Sequential Design of Computer Experiments for Numerical Dosimetry

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Motivation

Sequential Design of Computer Experiments ...

Estimation of the $\alpha$-quantile $q_\alpha$ of the distribution of $Y = f(X)$, for a given $\alpha$ in $(0, 1)$,

$$q_\alpha = \inf \{ q : \mathbb{P}(Y \leq q) > \alpha \} .$$

- $f$ is an unknown, expensive-to-evaluate real-valued function
- $X$ is a random vector having a known distribution on a compact subset $A \subseteq \mathbb{R}^d$.

We aim at estimating $q_\alpha$ by using as few evaluations of $f$ as possible

... for Numerical Dosimetry

At which level are fetuses exposed to Radio Frequency Electromagnetic Fields?
Background: Gaussian Process Modelling

Assume that $f$ is a sample of a zero-mean Gaussian process (GP) having a covariance function $k: \text{GP}(0, k(., .))$

Conditionally to $y_t = (y_1, \ldots, y_t)'$, the mean $\mu_t(u)$ and covariance $k_t(u, \nu)$ are given by

$$\mu_t(u) = k_t(u)'K_t^{-1}y_t,$$
$$k_t(u, \nu) = k(u, \nu) - k_t(u)'K_t^{-1}k_t(\nu),$$

where $k_t(u) = [k(x_1, u) \ldots k(x_t, u)]'$, ' denotes the matrix transposition, $K_t = [k(x_i, x_j)]_{1 \leq i, j \leq t}$, $u$ and $\nu$ and the $x_i$'s are in $A$.

Covariance function

Since the SAR is supposed to be smooth, we shall use the square exponential covariance function

$$k_{\text{SE}}(u, \nu) = \exp \left( -\frac{\|u - \nu\|^2}{2\ell^2} \right), u, \nu \in A, \ell > 0,$$

where $\|u\|$ denotes the euclidean norm of $u$ in $\mathbb{R}^d$. 
Background: Methodologies

Sequential strategies
Bayesian optimization: find the maximum of $f$, optimizing an acquisition function
- Expected Improvement [Vazquez et al., 2010]
- Confidence Bound Criteria (GP-UCB [Srinivas et al., 2010], Branch and Bounds [De Freitas et al., 2012])

EI has been adapted for
- Contour estimation [Ranjan et al., 2009]
- Estimation of $\mathbb{P}(Y \geq s)$ where $s$ is a given threshold (SUR) [Bect et al., 2012]

Quantile estimation
- Non sequential approach [Oakley, 2004]
- Extension of the SUR criterion [Arnaud et al., 2010]

We really need a sequential strategy, but improvement based criteria demand Monte Carlo samplings of the GP and the conditional GPs, which made them difficult to use for $d > 2$
Quantile estimation

We shall compare the quantile estimators with $\tilde{q}_{\alpha,m}$ defined by

$$\tilde{q}_{\alpha,m} = \inf \left\{ q : \frac{1}{m} \sum_{i=1}^{m} 1_{\{f(x_i) \leq q\}} > \alpha \right\} ,$$

where $x_1, \ldots, x_m$ are $m$ fixed points in $A$.

Let $A = \{x_1, \ldots, x_m\} \subset A$.

Pure exploration criterion

- Minimizes the global uncertainty on the estimation of $f$
- New point $x_{t+1}$ to add to the set of $t$ observations:

$$x_{t+1} \in \arg \max_{x \in A} \sigma_t(x) .$$

- Propose methodologies more adapted to our quantile estimation issue to realize the exploration-exploitation trade-off
Let \( \mu_t^U(x) = \mu_t(x) + \sqrt{\beta_t} \sigma_t(x) \) and \( \mu_t^L(x) = \mu_t(x) - \sqrt{\beta_t} \sigma_t(x) \)

with \( \beta_t = 2 \ln \left( \frac{\pi^2 t^2}{6} \right) + 2 \ln \left( \frac{m}{\delta} \right) \) where \( m \) is the cardinal of \( A \)

Let \( \hat{q}_{\alpha,t}^U \) and \( \hat{q}_{\alpha,t}^L \) be the estimators of the \( \alpha \)-quantile of \( \mu_t^U \) and \( \mu_t^L \)

\[
\hat{q}_{\alpha,t}^U = \inf \left\{ q : \frac{1}{m} \sum_{i=1}^{m} 1_{\left\{ \mu_t^U(x_i) \leq q \right\}} > \alpha \right\}
\]

\[
\hat{q}_{\alpha,t}^L = \inf \left\{ q : \frac{1}{m} \sum_{i=1}^{m} 1_{\left\{ \mu_t^L(x_i) \leq q \right\}} > \alpha \right\}
\]

**Proposition**

For all \( \delta \) in \( (0, 1) \), for all \( t \geq 1 \), with probability greater than \( (1 - \delta) \),

\[
\tilde{q}_{\alpha,m} \in [\hat{q}_{\alpha,t}^L, \hat{q}_{\alpha,t}^U]
\]
Let $U_{\alpha,t}$ and $L_{\alpha,t}$ be the following sets:

$$U_{\alpha,t} = \left\{ x \in A : \mu_t^U(x) \geq \hat{q}_{\alpha,t} \right\} \text{ and } L_{\alpha,t} = \left\{ x \in A : \mu_t^L(x) \leq \hat{q}_{\alpha,t} \right\}, \quad t \geq 1.$$ 

**Proposition**

With probability greater than $(1 - \delta)$, for all $t \geq 1$,

$$|\hat{q}_{\alpha,t} - \tilde{q}_{\alpha,m}| \leq \sqrt{\beta_t} \sup_{x \in U_{\alpha,t}} \sigma_t(x).$$

**Criterion**

$x_{t+1}$ to add to the set of $t$ observations is such that:

$$x_{t+1} \in \arg \max_{x \in U_{\alpha,t}} \sigma_t(x).$$
Illustration: 1D Gaussian Process sample path

$t = 3$

$t = 4$

$t = 6$

$t = 8$

$t = 10$

$t = 12$
Let $S_{\alpha,t} \subseteq A$ be the compact subset such that $S_{\alpha,t} = \prod_{i=1}^{d} [x_{\min,t}^{(i)}, x_{\max,t}^{(i)}] \times \cdots \times [x_{\min}^{(d)}, x_{\max}^{(d)}]$. Here $x_{\min,t}^{(i)}$ and $x_{\max,t}^{(i)}$ denote the smallest (resp. the largest) $i$th component of the points in $\bar{U}_{\alpha,t}$

where $\bar{U}_{\alpha,t} = \left\{ x \in S_{\alpha,t-1} : \mu_t^{U}(x) \geq \hat{q}_{\alpha,t}^L \right\}$

where $S_{\alpha,t} = \{x_{t,1}, \ldots, x_{t,m_t}\} \cup \bar{U}_{\alpha,t}$,

where $\{x_{t,1}, \ldots, x_{t,m_t}\}$ are $m_t$ points randomly chosen in $S_{\alpha,t}$

By convention $S_{\alpha,0} = A$.

Criterion

$x_{t+1}$ to add to the set of $t$ observations is such that:

$$x_{t+1} \in \arg \max_{x \in U_{\alpha,t}} \sigma_t(x)$$

Note: Since the size of the grid varies at each iteration of the process, we use $\beta_t = 2 \ln \left( \frac{\pi^2 t^2}{6} \right) + 2 \ln \left( \frac{|S_{\alpha,t-1}|}{\delta} \right)$. 
Illustration: 2D Gaussian Process sample path

$t = 2$

$t = 62$

$t = 102$

$t = 162$
Numerical Dosimetry?

In general
Virtually expose human 3D-models to one source of EMF in order to evaluate the Specific Absorption Rate (the SAR, in $W.kg^{-1}$)
SAR computation in our case is done through Finite Difference in Time Domain (FDTD) method
The SAR depends on
- the geometry of the models
- the dielectric properties of the tissues
- the type and position of the EMF source

Fetus exposure
- Very few models are available
- The simulations are expensive in terms of computational load
- The preparation of the simulations is very complex

We focus on the fetal brain exposure
Application I: GPS, Japanese model and plane wave

- Plane wave exposure: far field sources (base stations antennas, WiFi boxes)
- 900 MHz vertically polarized electromagnetic plane waves with a 1 Volt per meter amplitude
- Start by performing 5 randomly chosen evaluations of the SAR in order to have an estimation of $I$
Application I: GPS, Japanese model and plane wave (cont.)

3D-plot

Contour plot and observations

Relative errors

Quantile convergence
Application II: GPS+, Victoria and Samsung Galaxy Tab

- Model Victoria is sitting working on her Samsung Galaxy Tab at 3G frequency (1940 MHz)
- 3 parameters: height, nearness and slope of the tablet
- Start by performing 20 evaluations of the SAR from a LHS in order to have an estimation of /
Application II: GPS+, Victoria and Samsung Galaxy Tab (cont.)

Quantile convergence

ℓ convergence
Conclusion

- We propose two novel sequential approaches for quantile estimation
- Successfully applied to real data coming from numerical dosimetry