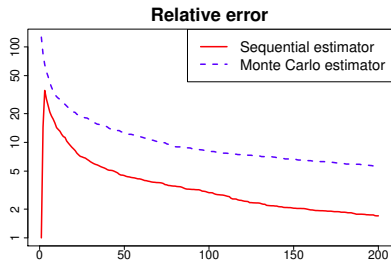
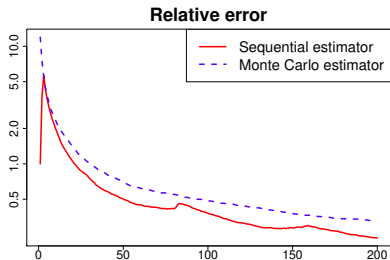
Left:  $p = 10^{-2}$ . Right:  $p = 10^{-4}$

$d = 5$



Left:  $p = 10^{-2}$ . Right:  $p = 10^{-4}$

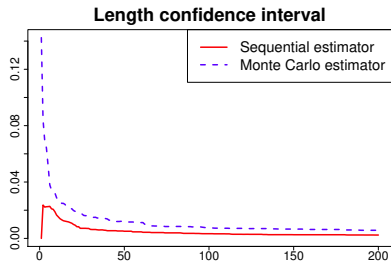
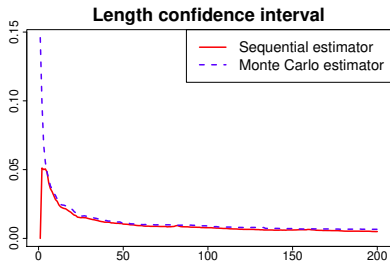
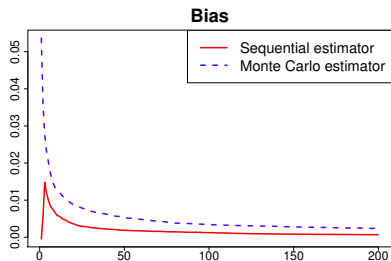
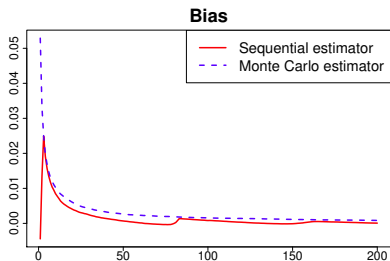
$d = 7$



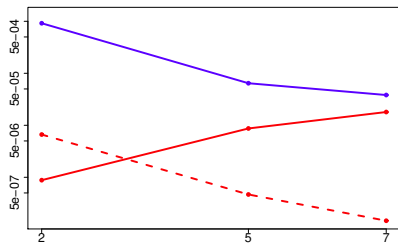
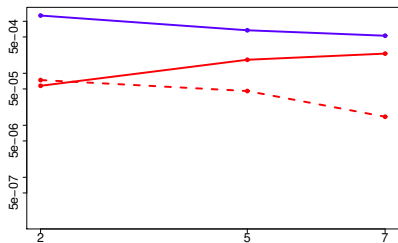
Left:  $p = 10^{-2}$ . Right:  $p = 10^{-4}$



$d = 7$



Left:  $p = 10^{-2}$ . Right:  $p = 10^{-4}$



**Left:**  $p = 10^{-2}$ . **Right:**  $p = 10^{-4}$

## Conclusion

- A central limit theorem can be obtained to control the estimator ?
- Instead a uniform sequential sampling, use a sequential importance sampling to accelerate the estimation of  $F(q)$  then to apply on quantile estimation
- Comparing this method with existing method (Guyader, Morio...)