Quantile Estimation via a Combination of Conditional Monte Carlo and Latin Hypercube Sampling

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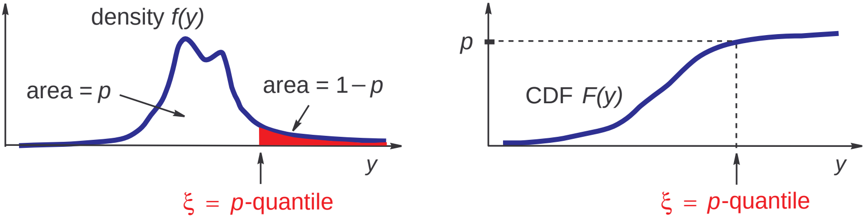
Evaluating Risk

Fukushima Daiichi Nuclear Power Plant, 2011 (Photo: Tepco)

- Complex stochastic system operating in uncertain environment.
  - Financial markets
  - Critical infrastructure
- Model's complexity makes it analytically intractable.
- Use (quasi) Monte Carlo simulation to evaluate risk.
- Risk often measured with quantile.

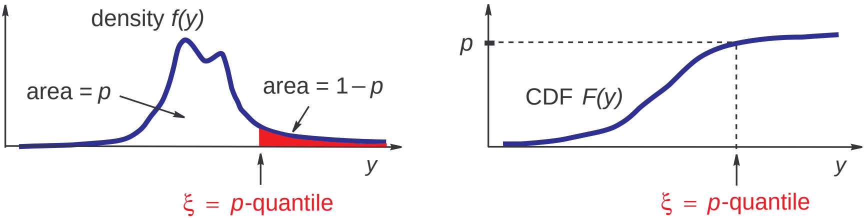


- Simulation model outputs random variable (RV) Y.
  - Can't evaluate CDF F nor density f of Y.
- For $0 < p < 1$, the p-quantile of F (or Y) is

$$\xi = F^{-1}(p) \equiv \inf\{y : F(y) \geq p\}$$

  - Median is the 0.5-quantile.
  - p-quantile also called $100p$th percentile.
- Quantiles often used to measure risk.

Application: Value-at-Risk (VaR)



- In finance, quantile called value-at-risk (VaR).
- Stochastic model of loss of portfolio.
- Y = Loss of portfolio over time horizon, e.g., two weeks.
- Basel II Accord
  - Capital requirements specified in terms of 0.99-quantile of Y.

Application: Nuclear Power Plants

Springfield Nuclear Power Plant (Image: The Simpsons)

- Probabilistic safety assessment (PSA) using simulation
  - Computationally expensive
- Y = **peak cladding temperature** during hypothesized accident
- "95/95 criterion" of Nuclear Regulatory Commission (NRC).
  - 95% confidence that 0.95-quantile $\leq$ mandated **fixed** capacity.
- Need confidence interval (CI) for quantile.

Variance-Reduction Techniques (VRTs) for Quantile Estimation

- Simple random sampling (SRS) estimator of p-quantile ξ may have large sampling error.
  - Especially when $p \approx 0$ or $p \approx 1$.
- VRTs for quantile estimation.
  - Importance sampling (IS): Glynn (1996), Glasserman et al. (2000), Sun & Hong (2010), Chu & N. (2012)
  - Control variates (CV): Hsu & Nelson (1990), Hesterberg & Nelson (1998), Chu & N. (2012)
  - Antithetic variates (AV): Chu & N. (2012)
  - Conditional Monte Carlo (CMC): N. (2014), Asmussen (2018)
  - Latin hypercube sampling (LHS): Avramidis & Wilson (1998), Jin et al. (2003), Dong & N. (2017a)
- General approach
  1. Use VRT to estimate CDF F.
  2. Invert CDF estimator to obtain estimator of quantile $\xi = F^{-1}(p)$.
- This talk combines CMC+LHS to estimate quantile [Dong & N. (2017b,2018)].

- Goal: use simulation to estimate p-quantile ξ of CDF F

Assumptions

1. $Y = c_Y(U_1, U_2, \ldots, U_d) \sim F$
    - $c_Y : \Re^d \to \Re$
    - $U_1, U_2, \ldots, U_d$ i.i.d. unif$[0, 1)$
2. $f(\xi) \equiv F'(\xi)$ exists and $f(\xi) > 0$.

- Next review simple random sampling (SRS) [Serfling (1980)].

Quantile Estimation via Simple Random Sampling (SRS)

- Generate $n \times d$ i.i.d. unif$[0,1)$ RVs $U_{i,j}$:

$$\boxed{\begin{array}{lcll} Y_1 & = & c_Y(\, U_{1,1},\, U_{1,2}, \ldots, U_{1,d}\,) & \sim \quad F \\ Y_2 & = & c_Y(\, U_{2,1},\, U_{2,2}, \ldots, U_{2,d}\,) & \sim \quad F \\ & \vdots & & \\ Y_n & = & c_Y(\, U_{n,1},\, U_{n,2}, \ldots, U_{n,d}\,) & \sim \quad F \end{array}}$$

- SRS estimator of CDF $F(y) = P(Y \leq y) = E[\, I(Y \leq y)\,]$ is

$$\hat{F}_n(y) = \frac{1}{n} \sum_{i=1}^{n} I(Y_i \leq y).$$

- SRS estimator of p-quantile $\xi = F^{-1}(p)$ is

$$\hat{\xi}_n = \hat{F}_n^{-1}(p) = Y_{\lceil np \rceil : n},$$

where $Y_{1:n} \leq Y_{2:n} \leq \cdots Y_{n:n}$ are order statistics.

CLT Follows From Bahadur Representation

- SRS CLT [Smirnov (1952)]:

$$\sqrt{n}\left[\hat{\xi}_n - \xi\right] \Rightarrow N(0, \tau^2_{\mathrm{SRS}}), \quad n \to \infty,$$

$$\tau^2_{\mathrm{SRS}} = \frac{\psi^2_{\mathrm{SRS}}}{f^2(\xi)} \quad \text{with} \quad \psi^2_{\mathrm{SRS}} = \mathrm{Var}[I(Y \le \xi)] = p(1-p)$$

- CLT follows from Bahadur representation

$$\boxed{\hat{\xi}_n \;=\; \xi \;-\; \frac{\hat{F}_n(\xi) - p}{f(\xi)} + R_n}, \qquad R_n = \text{remainder}$$

- **Idea:** Approximate (complicated) quantile estimator

$$\hat{\xi}_n = \hat{F}_n^{-1}(p)$$

in terms of (simpler) CDF estimator

$$\hat{F}_n(y) = \frac{1}{n}\sum_{j=1}^{n} I(Y_j \le y)$$

Basic idea of proof:

- Suppose $f(\xi) > 0$, where $f = F'$.
- Uniformly for x in nbhd $B_n(\xi)$ of ξ,

$$\hat{F}_n(x) \approx \hat{F}_n(\xi) + F(x) - F(\xi)$$

- $\hat{\xi}_n \in B_n(\xi)$ for sufficiently large n, so

$$\begin{aligned} p &\approx \hat{F}_n(\hat{\xi}_n) \\ &\approx \hat{F}_n(\xi) + F(\hat{\xi}_n) - F(\xi) \\ &\approx \hat{F}_n(\xi) + f(\xi)\,(\hat{\xi}_n - \xi) \qquad \text{[by Taylor approx]} \end{aligned}$$

- Rearranging terms gives

$$\boxed{\hat{\xi}_n \approx \xi - \frac{\hat{F}_n(\xi) - p}{f(\xi)}}$$

Bahadur Representation when using SRS

- More precisely: replace $\approx$ with $=$ by introducing error term R_n

$$\hat{\xi}_n = \xi - \frac{\hat{F}_n(\xi) - p}{f(\xi)} + R_n$$

  - Bahadur (1966): If $f(\xi) > 0$ and $f'(x)$ bdd in nbhd of ξ,

$$R_n = O(n^{-3/4} \log n) \text{ a.s.}$$

  - Ghosh (1971): If $f(\xi) > 0$,

$$\sqrt{n}\, R_n \Rightarrow 0$$

- CLT: Because $\hat{F}_n(\xi) = \frac{1}{n}\sum_{i=1}^{n} I(Y_i \le \xi)$ with $\text{Var}[I(Y \le \xi)] = \psi^2_{\text{SRS}}$,

$$\sqrt{n}\left[\hat{\xi}_n - \xi\right] = \underbrace{-\sqrt{n}\left(\frac{\hat{F}_n(\xi) - p}{f(\xi)}\right)}_{\Rightarrow N\left(0,\ \frac{\psi^2_{\text{SRS}}}{f^2(\xi)}\right)} + \underbrace{\sqrt{n}\, R_n}_{\Rightarrow 0}$$

Bahadur Representation when using VRT

Theorem

- *Consider VRT estimator* $\hat{F}_n$ *of* F.
- *Assume* $f(\xi) > 0$, $\hat{F}_n(\xi)$ *obeys CLT, and regularity conditions on* $\hat{F}_n$.
- *Then VRT p-quantile estimator* $\hat{\xi}_n = \hat{F}_n^{-1}(p)$ *satisfies Bahadur rep.*

$$\boxed{\hat{\xi}_n \ = \ \xi \ - \ \frac{\hat{F}_n(\xi) - p}{f(\xi)} \ + \ R_n}$$

where

$$\boxed{\sqrt{n}\, R_n \ \Rightarrow \ 0}$$

Bahadur Representation when using VRT

Theorem

- *Consider VRT estimator $\hat{F}_n$ of F.*
- *Assume $f(\xi) > 0$, $\hat{F}_n(\xi)$ obeys CLT, and regularity conditions on $\hat{F}_n$.*
- *Then VRT p-quantile estimator $\hat{\xi}_n = \hat{F}_n^{-1}(p)$ satisfies Bahadur rep.*

$$\boxed{\hat{\xi}_n \;=\; \xi \;-\; \frac{\hat{F}_n(\xi) - p}{f(\xi)} \;+\; R_n}$$

where

$$\boxed{\sqrt{n}\, R_n \;\Rightarrow\; 0}$$

- Sun and Hong (2010): a.s. Bahadur rep. for importance sampling (IS)
- Chu and N. (2012): weak Bahadur rep. for IS+SS, CV, AV
- Dong and N. (2017a): weak Bahadur rep. for LHS
- Dong and N. (2018): weak Bahadur rep. for CMC+LHS

This Talk: Combine CMC and LHS

- **This talk:** quantile estimation via combination of CMC+LHS
  - Avramidis & Wilson (1996) use CMC+LHS to estimate mean.
- **Key insight:** LHS substantially reduces variance when response is nearly additive function of inputs.
  - SRS and LHS response is indicator,

$$\hat{F}_{\mathrm{LHS},n}(\xi) = \frac{1}{n}\sum_{i=1}^{n} I(Y_i \leq \xi),$$

    so poor additive fit.
  - CMC has smoother response, so better additive fit.

Latin Hypercube Sampling (LHS)

- LHS: McKay, Beckman, Conover (1979).
  - Efficient extension stratified sampling to high dimensions.
  - Reduces variance by inducing negative correlation among responses.
- **Basic idea:** generate correlated sample outputs, n at a time.
  - Recall: $c_Y(\, U_1,\, U_2,\, \ldots,\, U_d\,) \sim F$ if $U_j \sim$ unif[0, 1) i.i.d.
  - Generate $(V_{i,1}, V_{i,2}, \ldots, V_{i,d})$ as d-vector of i.i.d. unif[0, 1).

$$
\begin{array}{ccccc}
Y_1 & = & c_Y(\, V_{1,1},\, V_{1,2}, \ldots, V_{1,d}\,) & \sim & F \\
Y_2 & = & c_Y(\, V_{2,1},\, V_{2,2}, \ldots, V_{2,d}\,) & \sim & F \\
 & \vdots & & & \\
Y_n & = & c_Y(\, V_{n,1},\, V_{n,2}, \ldots, V_{n,d}\,) & \sim & F
\end{array}
$$

  - Columns are independent.
  - Rows are dependent.
- $Y_1, Y_2, \ldots, Y_n$ are dependent and called LHS sample of size n.

Latin Hypercube Sampling (LHS)

- Generate $n \times d$ independent unif RVs:

$$\boxed{\begin{array}{cccc} U_{1,1} & U_{1,2} & \cdots & U_{1,d} \\ U_{2,1} & U_{2,2} & \cdots & U_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ U_{n,1} & U_{n,2} & \cdots & U_{n,d} \end{array}} \quad \begin{array}{lll} \sim & \text{unif}[0, \frac{1}{n}) & \text{i.i.d.} \\ \sim & \text{unif}[\frac{1}{n}, \frac{2}{n}) & \text{i.i.d.} \\ & \vdots & \\ \sim & \text{unif}[\frac{n-1}{n}, 1) & \text{i.i.d.} \end{array}$$

- Randomly permute entries in each column independently to get

$$\boxed{\begin{array}{cccc} V_{1,1} & V_{1,2} & \cdots & V_{1,d} \\ V_{2,1} & V_{2,2} & \cdots & V_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ V_{n,1} & V_{n,2} & \cdots & V_{n,d} \end{array}} \quad \begin{array}{lll} \sim & \text{unif}[0, 1) & \text{i.i.d.} \\ \sim & \text{unif}[0, 1) & \text{i.i.d.} \\ & \vdots & \\ \sim & \text{unif}[0, 1) & \text{i.i.d.} \end{array}$$

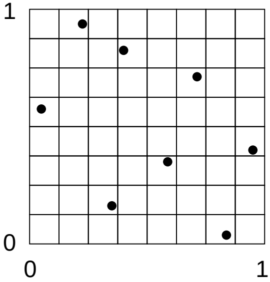
  - Each row consists of d i.i.d. unif$[0, 1)$.
  - Rows dependent because entries in each column permuted.

$$\begin{array}{rcl} Y_1 & = & c_Y(\, V_{1,1},\, V_{1,2},\, \ldots,\, V_{1,d}\,) \sim F \\ Y_2 & = & c_Y(\, V_{2,1},\, V_{2,2},\, \ldots,\, V_{2,d}\,) \sim F \\ & \vdots & \\ Y_n & = & c_Y(\, V_{n,1},\, V_{n,2},\, \ldots,\, V_{n,d}\,) \sim F \end{array}$$

- Each row consists of d i.i.d. unif$[0,1)$, so each $Y_i \sim F$.
- $Y_1, Y_2, \ldots, Y_n$ dependent because each column permuted.

Example

- LHS sample of size $n = 8$ in dimension $d = 2$
- Plot $(V_{i,1}, V_{i,2})$, $i = 1, 2, \ldots, n$.
- Each coordinate stratified.



Quantile Estimation via LHS

- Generate LHS sample $Y_1, Y_2, \ldots, Y_n$
  - Each $Y_i \sim F$
  - $Y_1, Y_2, \ldots, Y_n$ dependent
- LHS estimator of CDF $F(y) = P(Y \leq y) = E[\, I(Y \leq y)\,]$ is

$$\hat{F}_{\mathrm{LHS},n}(y) = \frac{1}{n} \sum_{i=1}^{n} I(Y_i \leq y).$$

- LHS estimator of p-quantile $\xi = F^{-1}(p)$ is

$$\hat{\xi}_{\mathrm{LHS},n} = \hat{F}^{-1}_{\mathrm{LHS},n}(p) = Y_{\lceil np \rceil :n}.$$

- CLT [Avramidis & Wilson (1998)]: $\sqrt{n} \left[\hat{\xi}_{\mathrm{LHS},n} - \xi \right] \Rightarrow N(0, \tau^2_{\mathrm{LHS}})$,

$$\tau^2_{\mathrm{LHS}} = \frac{\psi^2_{\mathrm{LHS}}}{f^2(\xi)}$$

- Numerator ψ^2_{LHS} is from CLT for CDF estimator:

$$\sqrt{n} \left[\hat{F}_{\mathrm{LHS},n}(\xi) - F(\xi) \right] \Rightarrow N(0, \psi^2_{\mathrm{LHS}})$$

Numerator of LHS Variance

- LHS removes variance of additive part of CDF estimator $\hat{F}_n(\xi)$ [Avramidis & Wilson (1998)]
  - $\hat{F}_{\mathrm{LHS},n}(\xi)$ averages identically distrib. but dependent copies of response

$$I(Y \le \xi) = I\left(c_Y(V_1, \ldots, V_d) \le \xi\right) \equiv A(V_1, \ldots, V_d) \equiv A$$

  - Additive approximation using ANOVA decomp [Hoeffding (1948)] with residual ϵ:

$$A(V_1, \ldots, V_d) \;=\; F(\xi) + \sum_{j=1}^{d} \Big(E\left[\, A \mid V_j \,\right] - F(\xi) \Big) + \epsilon$$

  - Numerator ψ^2_{LHS} of LHS quantile estimator's asymptotic variance

$$\psi^2_{\mathrm{LHS}} \;=\; \mathrm{Var}[\epsilon] \;=\; \psi^2_{\mathrm{SRS}} - \textstyle\sum_{j=1}^{d} \mathrm{Var}\Big[\, E\left[\, A \mid V_j \,\right] \Big]$$

- If response is nearly additive, LHS substantially reduces variance.
- But poor additive approximation for indicator response A, so LHS may not reduce variance much.

CMC: Trotter and Tukey (1954), Hammersley (1956)

- Analytically integrate out some variability to reduce variance

$$F(y) = E\,[I(Y \le y)] = E\Big[\, E\,[I(Y \le y) \mid \boldsymbol{X}] \,\Big] \equiv E\,[\, q(\boldsymbol{X}, y)\,]$$

- $\boldsymbol{X}$ is auxiliary random vector
- Assume we can compute

$$q(\boldsymbol{X}, y) = E\,[I(Y \le y) \mid \boldsymbol{X}] = P(Y \le y \mid \boldsymbol{X})$$

- Variance decomposition

$$\begin{aligned}\mathrm{Var}[I(Y \le y)] &= \mathrm{Var}\Big[E[I(Y \le y) \mid \boldsymbol{X}]\Big] + E\Big[\mathrm{Var}[I(Y \le y) \mid \boldsymbol{X}]\Big] \\ &\ge \mathrm{Var}\Big[E[I(Y \le y) \mid \boldsymbol{X}]\Big] = \mathrm{Var}[\, q(\boldsymbol{X}, y)\,]\end{aligned}$$

CMC quantile estimation [Nakayama (2014), Asmussen (2018)]

- Generate $\boldsymbol{X}_1, \boldsymbol{X}_2, \ldots, \boldsymbol{X}_n$ as i.i.d. copies of $\boldsymbol{X}$.
- CMC estimator of CDF $F(y) = P(Y \leq y) = E[q(\boldsymbol{X}, y)]$:

$$\hat{F}_{\mathrm{CMC},n}(y) = \frac{1}{n} \sum_{i=1}^{n} q(\boldsymbol{X}_i, y)$$

- CMC estimator of p-quantile $\xi = F^{-1}(p)$

$$\hat{\xi}_{\mathrm{CMC},n} = \hat{F}^{-1}_{\mathrm{CMC},n}(p)$$

- Computing $\hat{\xi}_{\mathrm{CMC},n}$ typically requires root-finding method.

Combining CMC+LHS

- Assume conditioning vector $\boldsymbol{X}$ satisfies

$$\begin{aligned}(Y, \boldsymbol{X}) &= c_*(U_1, U_2, \ldots, U_d) \\ &= (\, c_Y(U_1, U_2, \ldots, U_d), c_X(U_1, U_2, \ldots, U_{d'})\,)\end{aligned}$$

  - Y and $\boldsymbol{X}$ generated from same i.i.d. uniforms $U_1, U_2, \ldots, U_d$.
  - But $\boldsymbol{X}$ only requires the first $d' \leq d$ of the uniforms.
  - Avramidis & Wilson (1996): similar assumption for estimating a mean.
- CMC+LHS: generate dependent $\boldsymbol{X}$'s using LHS grid of unif $V_{i,j}$:

$$\boxed{\begin{array}{rcl} \boldsymbol{X}_1 & = & c_X(\, V_{1,1},\, V_{1,2},\, \ldots,\, V_{1,d'}\,) \\ \boldsymbol{X}_2 & = & c_X(\, V_{2,1},\, V_{2,2},\, \ldots,\, V_{2,d'}\,) \\ & \vdots & \\ \boldsymbol{X}_n & = & c_X(\, V_{n,1},\, V_{n,2},\, \ldots,\, V_{n,d'}\,) \end{array}}$$

- Estimate $F(y) = E[q(\boldsymbol{X}, y)]$ and p-quantile $\xi = F^{-1}(p)$ by

$$\hat{F}_{\mathrm{CMC+LHS},n}(y) = \frac{1}{n}\sum_{i=1}^{n} q(\boldsymbol{X}_i, y) \;\;\&\;\; \hat{\xi}_{\mathrm{CMC+LHS},n} = \hat{F}^{-1}_{\mathrm{CMC+LHS},n}(p)$$

CMC+LHS: Asymptotic Variance

- CMC+LHS CLT:

$$\sqrt{n}\left[\hat{\xi}_{\mathrm{CMC+LHS},n} - \xi\right] \Rightarrow N(0, \tau^2_{\mathrm{CMC+LHS}}), \quad n \to \infty,$$

$$\tau^2_{\mathrm{CMC+LHS}} = \frac{\psi^2_{\mathrm{CMC+LHS}}}{f^2(\xi)}$$

- Numerator $\psi^2_{\mathrm{CMC+LHS}}$ is from CLT for CDF estimator:

$$\sqrt{n}\left[\hat{F}_{\mathrm{CMC+LHS},n}(\xi) - F(\xi)\right] \Rightarrow N(0, \psi^2_{\mathrm{CMC+LHS}})$$

- $\hat{F}_{\mathrm{CMC+LHS},n}(\xi)$ averages dependent copies of response

$$q(\boldsymbol{X}, \xi) = q(c_X(V_1, \ldots, V_{d'}), \xi) \equiv A'(V_1, \ldots, V_{d'}) \equiv A'$$

CMC+LHS: Numerator of Variance

CMC+LHS removes variance of additive part of CMC response

$$q(\boldsymbol{X}, \xi) = q(c_X(V_1, \ldots, V_{d'}), \xi) \equiv A'(V_1, \ldots, V_{d'}) \equiv A'$$

- Additive approximation using ANOVA decomp with residual ϵ':

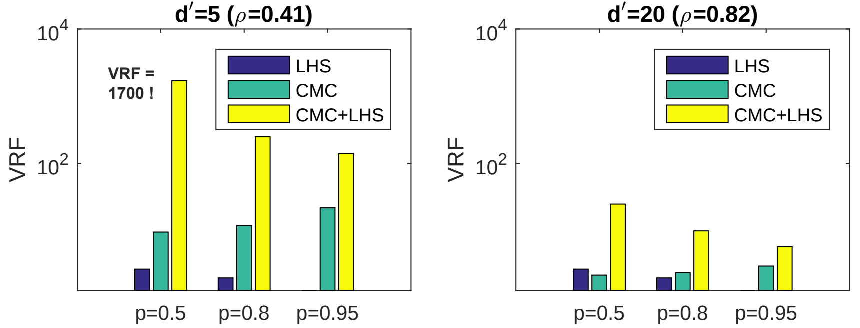
$$A'(V_1, \ldots, V_{d'}) \;=\; F(\xi) + \sum_{j=1}^{d'} \Big(E\left[\, A' \mid V_j \,\right] - F(\xi) \Big) + \epsilon'$$

- Numerator $\psi^2_{\mathrm{CMC+LHS}}$ of CMC+LHS quantile estimator's asymptotic variance

$$\psi^2_{\mathrm{CMC+LHS}} \;=\; \mathrm{Var}[\epsilon'] \;=\; \psi^2_{\mathrm{CMC}} - \textstyle\sum_{j=1}^{d} \mathrm{Var}\Big[\, E\left[\, A' \mid V_j \,\right] \Big]$$

- Additive fit for CMC+LHS much better than for LHS.
- CMC+LHS can reduce variance much more than LHS.

- (Y, X) bivariate normal
  - $Y = \sum_{j=1}^{d} \Phi^{-1}(U_j) \sim F = N(0, d)$ for $d = 30$
  - $X = \sum_{j=1}^{d'} \Phi^{-1}(U_j)$, so correlation $\rho(Y, X) = \sqrt{d'/d}$.
- Estimated p-quantile $\xi = F^{-1}(p)$ via SRS, LHS, CMC, CMC+LHS.
- Sample size $n = 1600$, 10^4 indep experiments
- Variance-reduction factor of method x: $\mathrm{VRF} = \mathrm{Var}[\hat{\xi}_{\mathrm{SRS},n}]/\mathrm{Var}[\hat{\xi}_{\mathrm{x},n}]$



VRT Confidence Interval (CI) for Quantile

- For SRS, can build CI for ξ by exploiting binomial property of

$$n\hat{F}_n(\xi) = \sum_{j=1}^{n} I(Y_j \leq \xi)$$

  - With VRT, binomial property no longer holds.

- For VRT, can build CI for ξ by consistently estimating CLT's asymptotic variance:

$$\sqrt{n}\left[\hat{\xi}_n - \xi\right] \Rightarrow N(0, \tau^2), \quad n \to \infty,$$

$$\tau^2 = \frac{\psi^2(\xi)}{f^2(\xi)}$$

  - Nontrivial to develop consistent estimator of τ^2.

- Instead examine methods that avoid consistently estimating τ^2.

VRT Batching Confidence Interval for Quantile

- Use VRT to generate $b \geq 2$ i.i.d. batches, each with m outputs.
- Total outputs $n = bm$.

$$n \text{ outputs: } \underbrace{1, \ldots, m,}_{\text{Batch 1}} \quad \underbrace{m+1, \ldots, 2m,}_{\text{Batch 2}} \quad \ldots, \quad \underbrace{(b-1)m+1, \ldots, bm}_{\text{Batch } b}$$

$$\Downarrow \qquad \Downarrow \qquad \Downarrow$$

$$b \text{ quantile estimates: } \tilde{\xi}_1 = \tilde{F}_1^{-1}(p) \quad \tilde{\xi}_2 = \tilde{F}_2^{-1}(p) \quad \tilde{\xi}_b = \tilde{F}_b^{-1}(p)$$

VRT Batching Confidence Interval for Quantile

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$$b \text{ quantile estimates: } \quad \tilde{\xi}_1 = \tilde{F}_1^{-1}(p) \quad \tilde{\xi}_2 = \tilde{F}_2^{-1}(p) \quad \tilde{\xi}_b = \tilde{F}_b^{-1}(p)$$

- Batching CI

$$CI_{b,m} = \left(\bar{\xi}_{b,m} \pm \tau_{b-1,\alpha} \frac{S}{\sqrt{b}} \right)$$

  - batching point estimator $\bar{\xi}_{b,m} = \frac{1}{n} \sum_{j=1}^{b} \tilde{\xi}_j$
  - sample variance $S^2 = \frac{1}{b-1} \sum_{j=1}^{b} \left(\tilde{\xi}_j - \bar{\xi}_{b,m} \right)^2$
  - $\tau_{b-1,\alpha} = (1 - \alpha/2)$-critical point of t-distn with $b-1$ d.f.

- Problem: CI centered at $\bar{\xi}_{b,m}$, which has large bias ($m < n$).

VRT Sectioning CI Centered at Overall Quantile Estimator

- Asmussen & Glynn (2007) develop sectioning for SRS.
- In batching CI, replace batching point estimator $\bar{\xi}_{b,m} = \frac{1}{b} \sum_{j=1}^{b} \tilde{\xi}_j$ with overall point estimator $\hat{\xi}_n = \hat{F}_n^{-1}(p)$
  - $\hat{\xi}_n$ less biased than $\bar{\xi}_{b,m}$ since $n = bm$ and $b \geq 2$

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  - $\hat{\xi}_n$ less biased than $\bar{\xi}_{b,m}$ since $n = bm$ and $b \geq 2$
- Sectioning CI:

$$\widehat{CI}_{b,m} = \left(\hat{\xi}_n \pm \tau_{b-1,\alpha} \frac{\hat{S}}{\sqrt{b}} \right)$$

Theorem (N. (2014), Dong & N. (2014,2017a,2018))

Suppose batches indep and VRT Bahadur rep holds. Then for any fixed # of batches $b \geq 2$ and $C_{b,m} = CI_{b,m}$ or $\widehat{CI}_{b,m}$,

$$\textit{coverage} \quad P(\xi \in C_{b,m}) \to 1 - \alpha \quad \textit{as} \quad m \to \infty.$$

Why Can Overall Estimator Replace Batching Estimator?

- By Bahadur representation

$$\text{Batch } j: \qquad \tilde{\xi}_j = \xi - \frac{\tilde{F}_j(\xi) - p}{f(\xi)} + R_{j,m}, \qquad \sqrt{m}\, R_{j,m} \Rightarrow 0.$$

$$\text{Overall:} \qquad \hat{\xi}_n = \xi - \frac{\hat{F}_n(\xi) - p}{f(\xi)} + R_n, \qquad \sqrt{n}\, R_n \Rightarrow 0,$$

Why Can Overall Estimator Replace Batching Estimator?

- By Bahadur representation

$$\text{Batch } j: \qquad \tilde{\xi}_j = \xi - \frac{\tilde{F}_j(\xi) - p}{f(\xi)} + R_{j,m}, \qquad \sqrt{m}\, R_{j,m} \Rightarrow 0.$$

$$\text{Overall: } \qquad \hat{\xi}_n = \xi - \frac{\hat{F}_n(\xi) - p}{f(\xi)} + R_n, \qquad \sqrt{n}\, R_n \Rightarrow 0,$$

- Batching point estimator satisfies

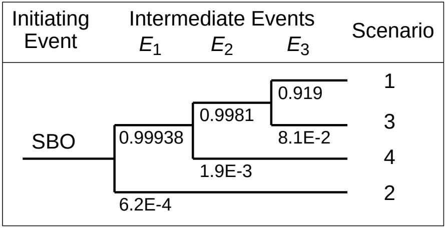
$$\begin{aligned}
\bar{\xi}_{b,m} = \frac{1}{b}\sum_{j=1}^{b} \tilde{\xi}_j &= \frac{1}{b}\sum_{j=1}^{b}\left(\xi - \frac{\tilde{F}_j(\xi) - p}{f(\xi)} + R_{j,m}\right) \\
&= \xi - \frac{\boxed{\frac{1}{b}\sum_{j=1}^{b} \tilde{F}_j(\xi)} - p}{f(\xi)} + \frac{1}{b}\sum_{j=1}^{b} R_{j,m} \\
&= \xi - \frac{\boxed{\hat{F}_n(\xi)} - p}{f(\xi)} + \frac{1}{b}\sum_{j=1}^{b} R_{j,m}
\end{aligned}$$

avg of avgs
= overall avg

- So $\sqrt{m}\left[\hat{\xi}_n - \bar{\xi}_{b,m}\right] = \sqrt{m}\left[R_n - \frac{1}{b}\sum_{j=1}^{b} R_{j,m}\right] \Rightarrow 0$ as batch size $m \to \infty$.

Numerical Results: Probabilistic Safety Assessment (PSA)

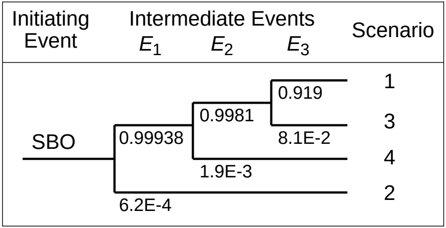
- PSA of station blackout (SBO) at nuclear power plant (NPP)
  - Stylized model inspired by Nutt & Wallis (2004), Sherry et al. (2013)
- Peak cladding temperature (PCT) during hypothesized SBO
  - Risk-informed safety-margin characterization (RISMC)
  - Random load $L \sim G_L$
  - Random capacity $C \sim G_C$
  - L and C independent [Sherry et al. (2013)]
- System fails when $L \geq C$
  - Equivalently, when safety margin $Y \equiv C - L \leq 0$
- NPP deemed "acceptably safe" if $\theta = P(L \geq C) \leq \theta_0 = 0.05$
  - Equivalently, when θ_0-quantile ξ of $Y \sim F$ satisfies $\xi \geq 0$.
- Goal: construct 95% lower confidence bound (LCB) for ξ



Event tree from Sherry et al. (2013)

- Load CDF $G_L(x) = P(L \leq x) = \sum_{s=1}^{4} \lambda_{\langle s \rangle} P(L_{\langle s \rangle} \leq x)$
- For each scenario $s = 1, 2, 3, 4$,
  - Lognormal load $L_{\langle s \rangle} = \exp(\sum_{j=1}^{10} X_{s,j})$, with $X_{s,j} \sim N(\mu_{s,j}, \sigma^2_{s,j})$
  - Scenario s occurs with prob. $\lambda_{\langle s \rangle}$, e.g., $\lambda_{\langle 1 \rangle} = 0.99938 \times 0.9981 \times 0.919$
- Capacity CDF G_C is $\mathrm{Tria}(1800, 2200, 2600)$ [Sherry et al. (2013)]
  - G_C does not depend on scenario

Numerical Results: NPP PSA



- Apply SRS, CMC, LHS, CMC+LHS to build LCB for $\xi = F^{-1}(\theta_0)$.
- CMC: L indep of $C \sim G_C$, so write CDF F of $Y = C - L$ as

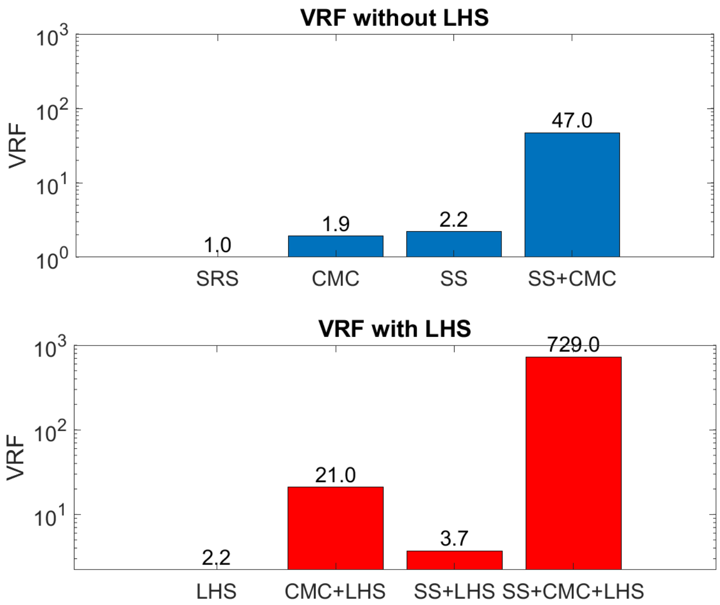
$$F(y) = P(C \le L + y) = E[P(C \le L + y \mid L)] = E[G_C(L + y)]$$

  - CMC estimator of $F(y)$ averages copies of $G_C(L + y)$ with $L \sim G_L$
- Also, sometimes combine with stratified sampling (SS):

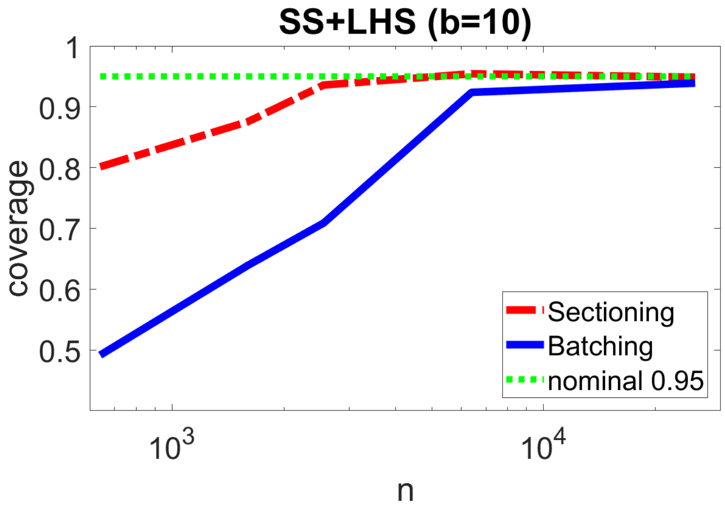
$$F(y) = P(C - L \le y) = \sum_{s=1}^{4} \lambda_{\langle s \rangle} F_{\langle s \rangle}(y)$$

where $F_{\langle s \rangle}(y) = P(C - L_{\langle s \rangle} \le y)$.

Numerical Results: Variance-Reduction Factor (wrt SRS)



Sectioning Can Improve Coverage



- 95% lower confidence bound: sectioning outperforms batching

Summary

- Quantile estimation using combination of conditional Monte Carlo and Latin hypercube sampling.
- Combination CMC+LHS outperforms each by itself.
- Synergism when combining CMC and LHS.
    - LHS removes variance from additive part of response.
    - Additive fit for CMC much better than for SRS.
    - CMC+LHS can greatly reduce variance.
- Constructed asymptotically valid confidence intervals for quantile using batching and sectioning.
- **Current work:** QMC and RQMC for constructing batching and sectioning CIs for quantile

Thank you!

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