Quantile Stein Variational Gradient Descent for Batch Bayesian Optimization


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Bayesian Optimization

- **Goal: black-box optimization**

\[
\max_x f(x), \quad f(\cdot): \text{expensive, black-box function.}
\]

- Bayesian Optimization:

Iteratively acquire new points based on an acquisition function:

\[
\begin{align*}
\mathcal{X}^{\text{new}} & \leftarrow \arg \max_x \alpha(x \mid \mathcal{D}), \\
\mathcal{D}^{\text{new}} & \leftarrow \mathcal{D} \cup \{x^{\text{new}}, f(x^{\text{new}})\},
\end{align*}
\]

**Acquisition function:**

\[
\alpha(x \mid \mathcal{D}) := \mathbb{E}_f[f(x) \mid \mathcal{D}] + \eta \sqrt{\text{var}_f[f(x) \mid \mathcal{D}].} \quad (UCB)
\]
**Batch Bayesian Optimization:**
Find multiple query points $\{x_i\}_{i=1}^m$ in parallel at every iteration.

Much more challenging; two desiderata:
- **Diversity**: Everyone should be unique.
- **Qualification**: Everyone should be good.

[Diagram showing acquisition function and next query points]
Optimizing the distribution $\rho$ of query points $\{x_i\}$ by

$$\max_\rho \left\{ F[\rho] := \mathbb{E}_\rho[\alpha(x)] + \eta H[\rho] \right\}.$$ 

$H[\rho]$ is the entropy. It encourages the **diversity**.

$\mathbb{E}_\rho[\cdot]$ is a quantile distorted expectation. It enforces **qualification**, 

$$\mathbb{E}_\rho[\alpha(x)] = \int_0^1 Q_{f,\rho}^\beta \omega(\beta) d\beta,$$

$Q_{f,\rho}^\beta$ is the $\beta$-th quantile of $\alpha(x)$, when $x \sim \rho$.

$\omega: [0, 1] \to \mathbb{R}_+$ is a distortion function:

- **Risk neutral**: $\omega(\beta) = 1$.
- **Risk aversion**: $\omega(\beta)$ is monotonic decreasing.
- **Risk seeking**: $\omega(\beta)$ is monotonic increasing.

We want risk aversion: Take $\omega(\beta) = \beta^{-\lambda}$, where $\lambda \geq 0$. 

Quantile Stein Variational Gradient Descent [Liu, Wang 16]

Idea: Find particle distributions

\[ \rho := \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i} / n \]

to approximately solve the optimization. The particles \( \{x_i\}_{i=1}^{n} \) are iteratively moved to maximize the objective by gradient-like updates

\[ x_i' \leftarrow x_i + \epsilon \phi^*(x_i), \quad \phi^* = \arg \max_{\phi \in \mathcal{H}} \left\{ \frac{d}{d\epsilon} F[\rho'] \bigg|_{\epsilon=0} \quad s.t. \quad ||\phi||_{\mathcal{H}} \leq 1 \right\}, \]

\( \epsilon \): step-size; \( \phi^* \): chosen to maximize the objective function as fast as possible. \( \mathcal{H} \): a reproducing kernel Hilbert space (RKHS) with positive definite kernel \( k(x, x') \).
Quantile Stein Variational Gradient Descent [Liu, Wang 16]

Optimization:

$$\max_{\rho} \left\{ F[\rho] := \mathbb{E}_{\rho}[\alpha(x)] + \eta H[\rho] \right\}.$$ 

Algorithm:

$$x_i \leftarrow x_i + \frac{\epsilon}{n} \sum_{j=1}^{n} \left[ \xi(x_j) \nabla x \alpha(x_j) k(x_j, x_i) + \eta \nabla x_j k(x_j, x_i) \right], \quad \forall i = 1, \ldots, n.$$ 

Here, each particle is assigned a weight to account the distortion function:

$$\xi(x_j) = \omega \left( \frac{\text{rank}(x_j)}{n} \right), \quad \text{rank}(x_j) = \sum_{\ell=1}^{n} \mathbb{I}[\alpha(x_\ell) \leq \alpha(x_j)].$$
### Empirical Results

#### Standard Benchmarks

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>LP-UCB</th>
<th>DPP</th>
<th>MACE</th>
<th>QSBO-UCB</th>
</tr>
</thead>
<tbody>
<tr>
<td>Branin</td>
<td>3.28e-4</td>
<td>9.63e-4</td>
<td><strong>2.85e-5</strong></td>
<td>5.14e-5</td>
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<td>Eggholder</td>
<td>51.34</td>
<td>82.81</td>
<td>74.14</td>
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<td>Dropwave</td>
<td>0.14</td>
<td>0.13</td>
<td>0.09</td>
<td><strong>0.07</strong></td>
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<tr>
<td>CrossInTray</td>
<td>6.83e-3</td>
<td>7.64e-3</td>
<td>3.78e-4</td>
<td><strong>1.35e-4</strong></td>
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<tr>
<td>gSobol5</td>
<td>1.85</td>
<td>2.34</td>
<td>1.14</td>
<td><strong>0.32</strong></td>
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<tr>
<td>gSobol10</td>
<td>1.04e2</td>
<td>1.07e3</td>
<td>48.92</td>
<td><strong>31.19</strong></td>
</tr>
<tr>
<td>gSobol15</td>
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<td>5.28e3</td>
<td>6.39e2</td>
<td><strong>3.61e2</strong></td>
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<tr>
<td>Ackley5</td>
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<td>3.74</td>
<td>2.36</td>
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<tr>
<td>Ackley10</td>
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<td>4.23</td>
<td>3.01</td>
<td><strong>2.41</strong></td>
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<tr>
<td>Alpine2</td>
<td>75.92</td>
<td>73.39</td>
<td><strong>63.29</strong></td>
<td>73.01</td>
</tr>
</tbody>
</table>

**Table:** Negative Rewards
Empirical Results

Automatic Chemical Design (Gomez-Bombarelli et. al., 2018; Griffiths, 2017)

<table>
<thead>
<tr>
<th></th>
<th>LP-UCB</th>
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<th>MACE</th>
<th>QSBO-UCB</th>
</tr>
</thead>
<tbody>
<tr>
<td>QED</td>
<td>0.91±0.05</td>
<td>0.91±0.06</td>
<td>0.92±0.03</td>
<td><strong>0.93±0.03</strong></td>
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<td>SAS</td>
<td>2.18±0.06</td>
<td>2.29±0.08</td>
<td>2.16±0.04</td>
<td><strong>2.08±0.05</strong></td>
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<td>LogP</td>
<td>0.50±0.11</td>
<td>0.47±0.07</td>
<td>0.41±0.06</td>
<td><strong>0.33±0.08</strong></td>
</tr>
</tbody>
</table>

Figure: Illustration of the search process of our QSBO-UCB.
Conclusions

1. A new algorithm (QSVGD) for risk-sensitive objective
2. Risk-aversion samples for batch Bayesian optimization
3. Good empirical results

Thank You

Poster #239, Today 06:30 PM –09:00 PM @ Pacific Ballroom