Online Supplement to “ Estimating Cycle Time Percentile Curves for Manufacturing Systems via Simulation”

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A. Appendix

The appendix is organized as follows: In Appendix A.1, we justify the specific forms of the regression models chosen to represent the CT-TH moment curves. In Appendix A.2, we define the notation that will be used in Appendix A.3–Appendix A.6. Appendix A.3 provides the statistical inference on the moment estimators $\{\widehat{\mu}_\nu(x) = \mu(x, \widehat{\boldsymbol{\theta}}_\nu), \nu = 1, 2, 3\}$. Appendix A.4 derives the normalized variances and covariances of the moment estimators in terms of the design parameters $[\mathbf{x}, \boldsymbol{\pi}]$. The numerical evaluation of the design criterion PM is explained in Appendix A.5, and the method for determining the number of additional replications ΔN is given in Appendix A.6.

A.1. Justification for the Metamodels

This subsection is devoted to justifying the specific form of the metamodels (4) and (5) adopted for the estimation of moment curves. Both models are motivated by some elementary queueing models as well as heavy-traffic analysis of queueing systems.

In Section 3, moment CT-TH curves are represented by Model (4) which consists of two parts: a polynomial function in the numerator, and $(1-x)^p$ in the denominator. Analytical results for some simple queueing systems have shown that the moment curves for these systems are of the form of (4). For example, the first three moment curves of the M/M/1 queue in steady state are

$$\begin{aligned}
\mathrm{E}[CT(x)] &= 1/(1-x) \\
\mathrm{E}[CT(x)^2] &= 2/(1-x)^2 \\
\mathrm{E}[CT(x)^3] &= 6/(1-x)^3.
\end{aligned}$$

In Whitt (1989), it has been shown that, at least as $x \to 1$, moment curves of many queueing systems will follow the form of (4). As explained in Yang et al. (2007), introducing parameter p in Model (4) is necessary because it has been demonstrated that the p value for the underlying CT-TH first-moment (mean) curves could deviate substantially from 1 for real manufacturing systems (Johnson et al. 2004).

Before we discuss the variance model (5), we first define the asymptotic variance of the sample mean $\sum_{h=1}^{H(x)}(CT_h(x))^\nu/H(x)$ as follows:

$$[\sigma_A^{(\nu)}(x)]^2 = \lim_{H(x)\to\infty} H(x)\mathrm{Var}\left[H(x)^{-1}\sum_{h=1}^{H(x)}(CT_h(x))^\nu\right].$$

We assume that $\{CT_h(x), h = 1, 2, 3, \ldots\}$ is a stationary discrete-time stochastic process. Whitt (1989) showed that for the M/M/1 queue, the asymptotic variance of $\sum_{h=1}^{H(x)} CT_h(x)/H(x)$ is given by

$$[\sigma_A^{(1)}(x)]^2 = \frac{x(2+5x-4x^2+x^3)}{(1-x)^4} \approx \frac{4}{(1-x)^4} \tag{27}$$

as x approaches 1. Under heavy traffic, (28) is consistent with Model (5). Furthermore, it has been shown by Whitt (2002) that the asymptotic variance of higher moments will also have form (5) in heavy traffic:

$$[\sigma_A^{(\nu)}(x)]^2 \approx \frac{\sigma^2}{(1-x)^{2\nu+2}}, \qquad \nu = 1, 2, 3, \ldots \tag{28}$$

A.2. Notation

We define the notation that will be used for the remainder of this appendix.

$\mathbf{n} = (n(x_1), n(x_2), \ldots, n(x_m))$ is the integer vector that represents the allocation of simulation replications to the m design points.

$\mathbf{Z}^{(\nu)} = (Z_1^{(\nu)}(x_1), \ldots, Z_{n(x_1)}^{(\nu)}(x_1), \ldots, Z_1^{(\nu)}(x_m), \ldots, Z_{n(x_m)}^{(\nu)}(x_m))'$ for $\nu = 1, 2, 3$, the transformed data vector consisting of independent observations collected at m different throughput levels.

$\mathbf{Z}^{(\nu)}(x) = (Z_1^{(\nu)}(x), Z_2^{(\nu)}(x), \ldots, Z_{n(x)}^{(\nu)}(x))'$ is the transformed data vector consisting of i.i.d. observations collected at throughput x.

$\mathrm{Cov}[\mathbf{Z}^{(k)}(x), \mathbf{Z}^{(\ell)}(x)]$ $(k, \ell = 1, 2, 3)$ is a diagonal matrix with identical diagonal elements, $\sigma_{k\ell}(x) \cdot \mathbf{I}_{n(x) \times n(x)}$.

$\mathrm{Cov}[\mathbf{Z}^{(k)}, \mathbf{Z}^{(\ell)}]$ $(k, \ell = 1, 2, 3, k \neq \ell)$ is a diagonal matrix given by:

$$\begin{pmatrix} \sigma_{k\ell}(x_1) \cdot \mathbf{I}_{n(x_1) \times n(x_1)} & & & \\ & \sigma_{k\ell}(x_2) \cdot \mathbf{I}_{n(x_2) \times n(x_2)} & & \\ & & \ddots & \\ & & & \sigma_{k\ell}(x_m) \cdot \mathbf{I}_{n(x_m) \times n(x_m)} \end{pmatrix}. \tag{29}$$

N: the total number of replications.

$\boldsymbol{\theta}_\nu = (\theta_{\nu 1}, \theta_{\nu 2}, \ldots, \theta_{\nu T_\nu})$: the unknown parameter vector of the ν^{th} $(\nu = 1, 2, 3)$ transformed moment model (7) including the coefficients $(c_0, c_1, \ldots, c_t)$ and the exponent parameter r. T_ν is the number of unknown parameters.

$\{\widehat{\mu}_\nu(x) = \mu(x, \widehat{\boldsymbol{\theta}}_\nu); \nu = 1, 2, 3\}$: the estimated moment model (4).

$\{\eta(x, \widehat{\boldsymbol{\theta}}_\nu); \nu = 1, 2, 3\}$: the estimated transformed moment model (7).

$\mathbf{u}(x, \boldsymbol{\theta}_\nu)$, the $T_\nu \times 1$ derivative vector with $\nu = 1, 2, 3$:

$$\begin{aligned} \mathbf{u}(x, \widehat{\boldsymbol{\theta}}_\nu) &= \left[u_1(x, \widehat{\boldsymbol{\theta}}_\nu), u_2(x, \widehat{\boldsymbol{\theta}}_\nu), \ldots, u_{T_\nu}(x, \widehat{\boldsymbol{\theta}}_\nu) \right] \\ &= \left[\frac{\partial \mu(x, \boldsymbol{\theta}_\nu)}{\partial \theta_{\nu 1}}, \frac{\partial \mu(x, \boldsymbol{\theta}_\nu)}{\partial \theta_{\nu 2}}, \ldots, \frac{\partial \mu(x, \boldsymbol{\theta}_\nu)}{\partial \theta_{\nu T_\nu}} \right]' \end{aligned} \tag{30}$$

$\widehat{\mathbf{V}}_\nu$: the $N \times T_\nu$ derivative matrix with elements $\{v_{kj}\}$ defined as

$$v_{kj}^{(\nu)} = v_j^{(\nu)}(x_k) = \frac{\partial \eta(x_k, \boldsymbol{\theta}_\nu)}{\partial \theta_{\nu j}} \Big|_{\boldsymbol{\theta}_\nu = \widehat{\boldsymbol{\theta}}_\nu} \quad k = 1, 2, \ldots, N; j = 1, 2, \ldots, T_\nu. \tag{31}$$

$\{s_\nu^2; \nu = 1,2,3\}$: the residual mean square error resulting from fitting the transformed model (7) for the ν^{th} moment.

A.3. Variance-Covariance Matrix of Moment Estimators

As can be seen from Section 5.2 of the paper, the variance of the percentile estimator $\widehat{\mathcal{C}}_\alpha(x)$ is a function of the variances and covariances of the moment estimators $\{\widehat{\mu}_\nu(x) = \mu(x, \widehat{\boldsymbol{\theta}}_\nu), \nu = 1,2,3\}$.

Consider the random vector of moment estimators $\widehat{\boldsymbol{\mu}}(x) = (\widehat{\mu}_1(x), \widehat{\mu}_2(x), \widehat{\mu}_3(x))'$ as a whole, and its variance-covariance matrix is:

$$\mathrm{Var}[\widehat{\boldsymbol{\mu}}(x)] = \begin{pmatrix} \mathrm{Var}[\widehat{\mu}_1(x)] & \mathrm{Cov}[\widehat{\mu}_1(x), \widehat{\mu}_2(x)] & \mathrm{Cov}[\widehat{\mu}_1(x), \widehat{\mu}_3(x)] \\ \mathrm{Cov}[\widehat{\mu}_1(x), \widehat{\mu}_2(x)] & \mathrm{Var}[\widehat{\mu}_2(x)] & \mathrm{Cov}[\widehat{\mu}_2(x), \widehat{\mu}_3(x)] \\ \mathrm{Cov}[\widehat{\mu}_1(x), \widehat{\mu}_3(x)] & \mathrm{Cov}[\widehat{\mu}_2(x), \widehat{\mu}_3(x)] & \mathrm{Var}[\widehat{\mu}_3(x)] \end{pmatrix}. \quad (32)$$

We provide an estimator for each element in the matrix.

A.3.1. Estimation of the Variances

As illustrated in Section 3 of the paper, the moment estimators $\{\mu(x, \widehat{\boldsymbol{\theta}}_\nu), \nu = 1,2,3\}$ are obtained indirectly from the estimated transformed model $\eta(x, \widehat{\boldsymbol{\theta}}_\nu)$:

$$\mu(x, \widehat{\boldsymbol{\theta}}_\nu) = \frac{\eta(x, \widehat{\boldsymbol{\theta}}_\nu)}{(1-x)^{\widehat{q}_\nu}}.$$

The fitting of $\eta(x, \widehat{\boldsymbol{\theta}}_\nu)$ is based on the transformed data set $\{\mathbf{Z}^{(\nu)}, \nu = 1,2,3\}$. From nonlinear regression analysis (Bates and Watts 1988), $\mathrm{Var}[\widehat{\boldsymbol{\theta}}_\nu]$ is estimated as

$$\begin{aligned} \widehat{\mathrm{Var}}[\widehat{\boldsymbol{\theta}}_\nu] &= \widehat{\mathrm{Var}}\left[(\widehat{\mathbf{V}}_\nu'\widehat{\mathbf{V}}_\nu)^{-1}\widehat{\mathbf{V}}_\nu'\mathbf{Z}_\nu\right] \\ &= (\widehat{\mathbf{V}}_\nu'\widehat{\mathbf{V}}_\nu)^{-1}\widehat{\mathbf{V}}_\nu'\widehat{\mathrm{Var}}[\mathbf{Z}_\nu]((\widehat{\mathbf{V}}_\nu'\widehat{\mathbf{V}}_\nu)^{-1}\widehat{\mathbf{V}}_\nu')' \\ &= s_\nu^2(\widehat{\mathbf{V}}_\nu'\widehat{\mathbf{V}}_\nu)^{-1}. \end{aligned} \quad (33)$$

For reasons explained in Yang et al. (2007), we assume that $q_\nu = \widehat{q}_\nu$ is known when making statistical inference on $\mu(x, \widehat{\boldsymbol{\theta}}_\nu)$. Since $\mu(x, \boldsymbol{\theta}_\nu)$ is nonlinear in the parameters $\boldsymbol{\theta}_\nu$, the first-order approximation by the delta method (Lehmann 1999) is used in the estimation of

$\mathrm{Var}[\mu(x, \widehat{\boldsymbol{\theta}}_\nu)]$:

$$\begin{aligned}
\mathrm{Var}[\mu(x, \widehat{\boldsymbol{\theta}}_\nu)] &\doteq \mathrm{Var}[\mu(x, \boldsymbol{\theta}_\nu) + \mathbf{u}'(x, \boldsymbol{\theta}_\nu)(\widehat{\boldsymbol{\theta}}_\nu - \boldsymbol{\theta}_\nu)] \\
&= \mathrm{Var}[\mathbf{u}'(x, \boldsymbol{\theta}_\nu)\widehat{\boldsymbol{\theta}}_\nu] \\
&= \mathbf{u}'(x, \boldsymbol{\theta}_\nu)\mathrm{Var}[\widehat{\boldsymbol{\theta}}_\nu]\mathbf{u}(x, \boldsymbol{\theta}_\nu). \qquad (34)
\end{aligned}$$

Plugging (33) into (34) and replacing $\boldsymbol{\theta}_\nu$ by $\widehat{\boldsymbol{\theta}}_\nu$, we have:

$$\widehat{\mathrm{Var}}[\mu(x, \widehat{\boldsymbol{\theta}}_\nu)] = s_\nu^2 \mathbf{u}'(x, \widehat{\boldsymbol{\theta}}_\nu)(\widehat{\mathbf{V}}_\nu' \widehat{\mathbf{V}}_\nu)^{-1}\mathbf{u}(x, \widehat{\boldsymbol{\theta}}_\nu). \qquad (35)$$

A.3.2. Estimation of the Covariances

A similar development applies to estimating $\{\mathrm{Cov}[\mu(x, \widehat{\boldsymbol{\theta}}_k), \mu(x, \widehat{\boldsymbol{\theta}}_\ell)]; k, \ell = 1, 2, 3, k \neq \ell\}$. By the first-order approximation of the delta method,

$$\begin{aligned}
\mathrm{Cov}[\widehat{\mu}(x, \widehat{\boldsymbol{\theta}}_k), \widehat{\mu}(x, \widehat{\boldsymbol{\theta}}_\ell)] &\doteq \mathrm{Cov}[\mu(x, \boldsymbol{\theta}_k) + \mathbf{u}'(x, \boldsymbol{\theta}_k)(\widehat{\boldsymbol{\theta}}_k - \boldsymbol{\theta}_k), \mu(x, \boldsymbol{\theta}_\ell) + \mathbf{u}'(x, \boldsymbol{\theta}_\ell)(\widehat{\boldsymbol{\theta}}_\ell - \boldsymbol{\theta}_\ell)] \\
&= \mathrm{Cov}[\mathbf{u}'(x, \boldsymbol{\theta}_k)\widehat{\boldsymbol{\theta}}_k, \mathbf{u}'(x, \boldsymbol{\theta}_\ell)\widehat{\boldsymbol{\theta}}_\ell] \\
&= \mathbf{u}'(x, \boldsymbol{\theta}_k)\mathrm{Cov}[\widehat{\boldsymbol{\theta}}_k, \widehat{\boldsymbol{\theta}}_\ell]\mathbf{u}(x, \boldsymbol{\theta}_\ell). \qquad (36)
\end{aligned}$$

And from nonlinear regression analysis of $\eta(x, \widehat{\boldsymbol{\theta}}_\nu)$, we have

$$\begin{aligned}
\widehat{\mathrm{Cov}}\left[\widehat{\boldsymbol{\theta}}_k, \widehat{\boldsymbol{\theta}}_\ell\right] &= \widehat{\mathrm{Cov}}[(\widehat{\mathbf{V}}_k'\widehat{\mathbf{V}}_k)^{-1}\widehat{\mathbf{V}}_k'\mathbf{Z}^{(k)}, (\widehat{\mathbf{V}}_\ell'\widehat{\mathbf{V}}_\ell)^{-1}\widehat{\mathbf{V}}_\ell'\mathbf{Z}^{(\ell)}] \\
&= (\widehat{\mathbf{V}}_k'\widehat{\mathbf{V}}_k)^{-1}\widehat{\mathbf{V}}_k'\widehat{\mathrm{Cov}}[\mathbf{Z}^{(k)}, \mathbf{Z}^{(\ell)}]((\widehat{\mathbf{V}}_\ell'\widehat{\mathbf{V}}_\ell)^{-1}\widehat{\mathbf{V}}_\ell')'. \qquad (37)
\end{aligned}$$

Combining (36) and (37), and substituting the parameter estimates $\{\widehat{\boldsymbol{\theta}}_\nu, \nu = 1, 2, 3\}$, we have:

$$\begin{aligned}
\widehat{\mathrm{Cov}}[\mu(x, \widehat{\boldsymbol{\theta}}_k), \mu(x, \widehat{\boldsymbol{\theta}}_\ell)] &= \mathbf{u}'(x, \widehat{\boldsymbol{\theta}}_k)(\widehat{\mathbf{V}}_k'\widehat{\mathbf{V}}_k)^{-1}\widehat{\mathbf{V}}_k'\widehat{\mathrm{Cov}}[\mathbf{Z}^{(k)}, \mathbf{Z}^{(\ell)}](\widehat{\mathbf{V}}_\ell(\widehat{\mathbf{V}}_\ell'\widehat{\mathbf{V}}_\ell)^{-1})\mathbf{u}(x, \widehat{\boldsymbol{\theta}}_\ell) \\
& \quad k, \ell = 1, 2, 3; \quad k \neq \ell. \qquad (38)
\end{aligned}$$

The only part left unsolved in (38) is the estimation of $\mathrm{Cov}[\mathbf{Z}^{(k)}, \mathbf{Z}^{(\ell)}]$, which is a diagonal matrix given by (29). The natural estimator of $\sigma_{k\ell}(x)$, the $k\ell$ element of the covariance matrix

$\mathrm{Cov}[\mathbf{Z}^{(k)}, \mathbf{Z}^{(\ell)}]$, is the sample covariance estimated at x:

$$\begin{aligned} \widetilde{\sigma}_{k\ell}(x) &= \frac{1}{n(x)-1}\sum_{j=1}^{n(x)}(Z_j^{(k)}(x) - \bar{Z}^{(k)}(x))(Z_j^{(\ell)}(x) - \bar{Z}^{(\ell)}(x)) \\ & \quad k, \ell = 1, 2, 3; \quad k \neq \ell \end{aligned} \tag{39}$$

where $\bar{Z}^{(\nu)}(x) = n(x)^{-1}\sum_{j=1}^{n(x)} Z_j^{(\nu)}(x)$ is the sample mean.

However, using the sample covariance (39) to estimate $\mathrm{Cov}[\mu(x, \widehat{\boldsymbol{\theta}}_k), \mu(x, \widehat{\boldsymbol{\theta}}_\ell)]$ may lead to a covariance matrix that is not positive semi-definite, which is a fundamental requirement on the variance-covariance matrix of any random vector. Therefore, we propose estimating $\sigma_{k\ell}(x)$ in the following way, which provides some consistency in how we estimate the variances and covariances, and preserves the positive semi-definite property of the estimated matrix (32). We estimate the sample correlation

$$\widetilde{\varrho}_{k\ell}(x) = \frac{\widetilde{\sigma}_{k\ell}(x)}{\sqrt{\widetilde{\sigma}_k^2(x)\widetilde{\sigma}_\ell^2(x)}} \tag{40}$$

where $\widetilde{\sigma}_{k\ell}(x)$ is the sample covariance (39), and $\widehat{\sigma}_\nu^2(x) = (n(x)-1)^{-1}\sum_{j=1}^{n(x)}(Z_j^{(\nu)}(x) - \bar{Z}^{(\nu)}(x))^2$ is the sample variance. Then an estimate of $\sigma_{ij}(x)$ can be obtained utilizing the residual error s_ν^2 which is also used in (33) for estimating $\mathrm{Var}[\mu(x, \widehat{\boldsymbol{\theta}}_\nu)]$:

$$\widehat{\sigma}_{ij}(x) = \widetilde{\varrho}_{ij}(x) \times s_i s_j. \tag{41}$$

Notice that the estimation discussed in this subsection is used either for making statistical inference on the percentile estimator or numerically evaluating the design criterion in search of the optimal design. The case worthy of mention is when the current design is to be expanded by including more design points. At those additional points, no simulation data have yet been collected, and we cannot directly obtain the corresponding covariance estimates $\widehat{\sigma}_{ij}(x)$ for the new design points. A simple approximation has been adopted in our procedure: we assign $\widehat{\sigma}_{ij}(x) = (\widehat{\sigma}_{ij}(x_L) + \widehat{\sigma}_{ij}(x_U)/2$ for those new design points to be included.

A.4. Normalized Variance and Covariance Derivation for Moment Estimators

In this section, we derive the normalized variances ($N\mathrm{Var}[\cdot]$) and covariances ($N\mathrm{Cov}[\cdot]$) of the moment estimators at a particular throughput rate $x \in [x_L, x_U]$ in terms of $\mathbf{x}$ and $\boldsymbol{\pi}$. This provides the basis for evaluating the normalized variances of percentile estimators, which is critical to the design of simulation experiments as shown later in Appendices A.5 and A.6.

The estimation is based on N replications allocated to m design points $\mathbf{x} = (x_1, x_2, \ldots, x_m)$ according to the loadings $\boldsymbol{\pi} = (\pi_1, \pi_2, \ldots, \pi_m)$. In the following derivations, we assume that the allocation of replications $n_i = N\pi_i$ $(i = 1, 2, \ldots, m)$ is an integer.

The estimated variance of $\widehat{\mu}_\nu(x)$ is given by (35) as

$$\widehat{\mathrm{Var}}[\widehat{\mu}_\nu(x)] = s_\nu^2 \mathbf{u}'(x, \widehat{\boldsymbol{\theta}}_\nu)(\widehat{\mathbf{V}}_\nu' \widehat{\mathbf{V}}_\nu)^{-1} \mathbf{u}(x, \widehat{\boldsymbol{\theta}}_\nu). \tag{42}$$

Let the matrix $\mathbf{A}^{(\nu)} = \widehat{\mathbf{V}}_\nu' \widehat{\mathbf{V}}_\nu$, with element $a_{st}^{(\nu)} = \sum_{i=1}^m n_i v_s^{(\nu)}(x_i) v_t^{(\nu)}(x_i)$. We can write the determinant of $A^{(\nu)}$ as

$$|\mathbf{A}^{(\nu)}| = \sum_{i_1=1}^m n_{i_1} v_1^{(\nu)}(x_{i_1}) \sum_{i_2=1}^m n_{i_2} v_2^{(\nu)}(x_{i_2}) \cdots \sum_{i_T=1}^m n_{i_T} v_T^{(\nu)}(x_{i_T}) \begin{vmatrix} v_1^{(\nu)}(x_{i_1}) & v_1^{(\nu)}(x_{i_2}) & \cdots & v_1^{(\nu)}(x_{i_T}) \\ v_2^{(\nu)}(x_{i_1}) & v_2^{(\nu)}(x_{i_2}) & \cdots & v_2^{(\nu)}(x_{i_T}) \\ \vdots & \vdots & \vdots & \vdots \\ v_T^{(\nu)}(x_{i_1}) & v_T^{(\nu)}(x_{i_2}) & \cdots & v_T^{(\nu)}(x_{i_T}) \end{vmatrix}.$$

Then $|\mathbf{A}^{(\nu)}|$, the determinant of $\mathbf{A}^{(\nu)}$, and $|\mathbf{A}_{st}^{(\nu)}|$, the cofactor of $\mathbf{A}^{(\nu)}$ can be written as follows:

$$\begin{aligned} |\mathbf{A}^{(\nu)}| &= \sum_{\substack{i_s \neq i_t \\ 1 \le i_1, \ldots, i_T \le m}} n_{i_1} n_{i_2} \cdots n_{i_T} v_1^{(\nu)}(x_{i_1}) v_2^{(\nu)}(x_{i_2}) \cdots v_T^{(\nu)}(x_{i_T}) \\ &\times \begin{vmatrix} v_1^{(\nu)}(x_{i_1}) & v_1^{(\nu)}(x_{i_2}) & \cdots & v_1^{(\nu)}(x_{i_T}) \\ v_2^{(\nu)}(x_{i_1}) & v_2^{(\nu)}(x_{i_2}) & \cdots & v_2^{(\nu)}(x_{i_T}) \\ \vdots & \vdots & \vdots & \vdots \\ v_T^{(\nu)}(x_{i_1}) & v_T^{(\nu)}(x_{i_2}) & \cdots & v_T^{(\nu)}(x_{i_T}) \end{vmatrix} \\ &= N^{T_\nu} b^{(\nu)}(\mathbf{x}, \boldsymbol{\pi}) \end{aligned} \tag{43}$$

$$
\begin{aligned}
|\mathbf{A}_{st}^{(\nu)}| &= \sum_{\substack{i_a \neq i_b \\ i_a \neq i_t \\ 1 \leq i_1, \ldots, i_T \leq m}} n_{i_1} \cdots n_{i_{t-1}} n_{i_{t+1}} \cdots n_{i_T} v_1^{(\nu)}(x_{i_1}) \cdots v_{t-1}^{(\nu)}(x_{i_{t-1}}) v_{t+1}^{(\nu)}(x_{i_{t+1}}) \cdots v_T^{(\nu)}(x_{i_T}) \\
&\times \begin{vmatrix}
v_1^{(\nu)}(x_{i_1}) & \cdots & v_1^{(\nu)}(x_{i_{t-1}}) & v_1^{(\nu)}(x_{i_{t+1}}) & \cdots & v_1^{(\nu)}(x_{i_T}) \\
\vdots & \vdots & \vdots & \vdots & \vdots & \\
v_{s-1}^{(\nu)}(x_{i_{s-1}}) & \cdots & v_{s-1}^{(\nu)}(x_{i_{t-1}}) & v_{s-1}^{(\nu)}(x_{i_{t+1}}) & \cdots & v_{s-1}^{(\nu)}(x_{i_T}) \\
v_{s+1}^{(\nu)}(x_{i_{s+1}}) & \cdots & v_{s+1}^{(\nu)}(x_{i_{t-1}}) & v_{s+1}^{(\nu)}(x_{i_{t+1}}) & \cdots & v_{s+1}^{(\nu)}(x_{i_T}) \\
\vdots & \vdots & \vdots & \vdots & \vdots & \\
v_T^{(\nu)}(x_{i_1}) & \cdots & v_T^{(\nu)}(x_{i_{t-1}}) & v_T^{(\nu)}(x_{i_{t+1}}) & \cdots & v_T^{(\nu)}(x_{i_T})
\end{vmatrix} \\
&= N^{T-1} b_{st}^{(\nu)}(\mathbf{x}, \boldsymbol{\pi}) \qquad (44)
\end{aligned}
$$

Equations (43) and (44) follow because $n_i = N\pi_i$. The functions $b^{(\nu)}(\mathbf{x}, \boldsymbol{\pi})$ and $b_{st}^{(\nu)}(\mathbf{x}, \boldsymbol{\pi})$ can be evaluated given $\mathbf{x}$ and $\boldsymbol{\pi}$. Then the inverse of $A_{st}^{(\nu)}$ can be obtained as

$$
[(\mathbf{A}^{(\nu)})^{-1}]_{st} = \frac{|\mathbf{A}_{st}^{(\nu)}|}{|\mathbf{A}^{(\nu)}|} = N^{-1} \frac{b_{st}^{(\nu)}(\mathbf{x}, \boldsymbol{\pi})}{b^{(\nu)}(\mathbf{x}, \boldsymbol{\pi})}. \qquad (45)
$$

Thus, $(\mathbf{A}^{(\nu)})^{-1} = N^{-1}\mathbf{B}^{(\nu)}(\mathbf{x}, \boldsymbol{\pi})$ where the (s, t) element of $\mathbf{B}^{(\nu)}(\mathbf{x}, \boldsymbol{\pi})$ is given by $\mathbf{B}_{st}^{(\nu)} = b_{st}^{(\nu)}(\mathbf{x}, \boldsymbol{\pi})/b^{(\nu)}(\mathbf{x}, \boldsymbol{\pi})$. The normalized variance of the ν^{th} moment estimator $\widehat{\mu}_\nu(x_0)$ can be expressed as:

$$
N \times \widehat{\mathrm{Var}}[\widehat{\mu}_\nu(x_0)] = s_\nu^2 \mathbf{u}'(x, \widehat{\boldsymbol{\theta}}_\nu) \mathbf{B}^{(\nu)}(\mathbf{x}, \boldsymbol{\pi}) \mathbf{u}(x, \widehat{\boldsymbol{\theta}}_\nu). \qquad (46)
$$

The covariances of the moment estimators are given in (38) as:

$$
\begin{aligned}
& \widehat{\mathrm{Cov}}[\widehat{\mu}_k(x), \widehat{\mu}_\ell(x)] \\
= \; & \mathbf{u}'(x, \widehat{\boldsymbol{\theta}}_k)(\widehat{\mathbf{V}}_k' \widehat{\mathbf{V}}_k)^{-1} \widehat{\mathbf{V}}_k' \widehat{\mathrm{Cov}}[\mathbf{Z}^{(k)}, \mathbf{Z}^{(\ell)}](\widehat{\mathbf{V}}_\ell (\widehat{\mathbf{V}}_\ell' \widehat{\mathbf{V}}_\ell)^{-1})' \mathbf{u}(x, \widehat{\boldsymbol{\theta}}_\ell) \qquad (47) \\
& k, \ell = 1, 2, 3; \quad k \neq \ell.
\end{aligned}
$$

The covariance matrix $\mathrm{Cov}[\mathbf{Z}^{(k)}, \mathbf{Z}^{(\ell)}]$ is given by (29), the elements of which $\sigma_{k\ell}(x)$ ($x = x_1, x_2, \ldots, x_m$) can be estimated by (41) as explained in Appendix A.3.

Using (45), we can easily derive

$$
\begin{aligned}
& N\widehat{\mathrm{Cov}}[\widehat{\mu}_k(x), \widehat{\mu}_\ell(x)] \\
= \; & \left(\sum_{i=1}^{m} \pi_i \widehat{\sigma}_{k\ell}(x_i) \left(\sum_{j=1}^{T_k} u_j(x, \widehat{\boldsymbol{\theta}}_k) d_{ji}^{(k)} \right) \left(\sum_{h=1}^{T_\ell} u_h(x, \widehat{\boldsymbol{\theta}}_\ell) d_{hi}^{(\ell)} \right) \right) \qquad (48)
\end{aligned}
$$

where

$$d_{ji}^{(\nu)} = \sum_{t=1}^{T_\nu} \frac{b_{jt}^{(\nu)}(\mathbf{x}, \boldsymbol{\pi})}{b^{(\nu)}(\mathbf{x}, \boldsymbol{\pi})} \times v_t^{(\nu)}(x_i), \tag{49}$$

and $u_j(x, \widehat{\boldsymbol{\theta}}_\ell)$ is defined in (30).

A.5. Numerical Evaluation of the Design Criterion

For convenience, we restate the design criterion in (22)

$$PM = N \sum_{\kappa \in \boldsymbol{\Omega}_x} \mathrm{Var}[\widehat{\mathcal{C}}_{\alpha_U}(\kappa)]. \tag{50}$$

In this section, we evaluate the design criterion numerically for given design $[\mathbf{x}, \boldsymbol{\pi}]$ in an effort to search for the optimal solution of (23). Recall that this evaluation is performed in the context where some simulation experiments have already been carried out. The key is to obtain the variances and covariances of the moment estimators $\{\widehat{\mu}_\nu(\kappa), \nu = 1, 2, 3\}$ for $\kappa \in \boldsymbol{\Omega}_x$, from which $\mathrm{Var}[\widehat{\mathcal{C}}_{\alpha_U}(\kappa)]$ can be approximately computed.

As we did in Yang et al. (2007), linear assumptions about the regression models for moment curves are made at the stage of designing experiments. More specifically, the unknown parameters, p_ν in the moment model (4) and q_ν in the variance model (5), are both assumed to be known and given as their best estimates obtained so far, $\widehat{p}_\nu$ and $\widehat{q}_\nu$. This assumption reduces the transformed model (7) to a linear model with the exponent r_ν being a known parameter given by $\widehat{q}_\nu - \widehat{p}_\nu$. In addition, we suppose that the expanded experiments with m design points are designed to estimate moment models (4) whose polynomial order is equal to $m - 1$.

Under these assumptions, the moment models and transformed moment models are (with superscript ν dropped for simplicity):

$$\mu(x, \boldsymbol{\theta}) = \frac{\sum_{\ell=0}^{m-1} c_\ell x^\ell}{(1-x)^p} \tag{51}$$

$$\eta(x, \boldsymbol{\theta}) = \left(\sum_{\ell=0}^{m-1} c_\ell x^\ell \right) (1-x)^r \tag{52}$$

where both p and r are assumed to be known, and the unknown linear parameters are $\boldsymbol{\theta} = (c_0, c_1, \ldots, c_{m-1})$.

As already noted, the design criterion (50) is a normalized variance measure, which depends on the design $[\mathbf{x}, \boldsymbol{\pi}]$. To search for the optimal $[\mathbf{x}, \boldsymbol{\pi}]$, we need to be able to evaluate (50) numerically for given $[\mathbf{x}, \boldsymbol{\pi}]$. With $\mu(x, \boldsymbol{\theta})$ and $\eta(x, \boldsymbol{\theta})$ defined as the linear models given by (51) and (52), we can numerically evaluate the normalized variances and covariances of the moment estimators for given $[\mathbf{x}, \boldsymbol{\pi}]$

$$N\mathrm{Var}[\mu(\kappa, \widehat{\boldsymbol{\theta}}_\nu)] \quad \nu = 1, 2, 3 \tag{53}$$

$$\text{and} \quad N\mathrm{Cov}[\mu(\kappa, \widehat{\boldsymbol{\theta}}_k), \mu(\kappa, \widehat{\boldsymbol{\theta}}_\ell)] \quad k, \ell = 1, 2, 3; k \neq \ell, \tag{54}$$

by following the derivation in Appendix A.4.

In addition, based on the data set already collected, $\{\mu(\kappa, \widehat{\boldsymbol{\theta}}_\nu); \kappa \in \boldsymbol{\Omega}_x, \nu = 1, 2, 3\}$, the distribution parameters of $G_\kappa(t; \widehat{a}(\kappa), \widehat{b}(\kappa), \widehat{k}(\kappa))$ can be estimated. Applying the delta method as illustrated in Section 5.2, we can approximately calculate $N\mathrm{Var}[\widehat{\mathcal{C}}_{\alpha_U}(\kappa)]$, which is a component of the sum formulation (50).

A.6. Incrementing the Number of Runs

As mentioned in Section 6.1.2, we need to determine ΔN, the number of replications to be added to the current design before solving the optimization problem (23) to obtain the optimal design for further simulation experiments. As explained in Yang et al. (2007), adding ΔN replications should help drive the precision level of the chosen estimators, in this case $\widehat{\mathcal{C}}_{\alpha_U}(x_U)$ and $\widehat{\mathcal{C}}_{\alpha_L}(x_L)$, down to the target $100\gamma\%$ (the definition of $100\gamma\%$ is given in Section 6.2). Conditional on the size of the current estimated relative error $100\widehat{\gamma}_c$, which indicates how precise the current estimate is, we set an intermediate target, say $100\gamma_1\% (\gamma \leq \gamma_1 < \gamma_c)$, for the expanded data set to achieve. Details regarding the choice of $100\gamma_1\%$ are discussed in Yang et al. (2007, Appendix 3).

Regarding the determination of ΔN, we follow the same logic as in Appendix 3 of Yang et al. (2007). In the remainder of this section, we illustrate how a rough estimate of ΔN is computed for achieving the desired precision level $100\gamma_1\%$ under the following assumptions:

(i) To obtain a rough estimate of ΔN needed for the follow-up design given the current data, the design points $\mathbf{x}$ to be included in the follow-up design have to be known. As noted in Section 6.2, there are two types of design augmentation involved in our procedure: adding more replications to the current design points; and expanding the current design by adding new design points to the initial design composed of the two points x_L and x_U. In the first case, the locations of the design points are known. In the second case, we simply assume that the design points in the augmented design will be evenly spaced throughout the throughput range.

(ii) The number of unknown parameters included in the estimated moment models $\{\widehat{\mu}_\nu(x), \nu = 1, 2, 3\}$ remains the same after the design augmentation.

(iii) The allocation of the total $N = N_c + \Delta N$ replications is not constrained by the fact that the N_c replications already performed cannot be reassigned.

The process for obtaining an estimate of N consists of two steps.

1. With $\mathbf{x}$ being given in Assumption (i), solve the following optimization problem for the optimal solution $\boldsymbol{\pi}^*$:

$$\begin{aligned} \min_{\boldsymbol{\pi}} PM &= N \sum_{\kappa \in \boldsymbol{\Omega}_x} \mathrm{Var}[\widehat{\mathcal{C}}_{\alpha_U}(\kappa)] \\ s.t. \sum_{i=1}^{m} \pi_i &= 1. \end{aligned} \tag{55}$$

   The objective PM is a function of $\boldsymbol{\pi}$ (independent of N) given the location of the design points $\mathbf{x}$. Under the assumptions above, the performance measure PM can be evaluated for given $\boldsymbol{\pi}$ as illustrated in Appendix A.5. Thus a numerical search will lead to the optimal solution $\boldsymbol{\pi}^*$.

2. Assuming the follow-up design is $[\mathbf{x}, \boldsymbol{\pi}^*]$, find the number of replications N that satisfy

$$\frac{2 \times \widehat{\mathrm{SE}}[\widehat{\mathcal{C}}_{\alpha_U}(x_U)]}{\widehat{\mathcal{C}}_{\alpha_U}(x_U)} \leq 100\gamma_1\%. \tag{56}$$

   Based on the current data set, an estimate of $\mathcal{C}_{\alpha_U}(x_U)$ is obviously available. Given design $[\mathbf{x}, \boldsymbol{\pi}^*]$, the normalized variance $N\mathrm{Var}[\widehat{\mathcal{C}}_{\alpha_U}(x_U)]$ can also be estimated: first, we estimate $\{N\mathrm{Var}[\widehat{\mu}_\nu(x_U)], \nu = 1,2,3\}$ and $\{N\mathrm{Cov}[\widehat{\mu}_k(x_U), \widehat{\mu}_\ell(x_U)], k, \ell = 1,2,3; k \neq \ell\}$ by following the derivation in Appendix A.4; then we estimate $N\mathrm{Var}[\widehat{\mathcal{C}}_{\alpha_U}(x_U)]$ by resorting to the delta method. The standard error is $\widehat{\mathrm{SE}} = \sqrt{N^{-1} \times (N\mathrm{Var}[\widehat{\mathcal{C}}_{\alpha_U}(x_U)])}$ with N being the unknown variable to be determined (the normalized variance $N\mathrm{Var}[\widehat{\mathcal{C}}_{\alpha_U}(x_U)]$ is independent of N). Therefore, by solving the inequality (56), we obtain N_{min}, the smallest number of replications required to satisfy (56). Then $\Delta N = N_{min} - N_c$.

Once the desired relative precision has been achieved on $\widehat{\mathcal{C}}_{\alpha_U}(x_U)$, we switch to use the precision of $\widehat{\mathcal{C}}_{\alpha_U}(x_L)$ to drive the procedure until $\widehat{\mathcal{C}}_{\alpha_U}(x_L)$ also achieves the prespecified precision level. The derivation for determining ΔN presented above can be applied directly to $\widehat{\mathcal{C}}_{\alpha_U}(x_L)$.

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