Uncertainty Quantification and Quasi-Monte Carlo

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Theorem (CBC error bound)

The generating vector $\boldsymbol{z} \in \mathbb{U}_n^s$ *constructed by the CBC algorithm, minimizing the squared shift-averaged worst-case error* $[e_{n,s}^{\mathrm{sh}}(\boldsymbol{z})]^2$ *for the weighted unanchored Sobolev space in each step, satisfies*

$$[e_{n,s}^{\mathrm{sh}}(\boldsymbol{z})]^2 \le \left(\frac{1}{\varphi(n)} \sum_{\varnothing \ne \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\right)^{|\mathfrak{u}|}\right)^{1/\lambda} \quad \text{for all } \lambda \in (1/2, 1], \tag{1}$$

where $\zeta(x) := \sum_{k=1}^{\infty} k^{-x}$ *denotes the Riemann zeta function for* $x > 1$.

Proof. Step $s = 1$: by direct calculation, it is easy to see that $[e_{n,1}^{\mathrm{sh}}(z_1)]^2 = \frac{\gamma_1}{6n^2}$ and this is less than or equal to $\left(\frac{1}{\varphi(n)}\gamma_1^{\lambda}\left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\right)\right)^{1/\lambda}$ for all $n \ge 1$, $\lambda \in (1/2, 1]$, and $\gamma_1 > 0$. Induction step: suppose that we have chosen the first $s-1$ components $z_1, \ldots, z_{s-1}$, and that (1) holds with s replaced by $s-1$.

We can write the squared worst-case error in dimension-recursive form as

$$[e^{\mathrm{sh}}_{n,s}(z_1,\dots,z_s)]^2 = \frac{1}{n}\sum_{\varnothing\neq\mathfrak{u}\subseteq\{1:s\}}\gamma_{\mathfrak{u}}\sum_{k=0}^{n-1}\prod_{j\in\mathfrak{u}}B_2\left(\left\{\frac{kz_j}{n}\right\}\right)$$
$$= [e^{\mathrm{sh}}_{n,s-1}(z_1,\dots,z_{s-1})]^2 + \theta(z_1,\dots,z_{s-1},z_s), \qquad (2)$$

where (suppressing the dependence of θ on $z_1,\dots,z_{s-1}$)

$$\theta(z_s) := \sum_{s\in\mathfrak{u}\subseteq\{1:s\}}\gamma_{\mathfrak{u}}\left(\frac{1}{n}\sum_{k=0}^{n-1}\prod_{j\in\mathfrak{u}}B_2\left(\left\{\frac{kz_j}{n}\right\}\right)\right) \qquad \text{(use Fourier expansion of } B_2\text{)}$$
$$= \sum_{s\in\mathfrak{u}\subseteq\{1:s\}}\frac{\gamma_{\mathfrak{u}}}{(2\pi^2)^{|\mathfrak{u}|}}\left(\frac{1}{n}\sum_{k=0}^{n-1}\sum_{\boldsymbol{h}_{\mathfrak{u}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{u}|}}\frac{\mathrm{e}^{2\pi\mathrm{i}k\boldsymbol{h}_{\mathfrak{u}}\cdot\boldsymbol{z}_{\mathfrak{u}}/n}}{\prod_{j\in\mathfrak{u}}h_j^2}\right)$$
$$= \sum_{s\in\mathfrak{u}\subseteq\{1:s\}}\frac{\gamma_{\mathfrak{u}}}{(2\pi^2)^{|\mathfrak{u}|}}\left(\sum_{\substack{\boldsymbol{h}_{\mathfrak{u}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{u}|}\\ \boldsymbol{h}_{\mathfrak{u}}\cdot\boldsymbol{z}_{\mathfrak{u}}\equiv 0 \pmod n}}\frac{1}{\prod_{j\in\mathfrak{u}}h_j^2}\right),$$

where we used the character property $\frac{1}{n}\sum_{k=0}^{n-1}\mathrm{e}^{2\pi\mathrm{i}k\boldsymbol{h}\cdot\boldsymbol{z}/n} = \begin{cases}1 & \text{if } \boldsymbol{h}\cdot\boldsymbol{z}\equiv 0 \pmod n\\ 0 & \text{otherwise}\end{cases}$.

Noting that $\boldsymbol{h}_{\mathfrak{u}}\cdot\boldsymbol{z}_{\mathfrak{u}}\equiv 0 \pmod n$ can be written equivalently as $\boldsymbol{h}_{\mathfrak{u}\setminus\{s\}}\cdot\boldsymbol{z}_{\mathfrak{u}\setminus\{s\}}\equiv -h_sz_s \pmod n$ for $s\in\mathfrak{u}\subseteq\{1:s\}$, we arrive at...

$$\theta(z_s) = \sum_{s\in\mathfrak{u}\subseteq\{1:s\}} \frac{\gamma_{\mathfrak{u}}}{(2\pi^2)^{|\mathfrak{u}|}} \Bigg(\sum_{h_s\in\mathbb{Z}\setminus\{0\}} \frac{1}{h_s^2} \sum_{\substack{\boldsymbol{h}_{\mathfrak{u}\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{u}|-1} \\ \boldsymbol{h}_{\mathfrak{u}\setminus\{s\}}\cdot\boldsymbol{z}_{\mathfrak{u}\setminus\{s\}}\equiv -h_s z_s \pmod{n}}} \frac{1}{\prod_{j\in\mathfrak{u}\setminus\{s\}} h_j^2} \Bigg)$$

If z_s^* denotes the value chosen by the CBC algorithm in dimension s, then we use the following principle:

Averaging argument: *The minimum is always smaller than or equal to the average.*

In particular, this implies for all $\lambda \in (0,1]$ that

$$[\theta(z_s^*)]^\lambda \le \frac{1}{\varphi(n)} \sum_{z_s\in\mathbb{U}_n} [\theta(z_s)]^\lambda$$

$$\le \frac{1}{\varphi(n)} \sum_{z_s\in\mathbb{U}_n} \Bigg[\sum_{s\in\mathfrak{u}\subseteq\{1:s\}} \frac{\gamma_{\mathfrak{u}}}{(2\pi^2)^{|\mathfrak{u}|}} \Bigg(\sum_{h_s\in\mathbb{Z}\setminus\{0\}} \frac{1}{h_s^2} \sum_{\substack{\boldsymbol{h}_{\mathfrak{u}\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{u}|-1} \\ \boldsymbol{h}_{\mathfrak{u}\setminus\{s\}}\cdot\boldsymbol{z}_{\mathfrak{u}\setminus\{s\}}\equiv -h_s z_s \pmod{n}}} \frac{1}{\prod_{j\in\mathfrak{u}\setminus\{s\}} h_j^2} \Bigg) \Bigg]^\lambda$$

$$\le \frac{1}{\varphi(n)} \sum_{z_s\in\mathbb{U}_n} \sum_{s\in\mathfrak{u}\subseteq\{1:s\}} \frac{\gamma_{\mathfrak{u}}^\lambda}{(2\pi^2)^{|\mathfrak{u}|\lambda}} \sum_{h_s\in\mathbb{Z}\setminus\{0\}} \frac{1}{|h_s|^{2\lambda}} \sum_{\substack{\boldsymbol{h}_{\mathfrak{u}\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{u}|-1} \\ \boldsymbol{h}_{\mathfrak{u}\setminus\{s\}}\cdot\boldsymbol{z}_{\mathfrak{u}\setminus\{s\}}\equiv -h_s z_s \pmod{n}}} \frac{1}{\prod_{j\in\mathfrak{u}\setminus\{s\}} |h_j|^{2\lambda}},$$

where we used the inequality $\left(\sum_k a_k\right)^\lambda \le \sum_k a_k^\lambda$, $a_k \ge 0$, $\lambda \in (0,1]$.

We separate the terms depending on whether or not h_s is a multiple of n. Note that this means

$$\sum_{h_s \in \mathbb{Z}\setminus\{0\}} \frac{1}{|h_s|^{2\lambda}} = \sum_{\substack{k=-\infty \\ k\neq 0}}^{\infty} \frac{1}{|kn|^{2\lambda}} + \sum_{\substack{h_s \in \mathbb{Z}\setminus\{0\} \\ h_s \not\equiv 0 \pmod{n}}} \frac{1}{|h_s|^{2\lambda}}$$

$$= \frac{2\zeta(2\lambda)}{n^{2\lambda}} + \sum_{c=1}^{n-1} \sum_{\substack{h_s \in \mathbb{Z}\setminus\{0\} \\ h_s \equiv c \pmod{n}}} \frac{1}{|h_s|^{2\lambda}}.$$

It will be convenient to carry out a change of variable to eliminate the dependence on h_s from the innermost sum on the previous slide. Denote by z_s^{-1} the multiplicative inverse of z_s in $\mathbb{U}_n$, i.e., $z_s z_s^{-1} \equiv 1 \pmod{n}$. Then

$$\frac{1}{\varphi(n)} \sum_{z_s \in \mathbb{U}_n} \sum_{s \in u \subseteq \{1:s\}} \frac{\gamma_u^\lambda}{(2\pi^2)^{|u|\lambda}} \sum_{h_s \in \mathbb{Z}\setminus\{0\}} \frac{1}{|h_s|^{2\lambda}} \sum_{\substack{\boldsymbol{h}_{u\setminus\{s\}} \in (\mathbb{Z}\setminus\{0\})^{|u|-1} \\ \boldsymbol{h}_{u\setminus\{s\}} \cdot \boldsymbol{z}_{u\setminus\{s\}} \equiv -h_s z_s \pmod{n}}} \frac{1}{\prod_{j\in u\setminus\{s\}} |h_j|^{2\lambda}}$$

$$= \sum_{s \in u \subseteq \{1:s\}} \frac{\gamma_u^\lambda}{(2\pi^2)^{|u|\lambda}} \frac{2\zeta(2\lambda)}{n^{2\lambda}} \sum_{\substack{\boldsymbol{h}_{u\setminus\{s\}} \in (\mathbb{Z}\setminus\{0\})^{|u|-1} \\ \boldsymbol{h}_{u\setminus\{s\}} \cdot \boldsymbol{z}_{u\setminus\{s\}} \equiv 0 \pmod{n}}} \frac{1}{\prod_{j\in u\setminus\{s\}} |h_j|^{2\lambda}}$$

$$+ \frac{1}{\varphi(n)} \sum_{z_s \in \mathbb{U}_n} \sum_{c=1}^{n-1} \sum_{s \in u \subseteq \{1:s\}} \frac{\gamma_u^\lambda}{(2\pi^2)^{|u|\lambda}} \sum_{\substack{h_s \in \mathbb{Z}\setminus\{0\} \\ h_s \equiv c \pmod{n}}} \frac{1}{|h_s|^{2\lambda}} \sum_{\substack{\boldsymbol{h}_{u\setminus\{s\}} \in (\mathbb{Z}\setminus\{0\})^{|u|-1} \\ \boldsymbol{h}_{u\setminus\{s\}} \cdot \boldsymbol{z}_{u\setminus\{s\}} \equiv -c z_s \pmod{n}}} \frac{1}{\prod_{j\in u\setminus\{s\}} |h_j|^{2\lambda}}.$$

We separate the terms depending on whether or not h_s is a multiple of n. Note that this means

$$\sum_{h_s\in\mathbb{Z}\setminus\{0\}}\frac{1}{|h_s|^{2\lambda}}=\sum_{\substack{k=-\infty\\k\neq 0}}^{\infty}\frac{1}{|kn|^{2\lambda}}+\sum_{\substack{h_s\in\mathbb{Z}\setminus\{0\}\\h_s\not\equiv 0 \pmod n}}\frac{1}{|h_s|^{2\lambda}}$$

$$=\frac{2\zeta(2\lambda)}{n^{2\lambda}}+\sum_{c=1}^{n-1}\sum_{\substack{h_s\in\mathbb{Z}\setminus\{0\}\\h_s\equiv c \pmod n}}\frac{1}{|h_s|^{2\lambda}}.$$

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$$\frac{1}{\varphi(n)}\sum_{z_s\in\mathbb{U}_n}\sum_{s\in u\subseteq\{1:s\}}\frac{\gamma_u^\lambda}{(2\pi^2)^{|u|\lambda}}\sum_{h_s\in\mathbb{Z}\setminus\{0\}}\frac{1}{|h_s|^{2\lambda}}\sum_{\substack{\boldsymbol{h}_{u\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|u|-1}\\ \boldsymbol{h}_{u\setminus\{s\}}\cdot\boldsymbol{z}_{u\setminus\{s\}}\equiv -h_s z_s \pmod n}}\frac{1}{\prod_{j\in u\setminus\{s\}}|h_j|^{2\lambda}}$$

$$=\sum_{s\in u\subseteq\{1:s\}}\frac{\gamma_u^\lambda}{(2\pi^2)^{|u|\lambda}}\frac{2\zeta(2\lambda)}{n^{2\lambda}}\sum_{\substack{\boldsymbol{h}_{u\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|u|-1}\\ \boldsymbol{h}_{u\setminus\{s\}}\cdot\boldsymbol{z}_{u\setminus\{s\}}\equiv 0 \pmod n}}\frac{1}{\prod_{j\in u\setminus\{s\}}|h_j|^{2\lambda}}$$

$$+\frac{1}{\varphi(n)}\sum_{z_s\in\mathbb{U}_n}\sum_{c=1}^{n-1}\sum_{s\in u\subseteq\{1:s\}}\frac{\gamma_u^\lambda}{(2\pi^2)^{|u|\lambda}}\sum_{\substack{h_s\in\mathbb{Z}\setminus\{0\}\\ h_s\equiv -cz_s^{-1}\pmod n}}\frac{1}{|h_s|^{2\lambda}}\sum_{\substack{\boldsymbol{h}_{u\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|u|-1}\\ \boldsymbol{h}_{u\setminus\{s\}}\cdot\boldsymbol{z}_{u\setminus\{s\}}\equiv c \pmod n}}\frac{1}{\prod_{j\in u\setminus\{s\}}|h_j|^{2\lambda}}.$$

For $c \in \{1, \ldots, n-1\}$, $\{\mathrm{mod}(cz_s^{-1}, n) : z_s \in \mathbb{U}_n\} = \{\mathrm{mod}(cz, n) : z \in \mathbb{U}_n\}$ and $\gcd(c/g, n/g) = 1$ with $g = \gcd(c, n)$. We obtain

$$\sum_{z_s \in \mathbb{U}_n} \sum_{\substack{h_s \in \mathbb{Z}\setminus\{0\} \\ h_s \equiv -cz_s^{-1} \pmod{n}}} \frac{1}{|h_s|^{2\lambda}} = \sum_{z \in \mathbb{U}_n} \sum_{\substack{h_s \in \mathbb{Z}\setminus\{0\} \\ h_s \equiv -cz \pmod{n}}} \frac{1}{|h_s|^{2\lambda}}$$

$$= \sum_{z \in \mathbb{U}_n} \sum_{m \in \mathbb{Z}} \frac{1}{|mn - cz|^{2\lambda}}$$

$$= g^{-2\lambda} \sum_{z \in \mathbb{U}_n} \sum_{m \in \mathbb{Z}} \frac{1}{|m(n/g) - (c/g)z|^{2\lambda}}$$

$$= g^{-2\lambda} \sum_{z \in \mathbb{U}_n} \sum_{\substack{h \in \mathbb{Z}\setminus\{0\} \\ h \equiv -(c/g)z \pmod{n/g}}} \frac{1}{|h|^{2\lambda}}$$

$$\leq g^{-2\lambda} g \sum_{a=1}^{n/g-1} \sum_{\substack{h \in \mathbb{Z}\setminus\{0\} \\ h \equiv a \pmod{n/g}}} \frac{1}{|h|^{2\lambda}} \leq g^{1-2\lambda} \sum_{h \in \mathbb{Z}\setminus\{0\}} \frac{1}{|h|^{2\lambda}} \leq 2\zeta(2\lambda),$$

where the last step holds since $g \geq 1$ and $\lambda > 1/2$. (The condition $\lambda > 1/2$ is needed to ensure that $\zeta(2\lambda) < \infty$.)

Hence

$$[\theta(z_s^*)]^\lambda \le \sum_{s\in\mathfrak{u}\subseteq\{1:s\}} \frac{\gamma_{\mathfrak{u}}^\lambda}{(2\pi^2)^{|\mathfrak{u}|\lambda}} \frac{2\zeta(2\lambda)}{n^{2\lambda}} \sum_{\substack{\boldsymbol{h}_{\mathfrak{u}\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{u}|-1} \\ \boldsymbol{h}_{\mathfrak{u}\setminus\{s\}}\cdot\boldsymbol{z}_{\mathfrak{u}\setminus\{s\}}\equiv 0 \pmod{n}}} \frac{1}{\prod_{j\in\mathfrak{u}\setminus\{s\}} |h_j|^{2\lambda}}$$

$$+ \frac{1}{\varphi(n)} \sum_{s\in\mathfrak{u}\subseteq\{1:s\}} \frac{\gamma_{\mathfrak{u}}^\lambda}{(2\pi^2)^{|\mathfrak{u}|\lambda}} 2\zeta(2\lambda) \sum_{\substack{\boldsymbol{h}_{\mathfrak{u}\setminus\{s\}}\in(\mathbb{Z}\setminus\{0\})^{|\mathfrak{u}|-1} \\ \boldsymbol{h}_{\mathfrak{u}\setminus\{s\}}\cdot\boldsymbol{z}_{\mathfrak{u}\setminus\{s\}}\not\equiv 0 \pmod{n}}} \frac{1}{\prod_{j\in\mathfrak{u}\setminus\{s\}} |h_j|^{2\lambda}}$$

$$\le \frac{1}{\varphi(n)} \sum_{s\in\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^\lambda \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^\lambda}\right)^{|\mathfrak{u}|},$$

where we used $\frac{1}{n^{2\lambda}} \le \frac{1}{\varphi(n)}$ for $n \ge 1$ and $\lambda \in (1/2, 1]$.[†]

[†] $\varphi(n) \le n \le n^{2\lambda} \Rightarrow \frac{1}{n^{2\lambda}} \le \frac{1}{\varphi(n)}$.

Returning to our original dimension-wise decomposition (2), using the bound on $\theta(z_s^*)$ and the induction hypothesis yield

$$
\begin{aligned}
&[e_{n,s}^{\mathrm{sh}}(z_1,\ldots,z_s)]^2 = [e_{n,s-1}^{\mathrm{sh}}(z_1,\ldots,z_{s-1})]^2 + \theta(z_1,\ldots,z_{s-1},z_s) \\
&\leq \left(\frac{1}{\varphi(n)} \sum_{\varnothing\neq \mathfrak{u}\subseteq\{1:s-1\}} \gamma_{\mathfrak{u}}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\right)^{|\mathfrak{u}|}\right)^{1/\lambda} + \left(\frac{1}{\varphi(n)} \sum_{s\in\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\right)^{|\mathfrak{u}|}\right)^{1/\lambda} \\
&\leq \left(\frac{1}{\varphi(n)} \sum_{\varnothing\neq \mathfrak{u}\subseteq\{1:s-1\}} \gamma_{\mathfrak{u}}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\right)^{|\mathfrak{u}|} + \frac{1}{\varphi(n)} \sum_{s\in\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\right)^{|\mathfrak{u}|}\right)^{1/\lambda} \\
&= \left(\frac{1}{\varphi(n)} \sum_{\varnothing\neq \mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\right)^{|\mathfrak{u}|}\right)^{1/\lambda},
\end{aligned}
$$

proving the assertion. □

Significance: Suppose that $f \in H_{s,\boldsymbol{\gamma}}$ for all $\boldsymbol{\gamma} = (\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1:s\}}$. Then for any given sequence of weights $\boldsymbol{\gamma}$, we can use the CBC algorithm to obtain a generating vector satisfying the error bound

$$\sqrt{\mathbb{E}_{\boldsymbol{\Delta}} |I_s f - Q_{n,s}^{\boldsymbol{\Delta}} f|^2} \le \left(\frac{1}{\varphi(n)} \sum_{\varnothing \ne \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}} \right)^{|\mathfrak{u}|} \right)^{1/(2\lambda)} \|f\|_{s,\boldsymbol{\gamma}} \quad (3)$$

for all $\lambda \in (1/2, 1]$. We can use the following strategy:

- For a given integrand f, estimate the norm $\|f\|_{s,\boldsymbol{\gamma}}$.
- Find weights $\boldsymbol{\gamma}$ which *minimize* the error bound (3).
- Using the optimized weights $\boldsymbol{\gamma}$ as input, use the CBC algorithm to find a generating vector which *satisfies* the error bound (3).

Remarks:

- If n is prime, then $\frac{1}{\varphi(n)} = \frac{1}{n-1}$. If $n = 2^k$, then $\frac{1}{\varphi(n)} = \frac{2}{n}$. For general (composite) $n \ge 3$, $\frac{1}{\varphi(n)} \le \frac{\mathrm{e}^{\gamma} \log\log n + \frac{3}{\log\log n}}{n}$, where $\gamma = 0.57721566\ldots$ (Euler–Mascheroni constant).
- The optimal convergence rate close to $\mathcal{O}(n^{-1})$ is obtained with $\lambda \to 1/2$, but note that $\lambda = 1/2$ is not permitted since $\zeta(2\lambda) \to \infty$ as $\lambda \to 1/2$.

Appendix

Let $a, b \in \mathbb{Z}$ and $m \in \mathbb{Z}_+$. Recall that

$$a \equiv b \pmod{m} \Leftrightarrow \frac{a-b}{m} \in \mathbb{Z} \Leftrightarrow a = km + b \text{ for some } k \in \mathbb{Z}.$$

Theorem (Bézout's identity)

Let $a, b \in \mathbb{Z}$. Then there exist $x, y \in \mathbb{Z}$ such that $ax + by = \gcd(a, b)$.

Corollary

Let $a, b \in \mathbb{Z}$ and $m \in \mathbb{Z}_+$.

- *The linear congruence $ax \equiv b \pmod{m}$ has a solution if and only if $\gcd(a, m) | b$.*
- *If $\gcd(a, m) | b$, then there are exactly $\gcd(a, m)$ solutions to the linear congruence $ax \equiv b \pmod{n}$.*

Let $z, n \in \mathbb{N}$ be such that $\gcd(z, n) = 1$. Then the above corollary implies that the linear congruence

$$xz \equiv 1 \pmod{n}$$

has exactly one solution (modulo n). This solution is called the *modular multiplicative inverse* and it is often denoted by $z^{-1} := x$.