Conditional Quantile Optimization via Branch-and-Bound Strategies

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1. Introduction to the hierarchical sequential optimistic optimization via the deterministic case

2. Hierarchical stochastic optimistic optimization

3. How to create confidence intervals?

4. Experiments
Introduction to the hierarchical sequential optimistic optimization via the deterministic case
Assuming there exists at least one $x^* \in \mathcal{X} = [0, 1]^d$ such that

$$f(x^*) = \max_{x \in \mathcal{X}} f(x).$$

Find

$$x^*_T \in \mathcal{X},$$

such that

$$f(x^*_T) \geq \max_{x \in \mathcal{X}} f(x) - \epsilon$$

using a minimal set of sequential observation $f(x_1), \cdots, f(x_T)$. 
Assumption on $f$

Define

$$\ell_{\beta,\gamma}(x, x') = \beta \|x - x'\|^\gamma, \quad \beta > 0, \quad \gamma > 0,$$

we assume

$$\forall x \in X, \ f(x) \geq f(x^*) - \ell_{\beta,\gamma}(x, x^*).$$

**Figure 1:** From [3], the function can be non smooth far from the maximum.

**Remark:** With this assumption we can have guarantees of convergence.
Hierarchical partition

The hierarchical partition $\mathcal{P} = \{\mathcal{P}_{h,j}\}_{h,j}$ is defined recursively as

$$\mathcal{P}_{0,1} = \mathcal{X} \quad \text{and} \quad \mathcal{P}_{h,j} = \bigcup_{i=0}^{K-1} \mathcal{P}_{h+1,kj-i}.$$ 

Hereafter

- $\mathcal{T}_t$ is a sub partition of $\mathcal{P}$.
- For all $\mathcal{P}_{h,j} \in \mathcal{T}_t$ we define $x_{h,j}$ the point at the center of the cell that we call a node.
- $\mathcal{L}_t$ is the set of cells in $\mathcal{T}_t$ that have not been expanded.
- Cells are hyper-rectangle of $[0, 1]^d$ of side $1/2^d$.
- The number of children that one cell can have is $K = 2^d$. 
Hierarchical partition

- $T_t$ is a sub partition of $P$.
- For all $P_{h,j} \in T_t$ we define $x_{h,j}$ the point at the center of the cell that we call a node.
- $L_t$ is the set of cells in $T_t$ that have not been expanded.
- Cells are hyper-scare of $[0,1]^d$ of side $1/2^{hd}$.
- The number of children that one cell can have is $K = 2^d$.

**Figure 2:** Example of hierarchical partitions with $d = 2$, bottom left $L_3 = \{P_{1,1}, P_{1,2}, P_{1,4}, P_{2,9}, P_{2,10}, P_{2,11}, P_{2,12}\}$. 
Given the past observations, in which cell do we sample $f$?

Assume $f$ is observed without noise. The Deterministic Optimistic Optimization (DOO [3]) algorithm associates a upper bound $\bar{u}_{h,j}$ to each $\mathcal{P}_{h,j}$

$$\bar{u}_{h,j} = f(x_{h,j}) + \beta \text{radius}(\mathcal{P}_{h,j})^\gamma$$

and sample at the center of $\mathcal{P}_{\tilde{h},\tilde{j}} = \arg \max_{\mathcal{P}_{h,j} \in \mathcal{P}} (\bar{u}_{h,j})$.

**Figure 3:** Example of DOO with $\beta = 4$ and $\gamma = 1$. 
Given the past observations, in which cell do we sample \( f \)?
Assume \( f \) is observed without noise. The Deterministic Optimistic Optimization (DOO [3]) algorithm associates a upper bound \( \bar{u}_{h,j} \) to each \( P_{h,j} \)

\[
\bar{u}_{h,j} = f(x_{h,j}) + \beta \text{ radius}(P_{h,j})^{\gamma}
\]
and sample at the center of \( \mathcal{P}_{h,j} = \arg \max_{P_{h,j} \in \mathcal{P}} (\bar{u}_{h,j}) \).

![Figure 4: Example of DOO with \( \beta = 4 \) and \( \gamma = 1 \).](image)
Optimistic principle: first approach with the determinist case

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Assume $f$ is observed without noise. The Deterministic Optimistic Optimization (DOO [3]) algorithm associates a upper bound $\bar{u}_{h,j}$ to each $P_{h,j}$

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and sample at the center of $P_{\bar{h},\bar{j}} = \arg \max_{P_{h,j} \in P}(\bar{u}_{h,j})$.

Figure 5: Example of DOO with $\beta = 4$ and $\gamma = 1$. 
Optimistic principle: first approach with the determinist case

**Given the past observations, in which cell do we sample \( f \)?**

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**Figure 6:** Example of DOO with \( \beta = 4 \) and \( \gamma = 1 \).
Given the past observations, in which cell do we sample $f$?

Assume $f$ is observed without noise. The Deterministic Optimistic Optimization (DOO [3]) algorithm associates a upper bound $\bar{u}_{h,j}$ to each $P_{h,j}$

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**Figure 7:** Example of DOO with $\beta = 4$ and $\gamma = 1$. 
Hierarchical stochastic optimistic optimization
Stochastic black box setting

- \( g : \mathcal{X} \times \Omega \to [0, 1] \) is considered as a black box function
- \( g(x, \cdot) = Y_x \) is a random variable of law \( P_x \).
- We are interested in \( f(x) = \psi(P_x) \) with \( \psi \) a real-valued functional.

For example \( f \) can be:

- The conditional expectation (StoOO, HOO, StoSOO, POO,...)
- The conditional quantile
- The CVAR (superquantile)

→ \( f \) is observed with noise
Stochastic Optimistic Optimization (StoOO)

How to take into account the noise?

→ Use repetitions as in the stochastic version of DOO named StoOO designed to optimize the conditional expectation.

Goals:

→ Estimate $f$ locally for all $x_{h,j} \in \mathcal{L}_t$.
→ Create a confidence interval on $f(x_{h,j})$ for all $x_{h,j} \in \mathcal{L}_t$.  


Repetitions, Upper confidence bounds, lower confidence bounds

**Definition**

Let $A$ be a subset of $\mathcal{X}$, we define $\mathcal{U}(A)$ the set of upper confidence bounds of $\sup_{x \in A} f(x)$ and $\mathcal{L}(A)$ the set of lower confidence bounds of $\sup_{x \in A} f(x)$ as

$$
\mathcal{U}(A) = \{\text{random variables } U, \sup_{x \in A} f(x) \leq U \text{ with high probability}\},
$$

$$
\mathcal{L}(A) = \{\text{random variables } L, \sup_{x \in A} f(x) \geq L \text{ with high probability}\}.
$$

**Use repetitions to explicit:**

$$
U_{h,j} \in \mathcal{U}(x_{h,j}) \text{ and } L_{h,j} \in \mathcal{L}(x_{h,j}).
$$

**Then define:**

$$
\bar{U}_{h,j} = U_{h,j} + \beta \text{ radius}(\mathcal{P}_{h,j})\gamma.
$$
How many times do we have to sample a point before expanded it?

Two sources of error in $\mathcal{P}_{h,j}$:

$$\bar{E}_{h,j} = E_{h,j} + B_{h,j}$$

with

$$E_{h,j} = U_{h,j} - L_{h,j} \quad \text{and} \quad B_{h,j} = \beta \text{radius}(\mathcal{P}_{h,j})^\gamma.$$ 

→ As soon as $E_{h,j} < B_{h,j}$, we expand the cell!
How many times do we have to sample a point before expansion?

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Sampling vs Expansion

How many times do we have to sample a point before expansion?

Two sources of error:

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with

\[ E_{h,j} = U_{h,j} - L_{h,j} \quad \text{and} \quad B_{h,j} = \beta \text{radius}(P_{h,j})^\gamma. \]

→ As soon as \( E_{h,j} < B_{h,j} \), we expand the cell!
Stochastic Risk Optimistic Optimization (StoROO)

Algorithm 1 StoROO

1: **Parameters:** error probability $\eta > 0$, number of children $K$, time horizon $T$, $\beta > 0$, $\gamma > 0$
2: **Define:** UCB, LCB
3: **Initialize:**
   Expand into $K$ sub-regions the root node $(0, 0)$ and sample one time each child
4: **while** $t \leq T$ **do**
5:   For each leaf $(h, j) \in L_t$, compute the UCB $U_{h,j}(t)$
6:   Select $(\tilde{h}, \tilde{j}) = \arg \max_{(h,j) \in L_t} \tilde{U}_{h,j}(t)$
7:   Compute the LCB $l_{h,j}(t)$
8:   **if** $U(x_{h,j})(t) - L(x_{h,j})(t) \leq \beta(\text{radius}(P_{h,j}))^\gamma$ **then** expand the node,
9:      remove $(\tilde{h}, \tilde{j})$ from $L_t$, add to $L_t$ the $K$ sub-regions of $P_{h,j}$ and sample each sub-region one time in its center
10: **else** Sample at $x_{h,j}$ and collect $y_{h,j}(t)$
11: **end if**
12: **end while**
13: Return the node having the highest LCB among those that have been expanded.
How to create confidence intervals?
Simple setting:
- We observe a sample $D_n = (Y_{1,x}, \ldots, Y_{n,x})$ of independent and identically distributed random variables.
- $n$ is a deterministic value.

StoOO setting:
- At time $t$ the instants and the number of times each node has been played is random.
- At time $t$ the size of $L_t$ is random.
How to create upper confidence bounds and lower confidence bounds? (Simple setting)

**Hoeffding’s inequality [2]**

Let $Y_1, \cdots, Y_n$ be independent random variables bounded by the interval $[0, 1]$ of expectation $\mathbb{E}(Y)$. Define the empirical mean of these variables by

$$\bar{Y}_n = \frac{1}{n} \sum_{i=1}^{n} Y_i,$$

then

$$\mathbb{P}( |\bar{Y}_n - \mathbb{E}(Y)| \geq \epsilon ) \leq 2 \exp(-2n\epsilon^2).$$

** Bounds for the conditional expectation**

Let $Y_1, \cdots, Y_n$ be independent random variables bounded by the interval $[0, 1]$, define $f(x) = \mathbb{E}_x(Y)$ then

$$\mathbb{P}( \bar{Y}_n - \epsilon \leq f(x) \leq \bar{Y}_n + \epsilon ) \geq 1 - 2 \exp(-2n\epsilon^2).$$
How to create upper confidence bounds and lower confidence bounds? (StoOO setting)

We want a UCB and a LCB for all time $1 \leq t \leq T$ and all nodes. Define

$$
\mathcal{A}_\eta = \bigcap_{t \leq T} \bigcap_{\mathcal{P}_h,j \in \mathcal{P}_t} \left\{ U_{\eta}^{h,j}(t) \geq f(x_{h,j}), \ L_{\eta}^{h,j}(t) \leq f(x_{h,j}) \right\}
$$

**Goal:** create $U_\eta$ and $L_\eta$ so that

$$
\mathbb{P}(\mathcal{A}_\eta) = 1 - \eta
$$

**Difficulty:** at time $t$ the number of node $W$ and the number of time each node has been sample $N_{h,j}(t)$ are random.

**A way to solve this problem:** Using a union bound over all $1 \leq N_{h,j}(t) \leq T$ and $1 \leq W \leq T$. 

How to create upper confidence bounds and lower confidence bounds? (StoOO setting)

**Bounds for the expectation [3]**

\[
\mathbb{P}(\bigcap_{t \leq T} \bigcap_{\mathcal{P}_{h,j} \in \mathcal{P}_t} \left\{ U_{h,j}^\eta(t) \geq f(x_{h,j}), \; L_{h,j}^\eta(t) \leq f(x_{h,j}) \right\}) \geq 1 - \eta,
\]

with

\[
U_{h,j}^\eta(t) = \tilde{Y}_{N_{h,j}(t)} + \epsilon_{h,j}^\eta(T),
\]

\[
L_{h,j}^\eta(t) = \tilde{Y}_{N_{h,j}(t)} - \epsilon_{h,j}^\eta(T),
\]

and

\[
\epsilon_{h,j}^\eta(T) = \sqrt{\frac{\log(2T^2/\eta)}{2N_{h,j}(t)}}.
\]
Bounds on the quantile

Let $Y_1, \ldots, Y_n$ be independent random variables. Define the empirical CDF of these variables by

$$
\hat{F}^n(q) = \frac{1}{n} \sum_{i=1}^{n} 1_{Y_i \leq q}
$$

$$
\hat{q}(\tau) = \hat{F}^- (q(\tau)) = \inf \{ q, \hat{F}(q) \geq \tau \}
$$
Define

\[ Z_i(q(\tau)) = \mathbb{1}_{Y_i \leq q(\tau)} \]

then

\[ \tilde{Z}_n = \hat{F}^n(q(\tau)) \text{ and } \mathbb{E}(Z(q(\tau))) = \tau \]

Using Hoeffding’s inequality:

\[ \mathbb{P}(\tau - \epsilon > \hat{F}^n(q(\tau)) \geq \tau + \epsilon) \geq 2 \exp(-2n\epsilon^2) \]
Bounds on the quantile

If \( \tau + \epsilon < 1 \)

\[
\hat{F}^n(q(\tau)) \geq \tau + \epsilon \iff q(\tau) \geq \hat{q}_{\tau+\epsilon}
\]

If \( \tau - \epsilon > 0 \)

\[
\hat{F}^n(q(\tau)) < \tau - \epsilon \iff q(\tau) \leq \hat{q}(\tau - \epsilon)
\]
Bounds on the quantile (Simple case)

If $\tau + \epsilon < 1$ and $\tau - \epsilon > 0$

$$P(\tau - \epsilon > \hat{F}_n(q(\tau)) \geq \tau + \epsilon) \leq P(\hat{q}(\tau - \epsilon) \geq q(\tau) \geq \hat{q}(\tau + \epsilon)) \leq 2 \exp(-2n\epsilon^2),$$

thus

$$P(\hat{q}(\tau - \epsilon) \leq q(\tau) \leq \hat{q}(\tau + \epsilon)) \geq P(\tau - \epsilon \leq \hat{F}_n(q(\tau)) < \tau + \epsilon) \geq 1 - 2 \exp(-2n\epsilon^2).$$

Define

$$U_x = \begin{cases} 
\inf\{q, \hat{F}_n(q) > \tau + \epsilon\} & \text{if } \tau + \epsilon > 1 \\
1 & \text{otherwise,}
\end{cases}$$

$$L_x = \begin{cases} 
\inf\{q, \hat{F}_n(q) \leq \tau + \epsilon\} & \text{if } \tau - \epsilon > 0 \\
0 & \text{otherwise,}
\end{cases}$$
How to create upper confidence bounds and lower confidence bounds for the quantile? (StoOO case)

**Bounds for the conditional quantile**

Define \( f(x_{h,j}) = q_{h,j}(\tau) \) and

\[
U_{\eta}^{h,j}(t) = \begin{cases} 
\inf\{q, \hat{F}^n(q) > \tau + \epsilon\} & \text{if } \tau + \epsilon > 1 \\
1 & \text{otherwise},
\end{cases}
\]

\[
L_{\eta}^{h,j}(t) = \begin{cases} 
\max\{q, \hat{F}^n(q) \leq \tau - \epsilon\} & \text{if } \tau - \epsilon > 0 \\
0 & \text{otherwise},
\end{cases}
\]

with

\[
\epsilon_{h,j}^\eta(T) = \sqrt{\frac{\log(2T^2/\eta)}{2N_{h,j}(t)}},
\]

then

\[
P\left( \bigcap_{t \leq T} \bigcap_{\mathcal{P}_{h,j} \in \mathcal{P}_t} \left\{ U_{\eta}^{h,j}(t) \geq f(x_{h,j}), \ L_{\eta}^{h,j}(t) \leq f(x_{h,j}) \right\} \right) \geq 1 - \eta.
\]
How to create upper confidence bounds and lower confidence bounds for the quantile?

\[
\epsilon_{h,j}(T) = \sqrt{\frac{\log(2 T^2 / \eta)}{2 N_{h,j}(t)}},
\]

Number of samples so that \(\varepsilon + \tau < 1\), \(\tau = 0.5\)
How to create upper confidence bounds and lower confidence bounds for the quantile?

\[
\epsilon^\eta_{h,j}(T) = \sqrt{\frac{\log(2T^2/\eta)}{2Nh,j(t)}},
\]

Number of samples so that \(\epsilon + \tau < 1\), \(\tau = 0.9\)
First, for \((p, q) \in [0, 1]^2\), let us introduce the definition of the Bernoulli Kullbach-Leibler divergence (KL)

\[
d(q, p) = p \log \frac{p}{q} + (1 - p) \log \frac{1 - p}{1 - q}.
\]

**Chernoff’s inequality for the CDF**

Let \(Y_1, \cdots, Y_n\) be independent and identically distributed random variables bounded by the interval \([0, 1]\). The Chernoff’s inequality implies

\[
P(\hat{F}^n(q(\tau)) \geq x) \leq \exp(-nd(x, \tau)).
\]
Can we do better?[1]

Chernoff’s inequality for the quantile

For all $1 \leq t \leq T$, $1 \leq h \leq t$ and $1 \leq j \leq K^h$, define

$$U_{\eta}^{h,j}(t) = \inf \{ q, \hat{F}_{h,j}^n(q) \geq \tau \text{ and } N_{h,j}(t) d(\hat{F}_{h,j}^n(q), \tau) \geq \log \frac{2t^2}{\eta} \},$$

$$L_{\eta}^{h,j}(t) = \inf \{ q, \hat{F}_{h,j}^n(q) \leq \tau \text{ and } N_{h,j}(t) d(\hat{F}_{h,j}^n(q), \tau) \leq \log \frac{2t^2}{\eta} \}.$$

Define $\mathcal{A}_t$

$$\mathcal{A}_t = \bigcap_{P_{h,j} \in \mathcal{T}_t} \left\{ U_{h,j}(t) \geq q_{h,j}(\tau), L_{h,j}(t) \leq q_{h,j}(\tau) \right\}.$$

The event $\mathcal{A}_t$ holds with probability at least $1 - \eta$. 
Can we do better?[1]

Number of samples so that $\varepsilon + \tau < 1$, $\tau = 0.5$

- KL
- Hoeffding

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Can we do better?[1]

Number of samples so that $\varepsilon + \tau < 1$, $\tau = 0.9$

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KL
Hoeffding
Experiments
Toy problem
Figure 8: Left $\tau = 0, 9$, right $\tau = 0, 1$. On top $\gamma = 1, \beta = 4$, bottom $\gamma = 1, \beta = 2$. 
Figure 9: On the top $\gamma = 1, \beta = 4$, bottom $\gamma = 1, \beta = 2$. Budget = 400.
Figure 10: On the top $\gamma = 1$, $\beta = 4$, bottom $\gamma = 1$, $\beta = 2$. Budget = 1000.
Figure 11: On the top $\gamma = 1$, $\beta = 4$, bottom $\gamma = 1$, $\beta = 2$. Budget = 10000.
Analysis of the regret

The simple regret

\[ r_T = q_{x^*}(\tau) - q_{x_T}(\tau) \]

Figure 12: Expectation of the simple regret for \( \tau = 0.9, \beta = 1, \gamma = 3. \)
Conclusion and perspectives

Conclusions

• We have designed an algorithm able to optimize the conditional quantile.
• The Chernoff bound shows better results.

Perspectives

• To adapt other optimistic algorithms to the optimization of the conditional quantile.
• Refine the confidence bounds. Do not use union bounds to take into account the random time we sample nodes and the random number of cells we have expanded. Using the "Peeling trick" seems promising.
Aurélien Garivier and Olivier Cappé.  
**The kl-ucb algorithm for bounded stochastic bandits and beyond.**  

Wassily Hoeffding.  
**Probability inequalities for sums of bounded random variables.**  

Rémi Munos et al.  
**From bandits to monte-carlo tree search: The optimistic principle applied to optimization and planning.**  
Thank you for your attention!