- Let \( \{F^k\}_{k=1}^{K} \) denote the set of computational outputs of interest with correlation coefficients \( \{\zeta_{1,k}\}_{k=2}^{K} \) and computational costs \( \{C_k\}_{k=1}^{K} \) that respectively satisfy

\[
|\zeta_{1,k-1}| > |\zeta_{1,k}| \quad \text{and} \quad \frac{C_{k-1}}{C_k} > \frac{\zeta_{1,k-1}^2 - \zeta_{1,k}^2}{\zeta_{1,k-1}^2 - \zeta_{1,k+1}^2}, \quad k = 2, \ldots, K.
\]  

(9)

The first requirement is easily satisfied by a reordering of the surrogate outputs of interest \( F^2, \ldots, F^K \). If, after that reordering, the second requirement is not satisfied for some \( k \in \{2, \ldots, K\} \), then \( F^K \) is removed from the list of surrogates.

- Let \( M_1, \ldots, M_{k-1} \) be given; these are all positive by construction.

- Also let \( M^*_k = \{M^*_k, k = k \} \) and \( \alpha^*_k = \{\alpha^*_k, k = k \} \), and let

\[
r^*_k, \frac{M^*_k}{M^*_k} = \frac{C_k}{C_{k'}} \left( \frac{\zeta_{1,k'}^2 - \zeta_{1,k}^2}{\zeta_{1,k'}^2 - \zeta_{1,k+1}^2} \right), \quad k' = k, \ldots, K.
\]

- Then, for each \( k = 1, \ldots, K \), the unique global minimizer \( (M^*_k, \alpha^*_k) \) of the functional \( L^k \) is given by

\[
M^*_k = \frac{B - \sum_{k'=1}^{k-1} C_{k'}}{\sum_{k'=k}^{K} C_{k'} r^*_{k,k'}},
\]

and

\[
M^*_k = \frac{C_k}{C_{k'}} \left( \frac{\zeta_{1,k}^2 - \zeta_{1,k'}^2}{\zeta_{1,k}^2 - \zeta_{1,k+1}^2} \right), \quad k' = k + 1, \ldots, K.
\]

(10)

Figure 1. Box A. Optimal non-integer sampling numbers for the modified MFMC method; see Gruber et al. (2022)

For \( k = 1, 2, \ldots, \)

Ia. if the minimization of the Lagrangian functional \( L^k \) constrained by \( M_{1,1} = M_{2,2} = \cdots = M_{k-1,k-1} = 1 \) results in all \( K - k + 1 \) members of the set \( \{M^*_k, k = k \} \) satisfying \( M_{k',k} \geq 1, k' = k, \ldots, K \). Then,

Ib. simply rounding downwards to the nearest integer produces integer sample numbers \( M^*_{k',k} \rightarrow \lfloor M^*_{k',k} \rfloor \) \( k' = k, \ldots, K \), so that the final set \( \{M^*_{k',k} = \lfloor M^*_{k',k} \rfloor \}, k' = k, \ldots, K \), of sampling number optimal under the constraint \( M_{1,1} = M_{2,2} = \cdots = M_{k-1,k-1} = 1 \) and preserves the computational budget. We then set \( \tilde{K} = k - 1 \) and exit to step IV.

Otherwise,

IIa. if \( M^*_{k,k} < 1 \), then it is rounded upwards \( M^*_{k,k} \rightarrow 1 \) and the function \( L^{k+1} \) is minimized to obtain the remaining \( K - k \) components of \( M^*_{k',k}, k' = k + 1, \ldots, K \).

This yields

IIb. a new set \( \{M^*_{1,1} = 1, M^*_{2,2} = 1, \ldots, M^*_{k,k} = 1 \} \bigcup \{M^*_{k',k} \}_{k'=k+1}^{K} \) which may or may not contain entries less than 1. If it does not, the model evaluation vector becomes \( M^* = \{M^*_{k',k} = 1 \}_{k'=1}^{K} \bigcup \{M^*_{k',k} \}_{k'=k+1}^{K} \). We then set \( \tilde{K} = k \) and exit to step IV.

Otherwise,

III. we increment \( k \rightarrow k + 1 \) and return to step Ia.

IV. The process terminates and the final set of sample numbers is given by \( \{M^*_{1,1} = 1, M^*_{2,2} = 1, \ldots, M^*_{\tilde{K},\tilde{K}} = 1 \} \bigcup \{M^*_{k',k} \}_{k'=1}^{K} \bigcup \{M^*_{k',k+1} \}_{k=k+1}^{K} \).

Figure 2. B. Practical near-optimal integer sampling numbers for the modified MFMC method; see Gruber et al. (2022).