Multifidelity write-up

Abstract

We derived the explicit sample size estimation in terms of the desired accuracy requirement.

1. Model problem

We have a high fidelity model denoted as $f_1 : \Omega \to Z$ we desire, and several low fidelity models (surrogates) f_k for $k \in \mathbb{N}$. Our objective is to approximate

$$\mathbb{E}\left(f_1(\omega)\right).$$

Note for each $f_i(\omega)$, its variance and Pearson product-moment correlation coefficient are

$$\sigma_i^2 = \mathbb{V}\left(f_i(\omega)\right), \qquad \rho_{i,j} = \frac{\mathrm{Cov}\left(f_i(\omega), f_j(\omega)\right)}{\sigma_i \sigma_j}, \quad i, j = 1, \ldots, K,$$

where $\mathbb{V}(f) := \mathbb{E}\left(\|f - \mathbb{E}(f)\|_Z^2\right)$.

2. Monte Carlo estimator

The Monte Carlo estimator for the expectation of each f_k is defined as the sample mean of N_k i.i.d realizations $\omega_1, \ldots, \omega_N$

$$A_{k,N_k}^{\mathrm{MC}} := \frac{1}{N_k} \sum_{i=1}^{N_k} f_k(\omega_i), \quad \forall k = 1, \ldots, K, \tag{1}$$

where $\mathbb{E}(A_{k,N_k}^{\mathrm{MC}}) = \mathbb{E}(f_k)$, $\mathbb{V}(A_{k,N_k}^{\mathrm{MC}}) = \mathbb{V}(f_k)/N_k$. Let C_k denote the average evaluation cost per sample for f_k, then the total sampling cost for each Monte Carlo estimator A_{k,N_k}^{MC} is

$$\mathcal{W}_{\mathrm{MC}}^k = C_k N_k.$$

We define the *normalized mean squared error* (nMSE), denoted as $\mathcal{E}_A^2$, with normalizing factor $\|\mathbb{E}(f)\|_Z^2$ for estimator A as

$$\mathcal{E}_A^2 := \frac{\mathbb{E}\left[\|\mathbb{E}(f) - A\|_Z^2\right]}{\|\mathbb{E}(f)\|_Z^2}.$$

If we use a Monte Carlo estimator to estimate $\mathbb{E}\left(f_1(\omega)\right)$,

$$\mathcal{E}_{A_{1,N_1}^{\mathrm{MC}}}^2 = \frac{\mathbb{E}\left[\left\|\mathbb{E}(f_1) - A_{1,N_1}^{\mathrm{MC}}\right\|_Z^2\right]}{\|\mathbb{E}(f_1)\|_Z^2} = \frac{\left\|\mathbb{E}(f_1) - \mathbb{E}(A_{1,N_1}^{\mathrm{MC}})\right\|_Z^2 + \mathbb{E}\left[\left\|\mathbb{E}(A_{1,N_1}^{\mathrm{MC}}) - A_{1,N_1}^{\mathrm{MC}}\right\|_Z^2\right]}{\|\mathbb{E}(f_1)\|_Z^2} = \frac{\mathbb{V}\left(f_1\right)}{N_1 \|\mathbb{E}(f_1)\|_Z^2}.$$

Given a target tolerance ϵ^2 for the nMSE, the sample size N_1 is estimated as

$$N_1 = \left\lceil \frac{\mathbb{V}(f_k)}{\epsilon^2 \|\mathbb{E}(f_k)\|_Z^2} \right\rceil \simeq \epsilon^{-2}.$$

So the total expense of sampling with N_1 samples using Monte Carlo method for $\mathbb{E}(f_1(\omega))$ is

$$\mathcal{W}_{\mathrm{MC}}^1 = C_1 N_1.$$

3. Multifidelity Monte Carlo

The Multifidelity Monte Carlo (MFMC) estimator is defined as

$$A_{\mathrm{MFMC}} := A_{1,N_1}^{\mathrm{MC}} + \sum_{k=2}^{K} \alpha_k \left(A_{k,N_k}^{\mathrm{MC}} - A_{k,N_{k-1}}^{\mathrm{MC}} \right), \tag{2}$$

where α_k are the coefficients to weight the correction term. In each correction term, the two Monte Carlo estimators are dependent in the sense that $A_{k,N_{k-1}}^{\mathrm{MC}}$ recycles the first N_{k-1} samples of A_{k,N_k}^{MC} so we require $N_{k-1} \le N_k$ for $k = 2, \ldots, K$. Using this property and (1), we can remove the dependent samples and rewrite (2) as

$$A^{\mathrm{MFMC}} = A_{1,N_1}^{\mathrm{MC}} + \sum_{k=2}^{K} \alpha_k \left[\left(\frac{N_{k-1}}{N_k} - 1 \right) A_{k,N_{k-1}}^{\mathrm{MC}} + \left(1 - \frac{N_{k-1}}{N_k} \right) A_{k,N_k - N_{k-1}}^{\mathrm{MC}} \right],$$

Now, the samples in $A_{k,N_{k-1}}^{\mathrm{MC}}$ and $A_{k,N_k-N_{k-1}}^{\mathrm{MC}}$ are independent with each other. Define $Y_1 := A_{1,N_1}^{\mathrm{MC}}$, $Y_k := \left(\frac{N_{k-1}}{N_k} - 1\right) A_{k,N_{k-1}}^{\mathrm{MC}} + \left(1 - \frac{N_{k-1}}{N_k}\right) A_{k,N_k-N_{k-1}}^{\mathrm{MC}}$ for $k = 2 \ldots, K$. Note that Y_k are independent with each other for $k = 2, \ldots, K$. Then

$$A^{\mathrm{MFMC}} = Y_1 + \sum_{k=2}^{K} \alpha_k Y_k.$$

So $\mathbb{E}(Y_k) = 0$ for $k \ge 2$ and $\mathbb{E}(A^{\mathrm{MFMC}}) = \mathbb{E}(f_1)$. For independent random variable, since each realization is uncorrelated to each other, this indicates that the sum of sample realizations and variance are interchangeable, therefore

$$\mathbb{V}(Y_1) = \frac{\sigma_1^2}{N_1}, \quad \mathbb{V}(Y_k) = \left(\frac{N_{k-1}}{N_k} - 1 \right)^2 \frac{\sigma_k^2}{N_{k-1}} + \left(\frac{N_{k-1}}{N_k} - 1 \right)^2 \frac{\sigma_k^2}{N_k - N_{k-1}} = \left(\frac{1}{N_{k-1}} - \frac{1}{N_k} \right) \sigma_k^2.$$

So,

$$\begin{aligned}
\mathbb{V}\left(A^{\mathrm{MFMC}}\right) &= \mathbb{V}(Y_1) + \mathbb{V}\left(\sum_{k=2}^{K} \alpha_k Y_k \right) + 2\,\mathrm{Cov}\left(Y_1, \sum_{k=2}^{K} \alpha_k Y_k \right), \\
&= \mathbb{V}(Y_1) + \sum_{k=2}^{K} \alpha_k^2 \mathbb{V}(Y_k) + 2 \sum_{2 \le k < j \le K} \alpha_k \alpha_j \,\mathrm{Cov}(Y_k, Y_j) + 2 \sum_{k=2}^{K} \alpha_k \,\mathrm{Cov}(Y_1, Y_k), \\
&= \frac{\sigma_1^2}{N_1} + \sum_{k=2}^{K} \left(\frac{1}{N_{k-1}} - \frac{1}{N_k} \right) \left(\alpha_k^2 \sigma_k^2 - 2\alpha_i \rho_{1,i} \sigma_1 \sigma_i \right),
\end{aligned} \tag{3}$$

where we use the fact that Y_k and Y_j are independent with each other for $k \geq 2$ and [1, Lemma 3.2]

$$\mathrm{Cov}(Y_1, Y_k) = \mathrm{Cov}\left(A^{\mathrm{MC}}_{1,N_1}, A^{\mathrm{MC}}_{k,N_k}\right) - \mathrm{Cov}\left(A^{\mathrm{MC}}_{1,N_1}, A^{\mathrm{MC}}_{k,N_{k-1}}\right) = -2\sum_{k=2}^{K} \alpha_k \left(\frac{1}{N_{k-1}} - \frac{1}{N_k}\right)\rho_{1,i}\sigma_1\sigma_i.$$

The nMSE error for the multifidelity Monte Carlo estimator is

$$\mathcal{E}^2_{A^{\mathrm{MFMC}}} = \frac{\mathbb{E}\left[\left\|\mathbb{E}(f_1) - A^{\mathrm{MFMC}}\right\|_Z^2\right]}{\|\mathbb{E}(f_1)\|_Z^2} = \frac{\left\|\mathbb{E}(f_1) - \mathbb{E}(A^{\mathrm{MFMC}})\right\|_Z^2 + \mathbb{E}\left[\left\|\mathbb{E}(A^{\mathrm{MFMC}}) - A^{\mathrm{MFMC}}\right\|_Z^2\right]}{\|\mathbb{E}(f_1)\|_Z^2} = \frac{\mathbb{V}\left(A^{\mathrm{MFMC}}\right)}{\|\mathbb{E}(f_1)\|_Z^2}.$$

The total sampling cost for MFMC estimator is

$$\sum_{k=1}^{K} C_k N_k.$$

Our next goal is to determine the sample size N_k such that the MFMC estimation satisfy the accuracy threshold $\mathcal{E}^2_{A^{\mathrm{MFMC}}} \leq \epsilon^2$. We formulate an following optimization problem to minimize the sampling cost subject to a bounded variance of MFMC estimator, and solve for sample size $N_k \in \mathbb{R}$ for $k = 1\ldots, K$ and $\alpha_k \in \mathbb{R}$ for $k = 2\ldots, K$ as

$$\begin{array}{lll}
\displaystyle\min_{N_1,\ldots N_K\in\mathbb{R},\alpha_2,\ldots,\alpha_K\in\mathbb{R}} & \sum_{k=1}^{K} C_k N_k, & \\
\text{s.t.} & -N_1 \leq 0, & \\
 & N_{k-1} - N_k \leq 0, & k = 2\ldots, K, \\
 & \mathbb{V}\left(A^{\mathrm{MFMC}}\right) \leq \|\mathbb{E}(f_1)\|_Z^2\,\epsilon^2. &
\end{array} \tag{4}$$

Theorem 1. *Let f_k be K models that satisfy the following conditions*

$$(i)\quad |\rho_{1,1}| > \ldots > |\rho_{1,k}| \qquad\qquad (ii)\quad \frac{C_{k-1}}{C_k} > \frac{\rho^2_{1,k-1} - \rho^2_{1,k}}{\rho^2_{1,k} - \rho^2_{1,k+1}}, \quad k = 2,\ldots,K.$$

Then the global minimizer to (4) *is*

$$\alpha_k^* = \frac{\rho_{1,k}\sigma_1}{\sigma_k}, \quad k = 2\ldots, K,$$

$$N_k^* = \frac{\sigma_1^2}{\|\mathbb{E}(f_1)\|_Z^2\,\epsilon^2}\sqrt{\frac{\rho^2_{1,k} - \rho^2_{1,k+1}}{C_k}}\sum_{j=1}^{K}\left(\sqrt{\frac{C_j}{\rho^2_{1,j} - \rho^2_{1,j+1}}} - \sqrt{\frac{C_{j-1}}{\rho^2_{1,j-1} - \rho^2_{1,j}}}\right)\rho^2_{1,j}, \quad k = 1\ldots, K,$$

with $\rho_{1,0} = \infty$ and $\rho_{1,K+1} = 0$.

Proof. First note that (*ii*) indicates a strict increasing sequence of sample size, the minimizer α_k^* and N_k^* satisfy the constraints (*i*) and (*ii*).

Our objective function

$$J^* = \sum_{k=1}^{K} C_k N_k^* = \frac{\sigma_1^2}{\|\mathbb{E}(f_1)\|_Z^2\,\epsilon^2}\sum_{k=1}^{K}\sqrt{\left(\rho^2_{1,k} - \rho^2_{1,k+1}\right)C_k}\sum_{k=1}^{K}\left(\sqrt{\frac{C_k}{\rho^2_{1,k} - \rho^2_{1,k+1}}} - \sqrt{\frac{C_{k-1}}{\rho^2_{1,k-1} - \rho^2_{1,k}}}\right)\rho^2_{1,k}$$

Consider another local minimum α_k^+ and N_k^+ of (4) such that $N_{k-1}^+ = N_k^+$ for some $k \geq 2$. Let index j_i be the first entry followed by equality for N_k,

$$N_{k_i}$$

□

4. Appendix

References

[1] B. Peherstorfer, K. Willcox, and M. Gunzburger. Optimal model management for multifidelity Monte Carlo estimation. SIAM J. Sci. Comput., 38(5):A3163–A3194, 2016.