

Uncertainty Quantification and Quasi-Monte Carlo

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Theorem (CBC error bound)

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

$$[e_{n,s}^{\text{sh}}(\mathbf{z})]^2 \leq \left(\frac{1}{\varphi(n)} \sum_{\emptyset \neq u \subseteq \{1:s\}} \gamma_u^\lambda \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^\lambda} \right)^{|u|} \right)^{1/\lambda} \quad \text{for all } \lambda \in (1/2, 1], \quad (1)$$

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 $[e_{n,1}^{\text{sh}}(z_1)]^2 = \frac{\gamma_1}{6n^2}$ 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 $n \geq 1$, $\lambda \in (1/2, 1]$, and $\gamma_1 > 0$. Induction step: suppose that we have chosen the first $s - 1$ components z_1, \dots, 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

$$\begin{aligned} [e_{n,s}^{\text{sh}}(z_1, \dots, z_s)]^2 &= \frac{1}{n} \sum_{\emptyset \neq u \subseteq \{1:s\}} \gamma_u \sum_{k=0}^{n-1} \prod_{j \in u} B_2 \left(\left\{ \frac{kz_j}{n} \right\} \right) \\ &= [e_{n,s-1}^{\text{sh}}(z_1, \dots, z_{s-1})]^2 + \theta(z_1, \dots, z_{s-1}, z_s), \end{aligned} \quad (2)$$

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

$$\begin{aligned} \theta(z_s) &:= \sum_{s \in u \subseteq \{1:s\}} \gamma_u \left(\frac{1}{n} \sum_{k=0}^{n-1} \prod_{j \in u} B_2 \left(\left\{ \frac{kz_j}{n} \right\} \right) \right) \quad (\text{use Fourier expansion of } B_2) \\ &= \sum_{s \in u \subseteq \{1:s\}} \frac{\gamma_u}{(2\pi^2)^{|u|}} \left(\frac{1}{n} \sum_{k=0}^{n-1} \sum_{\mathbf{h}_u \in (\mathbb{Z} \setminus \{0\})^{|u|}} \frac{e^{2\pi i k \mathbf{h}_u \cdot \mathbf{z}_u / n}}{\prod_{j \in u} h_j^2} \right) \\ &= \sum_{s \in u \subseteq \{1:s\}} \frac{\gamma_u}{(2\pi^2)^{|u|}} \left(\sum_{\substack{\mathbf{h}_u \in (\mathbb{Z} \setminus \{0\})^{|u|} \\ \mathbf{h}_u \cdot \mathbf{z}_u \equiv 0 \pmod{n}}} \frac{1}{\prod_{j \in u} h_j^2} \right), \end{aligned}$$

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

Noting that $\mathbf{h}_u \cdot \mathbf{z}_u \equiv 0 \pmod{n}$ can be written equivalently as

$\mathbf{h}_{u \setminus \{s\}} \cdot \mathbf{z}_{u \setminus \{s\}} \equiv -h_s z_s \pmod{n}$ for $s \in u \subseteq \{1:s\}$, we arrive at...

$$\theta(z_s) = \sum_{s \in u \subseteq \{1:s\}} \frac{\gamma_u}{(2\pi^2)^{|u|}} \left(\sum_{h_s \in \mathbb{Z} \setminus \{0\}} \frac{1}{h_s^2} \sum_{\substack{h_{u \setminus \{s\}} \in (\mathbb{Z} \setminus \{0\})^{|u|-1} \\ h_{u \setminus \{s\}} \cdot z_{u \setminus \{s\}} \equiv -h_s z_s \pmod{n}}} \frac{1}{\prod_{j \in u \setminus \{s\}} h_j^2} \right)$$

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

$$\begin{aligned} [\theta(z_s^*)]^\lambda &\leq \frac{1}{\varphi(n)} \sum_{z_s \in \mathbb{U}_n} [\theta(z_s)]^\lambda \\ &\leq \frac{1}{\varphi(n)} \sum_{z_s \in \mathbb{U}_n} \left[\sum_{s \in u \subseteq \{1:s\}} \frac{\gamma_u}{(2\pi^2)^{|u|}} \left(\sum_{h_s \in \mathbb{Z} \setminus \{0\}} \frac{1}{h_s^2} \sum_{\substack{h_{u \setminus \{s\}} \in (\mathbb{Z} \setminus \{0\})^{|u|-1} \\ h_{u \setminus \{s\}} \cdot z_{u \setminus \{s\}} \equiv -h_s z_s \pmod{n}}} \frac{1}{\prod_{j \in u \setminus \{s\}} h_j^2} \right) \right]^\lambda \\ &\leq \frac{1}{\varphi(n)} \sum_{z_s \in \mathbb{U}_n} \sum_{s \in u \subseteq \{1:s\}} \frac{\gamma_u^\lambda}{(2\pi^2)^{|u|\lambda}} \sum_{h_s \in \mathbb{Z} \setminus \{0\}} \frac{1}{|h_s|^{2\lambda}} \sum_{\substack{h_{u \setminus \{s\}} \in (\mathbb{Z} \setminus \{0\})^{|u|-1} \\ h_{u \setminus \{s\}} \cdot z_{u \setminus \{s\}} \equiv -h_s z_s \pmod{n}}} \frac{1}{\prod_{j \in u \setminus \{s\}} |h_j|^{2\lambda}}, \end{aligned}$$

where we used the inequality $(\sum_k a_k)^\lambda \leq \sum_k a_k^\lambda$, $a_k \geq 0$, $\lambda \in (0, 1]$.

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

$$\begin{aligned} \sum_{h_s \in \mathbb{Z} \setminus \{0\}} \frac{1}{|h_s|^{2\lambda}} &= \sum_{\substack{k=-\infty \\ k \neq 0}}^{\infty} \frac{1}{|kn|^{2\lambda}} + \sum_{\substack{h_s \in \mathbb{Z} \setminus \{0\} \\ h_s \not\equiv 0 \pmod{n}}} \frac{1}{|h_s|^{2\lambda}} \\ &= \frac{2\zeta(2\lambda)}{n^{2\lambda}} + \sum_{c=1}^{n-1} \sum_{\substack{h_s \in \mathbb{Z} \setminus \{0\} \\ h_s \equiv c \pmod{n}}} \frac{1}{|h_s|^{2\lambda}}. \end{aligned}$$

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

$$\begin{aligned} &\frac{1}{\varphi(n)} \sum_{z_s \in \mathbb{U}_n} \sum_{s \in u \subseteq \{1:s\}} \frac{\gamma_u^\lambda}{(2\pi^2)^{|u|\lambda}} \sum_{h_s \in \mathbb{Z} \setminus \{0\}} \frac{1}{|h_s|^{2\lambda}} \sum_{\substack{h_{u \setminus \{s\}} \in (\mathbb{Z} \setminus \{0\})^{|u|-1} \\ h_{u \setminus \{s\}} \cdot z_{u \setminus \{s\}} \equiv -h_s z_s \pmod{n}}} \frac{1}{\prod_{j \in u \setminus \{s\}} |h_j|^{2\lambda}} \\ &= \sum_{s \in u \subseteq \{1:s\}} \frac{\gamma_u^\lambda}{(2\pi^2)^{|u|\lambda}} \frac{2\zeta(2\lambda)}{n^{2\lambda}} \sum_{\substack{h_{u \setminus \{s\}} \in (\mathbb{Z} \setminus \{0\})^{|u|-1} \\ h_{u \setminus \{s\}} \cdot z_{u \setminus \{s\}} \equiv 0 \pmod{n}}} \frac{1}{\prod_{j \in u \setminus \{s\}} |h_j|^{2\lambda}} \\ &+ \frac{1}{\varphi(n)} \sum_{z_s \in \mathbb{U}_n} \sum_{c=1}^{n-1} \sum_{s \in u \subseteq \{1:s\}} \frac{\gamma_u^\lambda}{(2\pi^2)^{|u|\lambda}} \sum_{\substack{h_s \in \mathbb{Z} \setminus \{0\} \\ h_s \equiv c \pmod{n}}} \frac{1}{|h_s|^{2\lambda}} \sum_{\substack{h_{u \setminus \{s\}} \in (\mathbb{Z} \setminus \{0\})^{|u|-1} \\ h_{u \setminus \{s\}} \cdot z_{u \setminus \{s\}} \equiv -cz_s \pmod{n}}} \frac{1}{\prod_{j \in u \setminus \{s\}} |h_j|^{2\lambda}}. \end{aligned}$$

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

$$\begin{aligned}
& \sum_{z_s \in \mathbb{U}_n} \sum_{\substack{h_s \in \mathbb{Z} \setminus \{0\} \\ h_s \equiv -cz_s^{-1} \pmod{n}}} \frac{1}{|h_s|^{2\lambda}} = \sum_{z \in \mathbb{U}_n} \sum_{\substack{h_s \in \mathbb{Z} \setminus \{0\} \\ h_s \equiv -cz \pmod{n}}} \frac{1}{|h_s|^{2\lambda}} \\
&= \sum_{z \in \mathbb{U}_n} \sum_{m \in \mathbb{Z}} \frac{1}{|mn - cz|^{2\lambda}} \\
&= g^{-2\lambda} \sum_{z \in \mathbb{U}_n} \sum_{m \in \mathbb{Z}} \frac{1}{|m(n/g) - (c/g)z|^{2\lambda}} \\
&= g^{-2\lambda} \sum_{z \in \mathbb{U}_n} \sum_{\substack{h \in \mathbb{Z} \setminus \{0\} \\ h \equiv -(c/g)z \pmod{n/g}}} \frac{1}{|h|^{2\lambda}} \\
&\leq g^{-2\lambda} g^{\frac{n/g-1}{g}} \sum_{a=1}^{n/g-1} \sum_{\substack{h \in \mathbb{Z} \setminus \{0\} \\ h \equiv a \pmod{n/g}}} \frac{1}{|h|^{2\lambda}} \leq g^{1-2\lambda} \sum_{h \in \mathbb{Z} \setminus \{0\}} \frac{1}{|h|^{2\lambda}} \leq 2\zeta(2\lambda),
\end{aligned}$$

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

$$\begin{aligned}
[\theta(z_s^*)]^\lambda &\leq \sum_{s \in u \subseteq \{1:s\}} \frac{\gamma_u^\lambda}{(2\pi^2)^{|u|\lambda}} \frac{2\zeta(2\lambda)}{n^{2\lambda}} \sum_{\substack{\mathbf{h}_{u \setminus \{s\}} \in (\mathbb{Z} \setminus \{0\})^{|u|-1} \\ \mathbf{h}_{u \setminus \{s\}} \cdot \mathbf{z}_{u \setminus \{s\}} \equiv 0 \pmod{n}}} \frac{1}{\prod_{j \in u \setminus \{s\}} |h_j|^{2\lambda}} \\
&\quad + \frac{1}{\varphi(n)} \sum_{s \in u \subseteq \{1:s\}} \frac{\gamma_u^\lambda}{(2\pi^2)^{|u|\lambda}} 2\zeta(2\lambda) \sum_{\substack{\mathbf{h}_{u \setminus \{s\}} \in (\mathbb{Z} \setminus \{0\})^{|u|-1} \\ \mathbf{h}_{u \setminus \{s\}} \cdot \mathbf{z}_{u \setminus \{s\}} \not\equiv 0 \pmod{n}}} \frac{1}{\prod_{j \in u \setminus \{s\}} |h_j|^{2\lambda}} \\
&\leq \frac{1}{\varphi(n)} \sum_{s \in u \subseteq \{1:s\}} \gamma_u^\lambda \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^\lambda} \right)^{|u|},
\end{aligned}$$

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

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

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

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

proving the assertion. □

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

$$\sqrt{\mathbb{E}_{\Delta} |I_s f - Q_{n,s}^{\Delta} f|^2} \leq \left(\frac{1}{\varphi(n)} \sum_{\emptyset \neq u \subseteq \{1:s\}} \gamma_u^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}} \right)^{|u|} \right)^{1/(2\lambda)} \|f\|_{s,\gamma} \quad (3)$$

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

- For a given integrand f , estimate the norm $\|f\|_{s,\gamma}$.
- Find weights γ which *minimize* the error bound (3).
- Using the optimized weights γ 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) $n \geq 3$, $\frac{1}{\varphi(n)} \leq \frac{e^{\gamma} \log \log n + \frac{3}{\log \log n}}{n}$, where $\gamma = 0.57721566 \dots$ (Euler–Mascheroni constant).
- The optimal convergence rate close to $\mathcal{O}(n^{-1})$ is obtained with $\lambda \rightarrow 1/2$, but note that $\lambda = 1/2$ is not permitted since $\zeta(2\lambda) \rightarrow \infty$ as $\lambda \rightarrow 1/2$.

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 $\gcd(a, m) \mid b$.
- If $\gcd(a, m) \mid b$, then there are exactly $\gcd(a, m)$ solutions modulo m to the linear congruence $ax \equiv b \pmod{m}$.

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

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

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