Optimal Uncertainty Quantification of Quantiles Application to Industrial Risk Management.

Merlin Keller¹, Jérôme Stenger¹²

¹EDF R&D, France ²Institut Mathématique de Toulouse, France

ETICS 2018, Roscoff



2 Robust Bounds on Quantiles

◆□ → < 団 → < 三 → < 三 → < 三 → ○へ (~ 2/12)

Principle

Find optimal bounds for a quantity of interest $Q(\mu^{\dagger})$, functional of an uncertain probability measure μ^{\dagger} , known only to lie in some subset \mathcal{A} of $\mathcal{M}_1(\mathcal{X})$:

$$\underline{Q}(\mathcal{A}) \leq Q(\mu^{\dagger}) \leq \overline{Q}(\mathcal{A}),$$

with :

• $\underline{Q}(\mathcal{A}) = \inf_{\mu \in \mathcal{A}} Q(\mu)$

•
$$\overline{Q}(\mathcal{A}) = \sup_{\mu \in \mathcal{A}} Q(\mu)$$

• $\mathcal{A} = \{\mu \in \mathcal{M}_1(\mathcal{X}) \mid \Phi_j(\mu) \leq c_j, j = 1, \dots, N\}$ the *admissible* subset,

Distributionally Robust : Useful in risk-adverse situations when parametric assumptions are hard to justify

 \hookrightarrow Many applications in Industrial Risk Management (find two : exercise $\sharp 1$)

Principle

Find optimal bounds for a quantity of interest $Q(\mu^{\dagger})$, functional of an uncertain probability measure μ^{\dagger} , known only to lie in some subset \mathcal{A} of $\mathcal{M}_1(\mathcal{X})$:

$$\underline{Q}(\mathcal{A}) \leq Q(\mu^{\dagger}) \leq \overline{Q}(\mathcal{A}),$$

with :

• $\underline{Q}(\mathcal{A}) = \inf_{\mu \in \mathcal{A}} Q(\mu)$

•
$$\overline{Q}(\mathcal{A}) = \sup_{\mu \in \mathcal{A}} Q(\mu)$$

• $\mathcal{A} = \{\mu \in \mathcal{M}_1(\mathcal{X}) \mid \Phi_j(\mu) \leq c_j, j = 1, \dots, N\}$ the *admissible* subset,

Distributionally Robust : Useful in risk-adverse situations when parametric assumptions are hard to justify

- \hookrightarrow Many applications in Industrial Risk Management (find two : exercise $\sharp 1$)
 - Dyke Conception / Reliability Assessment

Principle

Find optimal bounds for a quantity of interest $Q(\mu^{\dagger})$, functional of an uncertain probability measure μ^{\dagger} , known only to lie in some subset \mathcal{A} of $\mathcal{M}_1(\mathcal{X})$:

$$\underline{Q}(\mathcal{A}) \leq Q(\mu^{\dagger}) \leq \overline{Q}(\mathcal{A}),$$

with :

• $\underline{Q}(\mathcal{A}) = \inf_{\mu \in \mathcal{A}} Q(\mu)$

•
$$\overline{Q}(\mathcal{A}) = \sup_{\mu \in \mathcal{A}} Q(\mu)$$

• $\mathcal{A} = \{\mu \in \mathcal{M}_1(\mathcal{X}) \mid \Phi_j(\mu) \leq c_j, j = 1, \dots, N\}$ the *admissible* subset,

Distributionally Robust : Useful in risk-adverse situations when parametric assumptions are hard to justify

- \hookrightarrow Many applications in Industrial Risk Management (find two : exercise $\sharp 1$)
 - Dyke Conception / Reliability Assessment : Q(µ) := ℙ_µ[Z − h > 0],
 - $Z \sim \mu$ water level, *h* dyke height, Z h overflow

Principle

Find optimal bounds for a quantity of interest $Q(\mu^{\dagger})$, functional of an uncertain probability measure μ^{\dagger} , known only to lie in some subset \mathcal{A} of $\mathcal{M}_1(\mathcal{X})$:

$$\underline{Q}(\mathcal{A}) \leq Q(\mu^{\dagger}) \leq \overline{Q}(\mathcal{A}),$$

with :

• $\underline{Q}(\mathcal{A}) = \inf_{\mu \in \mathcal{A}} Q(\mu)$

•
$$\overline{Q}(\mathcal{A}) = \sup_{\mu \in \mathcal{A}} Q(\mu)$$

• $\mathcal{A} = \{\mu \in \mathcal{M}_1(\mathcal{X}) \mid \Phi_j(\mu) \leq c_j, j = 1, \dots, N\}$ the *admissible* subset,

Distributionally Robust : Useful in risk-adverse situations when parametric assumptions are hard to justify

- \hookrightarrow Many applications in Industrial Risk Management (find two : exercise $\sharp 1$)
 - Dyke Conception / Reliability Assessment : Q(µ) := ℙ_µ[Z − h > 0],

• $Z \sim \mu$ water level, *h* dyke height, Z - h overflow

• Nuclear Accident Risk Assessment

Principle

Find optimal bounds for a quantity of interest $Q(\mu^{\dagger})$, functional of an uncertain probability measure μ^{\dagger} , known only to lie in some subset \mathcal{A} of $\mathcal{M}_1(\mathcal{X})$:

$$\underline{Q}(\mathcal{A}) \leq Q(\mu^{\dagger}) \leq \overline{Q}(\mathcal{A}),$$

with :

• $\underline{Q}(\mathcal{A}) = \inf_{\mu \in \mathcal{A}} Q(\mu)$

•
$$\overline{Q}(\mathcal{A}) = \sup_{\mu \in \mathcal{A}} Q(\mu)$$

• $\mathcal{A} = \{\mu \in \mathcal{M}_1(\mathcal{X}) \mid \Phi_j(\mu) \leq c_j, j = 1, \dots, N\}$ the *admissible* subset,

Distributionally Robust : Useful in risk-adverse situations when parametric assumptions are hard to justify

- \hookrightarrow Many applications in Industrial Risk Management (find two : exercise $\sharp 1$)
 - Dyke Conception / Reliability Assessment : Q(µ) := ℙ_µ[Z − h > 0],
 - $Z \sim \mu$ water level, *h* dyke height, Z h overflow
 - Nuclear Accident Risk Assessment : Q(µ) := sup{t > 0|ℙ_µ[T ≤ t] ≤ p},
 - $T \sim \mu$ maximal temperature inside nuclear reactor, p safety requirement

Principle

Find optimal bounds for a quantity of interest $Q(\mu^{\dagger})$, functional of an uncertain probability measure μ^{\dagger} , known only to lie in some subset \mathcal{A} of $\mathcal{M}_1(\mathcal{X})$:

$$\underline{Q}(\mathcal{A}) \leq Q(\mu^{\dagger}) \leq \overline{Q}(\mathcal{A}),$$

with :

• $\underline{Q}(\mathcal{A}) = \inf_{\mu \in \mathcal{A}} Q(\mu)$

•
$$\overline{Q}(\mathcal{A}) = \sup_{\mu \in \mathcal{A}} Q(\mu)$$

• $\mathcal{A} = \{\mu \in \mathcal{M}_1(\mathcal{X}) \mid \Phi_j(\mu) \leq c_j, j = 1, \dots, N\}$ the *admissible* subset,

Distributionally Robust : Useful in risk-adverse situations when parametric assumptions are hard to justify

- \hookrightarrow Many applications in Industrial Risk Management (find two : exercise $\sharp 1$)
 - Dyke Conception / Reliability Assessment : Q(µ) := ℙ_µ[Z − h > 0],
 - $Z \sim \mu$ water level, *h* dyke height, Z h overflow
 - Nuclear Accident Risk Assessment : Q(µ) := sup{t > 0|ℙ_µ[T ≤ t] ≤ p},
 - $\blacktriangleright~T\sim\mu$ maximal temperature inside nuclear reactor, p safety requirement
 - and also : Probabilistic Seismic Hazard Assessment (PSHA), Extreme weather forecasting, Environmental risk assessment, Ecotoxicology, ...

Robust Bayesian Inference (RBI) : [Rios Insua and Ruggeri, 2000]

RBI as a special case of OUQ

- μ prior distribution on parameter θ in statistical model $Y \sim f_{\theta} d\lambda$, belonging to a class A of admissible priors
- $P_Y(\mu)$ posterior distribution of θ given Y, according to Bayes' theorem :

$$dP_{Y}(\mu)(\theta) = \frac{f_{\theta}(Y)d\mu(\theta)}{\int_{\nu} f_{\nu}(Y)d\mu(\nu)}$$
(1)

- Derive optimal bounds on interest quantity of posterior distribution
 - replace $Q(\mu)$ by $Q(P_Y(\mu))$ (or Q by $Q \circ P_Y$)

Robust Bayesian Inference (RBI) : [Rios Insua and Ruggeri, 2000]

RBI as a special case of OUQ

- μ prior distribution on parameter θ in statistical model $Y \sim f_{\theta} d\lambda$, belonging to a class A of admissible priors
- $P_Y(\mu)$ posterior distribution of θ given Y, according to Bayes' theorem :

$$dP_{Y}(\mu)(\theta) = \frac{f_{\theta}(Y)d\mu(\theta)}{\int_{\nu} f_{\nu}(Y)d\mu(\nu)}$$
(1)

- Derive optimal bounds on interest quantity of posterior distribution
 - replace $Q(\mu)$ by $Q(P_Y(\mu))$ (or Q by $Q \circ P_Y$)

OUQ as a special case of RBI

- OUQ corresponds to the **no-data** case ($f_{\theta} := f$ does not depend on θ)
 - *Proof* : (1) reduces to $P_Y(\mu)$, whence $Q(P_Y(\mu))$ reduces to $Q(\mu)$

 \hookrightarrow both formulations are equivalent, and special cases of the Dempster Schaeffer Theory (DST) (M. Couplet, private conversation)

Main result

Theorem (Measure affine functionals over generalized moment classes) If :

- $Q(\mu)$ is measure affine (e.g. $Q(\mu) := \mathbb{E}_{\mu}[q], q$ bounded above or below)
- $\mathcal{A} = \{\mu \in \mathcal{M}_1(\mathcal{X}) | \mathbb{E}_{\mu}[\varphi_j] \le c_j, j = 1, \dots, N\}$ for measurable functions φ_j
- $\mathcal{A}_{\Delta} = \{\mu \in \mathcal{A} | \mu = \sum_{0=1}^{N} w_i \delta_{x_i}\}$ extremal admissible probability measures

Then :

• $\underline{Q}(\mathcal{A}) = \underline{Q}(\mathcal{A}_{\Delta})$; $\overline{Q}(\mathcal{A}) = \overline{Q}(\mathcal{A}_{\Delta})$

Main result

Theorem (Measure affine functionals over generalized moment classes)

If :

- $Q(\mu)$ is measure affine (e.g. $Q(\mu) := \mathbb{E}_{\mu}[q], q$ bounded above or below)
- $\mathcal{A} = \{\mu \in \mathcal{M}_1(\mathcal{X}) | \mathbb{E}_{\mu}[\varphi_j] \le c_j, j = 1, \dots, N\}$ for measurable functions φ_j
- $\mathcal{A}_{\Delta} = \{\mu \in \mathcal{A} | \mu = \sum_{0=1}^{N} w_i \delta_{x_i}\}$ extremal admissible probability measures

Then :

•
$$\underline{Q}(\mathcal{A}) = \underline{Q}(\mathcal{A}_{\Delta})$$
; $\overline{Q}(\mathcal{A}) = \overline{Q}(\mathcal{A}_{\Delta})$

Implementation

To find $\underline{Q}(\mathcal{A})$ (resp. $\overline{Q}(\mathcal{A})$) :

- Minimize (resp. Maximize) $Q(\mu) = \sum_{i=0}^{N} w_i q(x_i)$ wrt : $(w_i, x_i)_{0 \le i \le N}$
- subject to : $\sum_{i=0}^{N} w_i \varphi_j(x_i) \leq c_j$, for $j = 1, \dots, N$

 \hookrightarrow **Constrained optimization** problem, solvabe by (almost) off-the shelf methods if q, φ_j analytical functions : **Mystic framework** [McKerns et al., 2012]







A Simple Result

Theorem (Quantile-CDF duality)

Assume $\mathcal{X} = \mathbb{R}^+$ Let :

- $F_{\mu}(x) = \mathbb{P}_{\mu}[X \leq x]$ pointwise cdf evaluation functional
- $Q_{\mu}(p) = \inf\{x > 0 | F_{\mu}(x) \ge p\}$ order-p quantile

Then :

$$\overline{Q_{\mathcal{A}}}(p) = \inf\{x > 0 | \underline{F_{\mathcal{A}}}(x) \ge p\}$$

A Simple Result

Theorem (Quantile-CDF duality)

Assume $\mathcal{X} = \mathbb{R}^+$ Let :

• $F_{\mu}(x) = \mathbb{P}_{\mu}[X \leq x]$ pointwise cdf evaluation functional

• $Q_{\mu}(p) = \inf\{x > 0 | F_{\mu}(x) \ge p\}$ order-p quantile

Then :

$$\overline{Q_{\mathcal{A}}}(p) = \inf\{x > 0 | \underline{F_{\mathcal{A}}}(x) \ge p\}$$

Proof.

•
$$\forall \mu \in \mathcal{A} :$$

 $\{x > 0 | \underline{F}_{\mathcal{A}}(x) \ge p\} \subseteq \{x > 0 | F_{\mu}(x) \ge p\}$
 $\Rightarrow \inf\{x > 0 | \underline{F}_{\mathcal{A}}(x) \ge p\} \ge Q_{\mu}(p)$
 $\Rightarrow \inf\{x > 0 | \underline{F}_{\mathcal{A}}(x) \ge p\} \ge Q_{\mathcal{A}}(p).$
• Assuming a strict inequality, $\exists x_0, \text{ s.t. }:$
• $x_0 < \inf\{x > 0 | \underline{F}_{\mathcal{A}}(x) \ge p\}$
 $\Rightarrow \underline{F}_{\mathcal{A}}(x_0)
• $\overline{Q_{\mathcal{A}}}(p) < x_0$
 $\Rightarrow Q_{\mu}(p) < x_0 \Rightarrow F_{\mu}(x_0) \ge p,$
leading to a contradiction $\Box$$

Sequential construction of Quantile Upper Bound

• Initialization (t = 0): $(a_t, b_t) = (0, +\infty)$



イロト イロト イヨト イヨト 三日

Sequential construction of Quantile Upper Bound

- Initialization (t = 0): $(a_t, b_t) = (0, +\infty)$
- For t = 1, 2, ...:
 - Choose $x_t \in (a_{t-1}, b_{t-1})$
 - Calculate $\underline{F_A}(x_t)$
 - If $\underline{F_A}(x_t) \leq p$, set $a_t := x_t$
 - If $\overline{F_A}(x_t) > p$, set $b_t := x_t$
- Stop when $b_t a_t < \varepsilon$
- b_t is then an ε -approximation of $\overline{Q_A}(p)$



(ロ) (同) (E) (E) (E)

Sequential construction of Quantile Upper Bound

- Initialization (t = 0): $(a_t, b_t) = (0, +\infty)$
- For t = 1, 2, ...:
 - Choose $x_t \in (a_{t-1}, b_{t-1})$
 - Calculate $\underline{F_A}(x_t)$
 - If $\underline{F_A}(x_t) \leq p$, set $a_t := x_t$
 - If $\overline{F_A}(x_t) > p$, set $b_t := x_t$
- Stop when $b_t a_t < \varepsilon$
- b_t is then an ε -approximation of $\overline{Q_A}(p)$



(ロ) (同) (E) (E) (E)

Sequential construction of Quantile Upper Bound

- Initialization (t = 0): $(a_t, b_t) = (0, +\infty)$
- For t = 1, 2, ...:
 - Choose $x_t \in (a_{t-1}, b_{t-1})$
 - Calculate $\underline{F_{\mathcal{A}}}(x_t)$
 - If $\underline{F_A}(x_t) \leq p$, set $a_t := x_t$
 - If $\overline{F_A}(x_t) > p$, set $b_t := x_t$
- Stop when $b_t a_t < \varepsilon$
- b_t is then an ε -approximation of $\overline{Q_A}(p)$



Sequential construction of Quantile Upper Bound

- Initialization (t = 0): $(a_t, b_t) = (0, +\infty)$
- For t = 1, 2, ...:
 - Choose $x_t \in (a_{t-1}, b_{t-1})$
 - Calculate $\underline{F_{\mathcal{A}}}(x_t)$
 - If $\underline{F_A}(x_t) \leq p$, set $a_t := x_t$
 - If $\overline{F_A}(x_t) > p$, set $b_t := x_t$
- Stop when $b_t a_t < \varepsilon$
- b_t is then an ε -approximation of $\overline{Q_A}(p)$



4 ロ > 4 部 > 4 差 > 4 差 > 差 の Q (や 8/12

Sequential construction of Quantile Upper Bound

- Initialization (t = 0): $(a_t, b_t) = (0, +\infty)$
- For t = 1, 2, ...:
 - Choose $x_t \in (a_{t-1}, b_{t-1})$
 - Calculate $\underline{F_{\mathcal{A}}}(x_t)$
 - If $\underline{F_A}(x_t) \leq p$, set $a_t := x_t$
 - If $\overline{F_A}(x_t) > p$, set $b_t := x_t$

• Stop when
$$b_t - a_t < \varepsilon$$

• b_t is then an ε -approximation of $\overline{Q_A}(p)$

Challenges



(日) (종) (종) (종) (종)

Sequential construction of Quantile Upper Bound

- Initialization (t = 0): $(a_t, b_t) = (0, +\infty)$
- For t = 1, 2, ...:
 - Choose $x_t \in (a_{t-1}, b_{t-1})$
 - Calculate $\underline{F_A}(x_t)$
 - If $\underline{F}_{\mathcal{A}}(x_t) \leq p$, set $a_t := x_t$
 - If $\overline{F_A}(x_t) > p$, set $b_t := x_t$
- Stop when $b_t a_t < \varepsilon$
- b_t is then an ε -approximation of $\overline{Q_A}(p)$

Challenges

• How to 'choose' $x_t \in (a_{t-1}, b_{t-1})$?



(日) (종) (종) (종) (종)

Sequential construction of Quantile Upper Bound

- Initialization (t = 0): $(a_t, b_t) = (0, +\infty)$
- For t = 1, 2, ...:
 - Choose $x_t \in (a_{t-1}, b_{t-1})$
 - Calculate $\underline{F_{\mathcal{A}}}(x_t)$
 - If $\underline{F}_{\mathcal{A}}(x_t) \leq p$, set $a_t := x_t$
 - If $\overline{F_A}(x_t) > p$, set $b_t := x_t$
- Stop when $b_t a_t < \varepsilon$
- b_t is then an ε -approximation of $\overline{Q_A}(p)$

Challenges

- How to 'choose' $x_t \in (a_{t-1}, b_{t-1})$?
- Can we guarantee $\overline{Q_A}(p)$ is nontrivial $(<\infty)$?



(日) (종) (종) (종) (종)

Sequential construction of Quantile Upper Bound

- Initialization (t = 0): $(a_t, b_t) = (0, +\infty)$
- For t = 1, 2, ...:
 - Choose $x_t \in (a_{t-1}, b_{t-1})$
 - Calculate $\underline{F_{\mathcal{A}}}(x_t)$
 - If $\underline{F_A}(x_t) \le p$, set $a_t := x_t$
 - If $\underline{F_A}(x_t) > p$, set $b_t := x_t$
- Stop when $b_t a_t < \varepsilon$
- b_t is then an ε -approximation of $\overline{Q_A}(p)$

Challenges

- How to 'choose' $x_t \in (a_{t-1}, b_{t-1})$?
- Can we guarantee $\overline{Q_A}(p)$ is nontrivial $(<\infty)$?
- What if Q(μ) is an extreme quantile on Y = G(X), with X ~ μ and G a costly computer model? Can we develop an 'EGO-like' approach?



Alternative : Direct quantile optimization

$Q_{\mu}(p)$ not a measure affine functional

However, quantile-CDF duality ensures that main result still applies :

OUQ for quantiles

To find $\underline{Q_A}(p)$ (resp. $\overline{Q_A}(p)$) :

• Minimize (resp. Maximize) $Q_{\mu}(p) = x_{(i^*)}$ wrt : $(w_i, x_i)_{0 \le i \le N}$ where :

•
$$i^* = \min_{0 \le i \le N} |\sum_{\ell=0}^{i} w_{(i)} \ge p$$

$$> x_{(0)} \leq \ldots \leq x_{(N)}$$

•
$$w_i > 0$$
 and $\sum_{i=1}^{N} w_i = 1$

• subject to : $\sum_{i=0}^{N} w_i \varphi_j(x_i) \leq c_j$, for $j = 1, \dots, N$

Alternative : Direct quantile optimization

$Q_{\mu}(p)$ not a measure affine functional

However, quantile-CDF duality ensures that main result still applies :

OUQ for quantiles

To find $\underline{Q_A}(p)$ (resp. $\overline{Q_A}(p)$) :

• Minimize (resp. Maximize) $Q_{\mu}(p) = x_{(i^*)}$ wrt : $(w_i, x_i)_{0 \le i \le N}$ where :

•
$$i^* = \min_{0 \le i \le N} |\sum_{\ell=0}^{i} w_{(i)} \ge p$$

$$> x_{(0)} \leq \ldots \leq x_{(N)}$$

•
$$w_i > 0$$
 and $\sum_{i=1}^N w_i = 1$

• subject to : $\sum_{i=0}^{N} w_i \varphi_j(x_i) \leq c_j$, for $j = 1, \dots, N$

Main difficulty

• Objective function $Q_{\rho}(\mu) = Q_{\rho}((w_i, x_i)_{0 \le i \le N})$ irregular and non convex

Case study : Quantile of nonlinear transform under product measure

Problem specification (simplified version)

$$Q_{\mu}(p) = \sup\{y > 0, \mathbb{P}_{\mu}[G(X) \leq y] \leq p\},$$

where :

- $X = (X_1, \ldots, X_d) \sim \mu$ over $[0, 1]^d$
- $G:[0,1]^d
 ightarrow \mathbb{R}^+$ potentially costly

•
$$\mathcal{A} = \{\mu = \bigotimes_{k=1}^{d} \mu_k \mid \mathbb{E}_{\mu_k}[X_k] = m_k, 1 \le k \le d\}$$

Extreme set of product measures

[Owhadi et al., 2013] show that $\overline{Q}(\mathcal{A}) = \overline{Q}(\mathcal{A}_{\Delta})$ where :

• $Q(\mu)$ measure affine (extendable to quantiles by duality with CDF)

•
$$\mathcal{A}_{\Delta} = \{ \mu = \bigotimes_{k=1}^{d} \left(w_k \delta_{x_{k,0}} + (1 - w_k) \delta_{x_{k,1}} \right) \mid w_k x_{k,0} + (1 - w_k) x_{k,1} = m_k \}$$

To be continued...

THANKS FOR YOUR ATTENTION !!

< □ > < □ > < □ > < 亘 > < 亘 > < 亘 > < 亘 > ○ Q (~ 11/12

References

 McKerns, M., Owhadi, H., Scovel, C., Sullivan, T. J., and Ortiz, M. (2012).
 The optimal uncertainty algorithm in the mystic framework. *CoRR*, abs/1202.1055.

Owhadi, H., Scovel, C., Sullivan, T. J., McKerns, M., and Ortiz, M. (2013). Optimal Uncertainty Quantification . *SIAM Rev.*, 2(55) :271–345.

12/12

Rios Insua, D. and Ruggeri, F. (2000). *Robust Bayesian Analysis*. Springer-Verlag.