Efficient Learning for Clustering and Optimizing Context-Dependent Designs

Haidong Li
College of Engineering, Peking University, Beijing 100871, China, haidong.li@pku.edu.cn

Henry Lam
Department of Industrial Engineering and Operations Research, Columbia University, NY 10027, USA, henry.lam@columbia.edu

Yijie Peng
Department of Management Science and Information Systems, Guanghua School of Management, Peking University, Beijing 100871, China, pengyijie@pku.edu.cn

We consider a simulation optimization problem for context-dependent decision-making. Under a Gaussian mixture model based Bayesian framework, we develop a dynamic sampling policy to maximize the worst-case probability of correctly selecting the best design over all contexts, which utilizes both global clustering information and local performance information. In particular, we design a computationally efficient approximation method to learn these sources of information, thereby leading to an implementable dynamic sampling policy. The proposed sampling policy is proved to be consistent and achieve the asymptotically optimal sampling ratio. Numerical experiments show that the proposed approximation method makes a good balance between the performance and complexity, and the proposed sampling policy significantly improves the efficiency in context-dependent simulation optimization.

Key words: simulation, ranking and selection, context, performance clustering

Proofs and Supplementary Materials

EC.1. Gaussian mixture model for arbitrarily shaped clustering patterns

Figure EC.1 shows a general clustering pattern which is not grid-like. Arbitrarily shaped clustering patterns can be characterized by the following classic Gaussian mixture model:

$$y_i(\boldsymbol{x}) \sim \sum_{k=1}^{K\times L} \tau_k \phi(\cdot|\Lambda_k, \Xi_k^2)$$
$$\text{s.t.} \sum_{k=1}^{K\times L} \tau_k = 1.$$

The hidden state random variable $z_{i,j}[k]$ assigns design-context pair (i,j) to cluster k if $z_{i,j}[k]=1$, which means $y_i(\boldsymbol{x}_j)$ comes from a realization of distribution $\phi(\cdot|\Lambda_k,\Xi_k^2)$. The general model will have $K\times L$ weight parameters $(\tau_k, k=1,\dots,K\times L)$ and $n\times m\times K\times L$ hidden state random variables $(z_{i,j}[k], i=1,\dots,n, j=1,\dots,m, k=1,\dots,K\times L)$ to be estimated, whereas the GMM used in our paper only has $K+L$ weight parameters $(\tau_k, k=1,\dots,K$ and $\omega_\ell, \ell=1,\dots,L)$ and $n\times K+m\times L$ hidden state random variables $(z_i[k], i=1,\dots,n, k=1,\dots,K$ and $v_j[\ell], j=1,\dots,m, \ell=1,\dots,L)$. Compared with using general clustering pattern, our model is relatively parsimonious and less likely to overfit.

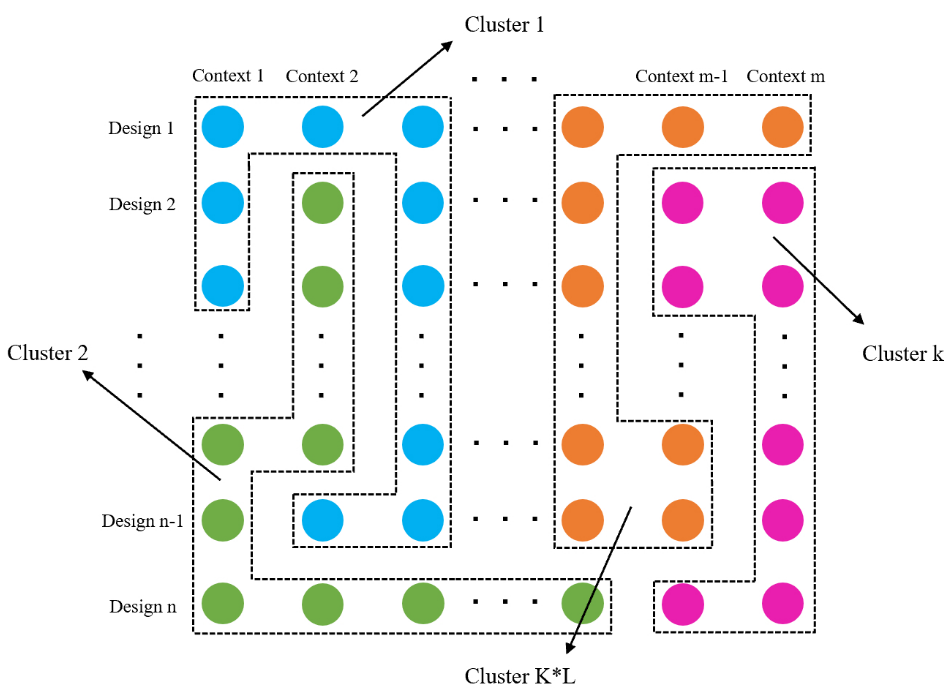

Figure EC.1 A general clustering pattern.

EC.2. Proof of Lemmas 1 and 2

Proof of Lemma 1 Given $\widehat{\theta}^{(t,s)}$, an analytical form for the likelihood of the observations can be obtained by integrating out $\boldsymbol{y}$, Z, and V as follow:

$$
\begin{aligned}
&\mathcal{L}(\mathcal{E}_t;\widehat{\theta}^{(t,s)})\\
&=\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L}}\left(\prod_{i=1}^{n}\widehat{\tau}_{k_i}^{(t,s)}\right)\left(\prod_{j=1}^{m}\widehat{\omega}_{\ell_j}^{(t,s)}\right)\prod_{i=1}^{n}\prod_{j=1}^{m}\left[\int_{\mathbb{R}}\phi\left(y_i(\boldsymbol{x}_j)|\widehat{\Lambda}_{k_i,\ell_j}^{(t,s)},(\widehat{\Xi}^2_{k_i,\ell_j})^{(t,s)}\right)\right.\\
&\quad\left.\times\prod_{h=1}^{t_{i,j}}\phi\left(Y_{i,h}(\boldsymbol{x}_j)|y_i(\boldsymbol{x}_j),\sigma_i^2(\boldsymbol{x}_j)\right)dy_i(\boldsymbol{x}_j)\right]\\
&=\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L}}\left(\prod_{i=1}^{n}\widehat{\tau}_{k_i}^{(t,s)}\right)\left(\prod_{j=1}^{m}\widehat{\omega}_{\ell_j}^{(t,s)}\right)\prod_{i=1}^{n}\prod_{j=1}^{m}\left[\frac{1}{\sqrt{2\pi(\widehat{\Xi}^2_{k_i,\ell_j})^{(t,s)}}}\prod_{h=1}^{t_{i,j}}\frac{1}{\sqrt{2\pi\sigma_i^2(\boldsymbol{x}_j)}}\right.\\
&\quad\left.\times\int_{\mathbb{R}}\exp\left\{-\frac{1}{2}\left[\frac{(y_i(\boldsymbol{x}_j)-\widehat{\Lambda}_{k_i,\ell_j}^{(t,s)})^2}{(\widehat{\Xi}^2_{k_i,\ell_j})^{(t,s)}}+\sum_{h=1}^{t_{i,j}}\frac{(Y_{i,h}(\boldsymbol{x}_j)-y_i(\boldsymbol{x}_j))^2}{\sigma_i^2(\boldsymbol{x}_j)}\right]\right\}dy_i(\boldsymbol{x}_j)\right]\\
&=\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L}}\left(\prod_{i=1}^{n}\widehat{\tau}_{k_i}^{(t,s)}\right)\left(\prod_{j=1}^{m}\widehat{\omega}_{\ell_j}^{(t,s)}\right)\prod_{i=1}^{n}\prod_{j=1}^{m}\left[C_{i,j}^{(t,s)}[k_i,\ell_j]\int_{\mathbb{R}}\phi(y_i(\boldsymbol{x}_j)|\mu_{i,j}^{(t,s)}[k_i,\ell_j],(\sigma^2_{i,j})^{(t,s)}[k_i,\ell_j])dy_i(\boldsymbol{x}_j)\right]\\
&=\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L}}\left(\prod_{i=1}^{n}\widehat{\tau}_{k_i}^{(t,s)}\right)\left(\prod_{j=1}^{m}\widehat{\omega}_{\ell_j}^{(t,s)}\right)\prod_{i=1}^{n}\prod_{j=1}^{m}C_{i,j}^{(t,s)}[k_i,\ell_j],
\end{aligned}
$$

where

$$
(\sigma^2_{i,j})^{(t,s)}[k_i,\ell_j]=1\Bigg/\left[\frac{t_{i,j}}{\sigma_i^2(\boldsymbol{x}_j)}+\frac{1}{(\widehat{\Xi}^2_{k_i,\ell_j})^{(t,s)}}\right],
$$

$$
\mu_{i,j}^{(t,s)}[k_i,\ell_j]=(\sigma^2_{i,j})^{(t,s)}[k_i,\ell_j]\left[\frac{\sum_{h=1}^{t_{i,j}}Y_{i,h}(\boldsymbol{x}_j)}{\sigma_i^2(\boldsymbol{x}_j)}+\frac{\widehat{\Lambda}_{k_i,\ell_j}^{(t,s)}}{(\widehat{\Xi}^2_{k_i,\ell_j})^{(t,s)}}\right],
$$

and

$$
C_{i,j}^{(t,s)}[k_i,\ell_j]=\left(\frac{1}{2\pi\sigma_i^2(\boldsymbol{x}_j)}\right)^{\frac{t_{i,j}}{2}}\sqrt{\frac{(\sigma^2_{i,j})^{(t,s)}[k_i,\ell_j]}{(\widehat{\Xi}^2_{k_i,\ell_j})^{(t,s)}}}\exp\left\{\frac{1}{2}\left[\frac{(\mu_{i,j}^{(t,s)}[k_i,\ell_j])^2}{(\sigma^2_{i,j})^{(t,s)}[k_i,\ell_j]}-\frac{\sum_{h=1}^{t_{i,j}}Y^2_{i,h}(\boldsymbol{x}_j)}{\sigma_i^2(\boldsymbol{x}_j)}-\frac{(\widehat{\Lambda}_{k_i,\ell_j}^{(t,s)})^2}{(\widehat{\Xi}^2_{k_i,\ell_j})^{(t,s)}}\right]\right\}.
$$

By the Bayes' rule, the posterior distribution of $\{z_i[k]=1\}$ conditional on $\mathcal{E}_t$ and given $\widehat{\theta}^{(t,s)}$ is

$$
\widehat{z}_i^{(t,s)}[k]=\frac{\sum_{k_{1:n}\in\mathcal{K},k_i=k}\sum_{\ell_{1:m}\in\mathcal{L}}\left(\prod_{i=1}^{n}\widehat{\tau}_{k_i}^{(t,s)}\right)\left(\prod_{j=1}^{m}\widehat{\omega}_{\ell_j}^{(t,s)}\right)\prod_{i=1}^{n}\prod_{j=1}^{m}C_{i,j}^{(t,s)}[k_i,\ell_j]}{\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L}}\left(\prod_{i=1}^{n}\widehat{\tau}_{k_i}^{(t,s)}\right)\left(\prod_{j=1}^{m}\widehat{\omega}_{\ell_j}^{(t,s)}\right)\prod_{i=1}^{n}\prod_{j=1}^{m}C_{i,j}^{(t,s)}[k_i,\ell_j]},
$$

the posterior distribution of $\{v_j[\ell]=1\}$ conditional on $\mathcal{E}_t$ and given $\widehat{\theta}^{(t,s)}$ is

$$
\widehat{v}_j^{(t,s)}[\ell]=\frac{\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L},\ell_j=\ell}\left(\prod_{i=1}^{n}\widehat{\tau}_{k_i}^{(t,s)}\right)\left(\prod_{j=1}^{m}\widehat{\omega}_{\ell_j}^{(t,s)}\right)\prod_{i=1}^{n}\prod_{j=1}^{m}C_{i,j}^{(t,s)}[k_i,\ell_j]}{\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L}}\left(\prod_{i=1}^{n}\widehat{\tau}_{k_i}^{(t,s)}\right)\left(\prod_{j=1}^{m}\widehat{\omega}_{\ell_j}^{(t,s)}\right)\prod_{i=1}^{n}\prod_{j=1}^{m}C_{i,j}^{(t,s)}[k_i,\ell_j]},
$$

and given $\widehat{\theta}^{(t,s)}$, the posterior distribution of $y_i(\boldsymbol{x}_j)$ conditional on $\{z_i[k]=1\}$, $\{v_j[\ell]=1\}$, and $\mathcal{E}_t$ is

$$\phi(y_i(\boldsymbol{x}_j)|\mu_{i,j}^{(t,s)}[k,\ell],(\sigma_{i,j}^2)^{(t,s)}[k,\ell]).$$

□

Proof of Lemma 2 The log-likelihood of the complete state variables has the following form:

$$\begin{aligned}
&\log\mathcal{L}(\mathcal{E}_t,\boldsymbol{y},Z,V;\theta)\\
=&\left(\sum_{i=1}^{n}\sum_{k=1}^{K}z_i[k]\log\tau_k\right)+\left(\sum_{j=1}^{m}\sum_{\ell=1}^{L}v_j[\ell]\log\omega_\ell\right)+\sum_{i=1}^{n}\sum_{j=1}^{m}\left\{-\sum_{h=1}^{t_{i,j}}\left[\frac{1}{2}\log(2\pi\sigma_i^2(\boldsymbol{x}_j))+\frac{(Y_{i,h}(\boldsymbol{x}_j)-y_i(\boldsymbol{x}_j))^2}{2\sigma_i^2(\boldsymbol{x}_j)}\right]\right.\\
&\left.-\sum_{k=1}^{K}\sum_{\ell=1}^{L}\left[\frac{1}{2}z_i[k]v_j[\ell]\log(2\pi\Xi_{k,\ell}^2)+z_i[k]v_j[\ell]\frac{(y_i(\boldsymbol{x}_j)-\Lambda_{k,\ell})^2}{2\Xi_{k,\ell}^2}\right]\right\}. \qquad \text{(EC.1)}
\end{aligned}$$

From the log-likelihood of complete state variables given by (EC.1), we have

$$\begin{aligned}
&\mathcal{Q}(\theta|\widehat{\theta}^{(t,s)})\\
=&\mathbb{E}\left[\log\mathcal{L}(\mathcal{E}_t,\boldsymbol{y},Z,V;\theta)|\mathcal{E}_t,\widehat{\theta}^{(t,s)}\right]\\
=&\mathbb{E}\left[\left(\sum_{i=1}^{n}\sum_{k=1}^{K}z_i[k]\log\tau_k\right)+\left(\sum_{j=1}^{m}\sum_{\ell=1}^{L}v_j[\ell]\log\omega_\ell\right)-\sum_{i=1}^{n}\sum_{j=1}^{m}\sum_{k=1}^{K}\sum_{\ell=1}^{L}\left[\frac{1}{2}z_i[k]v_j[\ell]\log(2\pi\Xi_{k,\ell}^2)\right.\right.\\
&\left.\left.+z_i[k]v_j[\ell]\frac{(y_i(\boldsymbol{x}_j)-\Lambda_{k,\ell})^2}{2\Xi_{k,\ell}^2}\right]\middle|\mathcal{E}_t,\widehat{\theta}^{(t,s)}\right]+C^{(t,s)},
\end{aligned}$$

where $C^{(t,s)}$ is a constant independent of θ. The estimate $\widehat{\tau}_k^{(t,s+1)}$ in the $(s+1)$-th iteration of the EM algorithm is obtained by solving the following optimization problem:

$$\max_{\tau}\sum_{i=1}^{n}\sum_{k=1}^{K}\widehat{z}_i^{(t,s)}[k]\log\tau_k,\ \text{s.t.}\sum_{k=1}^{K}\tau_k=1,\ \tau_k\geq 0,$$

which is given by

$$\widehat{\tau}_k^{(t,s+1)}=\frac{\sum_{i=1}^{n}\widehat{z}_i^{(t,s)}[k]}{n}.$$

Similarly,

$$\widehat{\omega}_\ell^{(t,s+1)}=\frac{\sum_{j=1}^{m}\widehat{v}_j^{(t,s)}[\ell]}{m}.$$

Posterior estimate $\widehat{\Lambda}_{k,\ell}^{(t,s+1)}$ is the solution of the follow equation:

$$\sum_{i=1}^{n}\sum_{j=1}^{m}\widehat{z}_i^{(t,s)}[k]\widehat{v}_j^{(t,s)}[\ell]\mathbb{E}\left[y_i(\boldsymbol{x}_j)-\Lambda_{k,\ell}\middle|z_i[k]=1,v_j[\ell]=1,\mathcal{E}_t,\widehat{\theta}^{(t,s)}\right]=0,$$

which yields

$$\widehat{\Lambda}_{k,\ell}^{(t,s+1)}=\frac{\sum_{i=1}^{n}\sum_{j=1}^{m}\widehat{z}_i^{(t,s)}[k]\widehat{v}_j^{(t,s)}[\ell]\mu_{i,j}^{(t,s)}[k,\ell]}{\sum_{i=1}^{n}\sum_{j=1}^{m}\widehat{z}_i^{(t,s)}[k]\widehat{v}_j^{(t,s)}[\ell]}.$$

To calculate $(\widehat{\Xi}^2_{k,\ell})^{(t,s+1)}$, we solve the follow equation:

$$\sum_{i=1}^{n}\sum_{j=1}^{m}\widehat{z}_i^{(t,s)}[k]\widehat{v}_j^{(t,s)}[\ell]\mathbb{E}\left[1-\frac{(y_i(\boldsymbol{x}_j)-\widehat{\Lambda}_{k,\ell}^{(t,s+1)})^2}{\Xi^2_{k,\ell}}\middle| z_i[k]=1, v_j[\ell]=1,\mathcal{E}_t,\widehat{\theta}^{(t,s)}\right]=0,$$

which leads to

$$(\widehat{\Xi}^2_{k,\ell})^{(t,s+1)}=\frac{\sum_{i=1}^{n}\sum_{j=1}^{m}\widehat{z}_i^{(t,s)}[k]\widehat{v}_j^{(t,s)}[\ell]\left[(\sigma^2_{i,j})^{(t,s)}[k,\ell]+\left(\mu_{i,j}^{(t,s)}[k,\ell]-\widehat{\Lambda}_{k,\ell}^{(t,s+1)}\right)^2\right]}{\sum_{i=1}^{n}\sum_{j=1}^{m}\widehat{z}_i^{(t,s)}[k]\widehat{v}_j^{(t,s)}[\ell]}.$$

□

EC.3. The asymptotic analysis of Theorem 1

PROPOSITION EC.1. *The posterior probability of $\{z_i[k]=1\}$ conditional on $\boldsymbol{y}$ and given $\widehat{\theta}^{(s)}$ is*

$$\widehat{z}_i^{(s)}[k]=\frac{\sum_{k_{1:n}\in\mathcal{K},k_i=k}\sum_{\ell_{1:m}\in\mathcal{L}}f_\tau^{(s)}(k_{1:n})f_\omega^{(s)}(\ell_{1:m})f_{\boldsymbol{y}}^{(s)}(k_{1:n},\ell_{1:m})}{\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L}}f_\tau^{(s)}(k_{1:n})f_\omega^{(s)}(\ell_{1:m})f_{\boldsymbol{y}}^{(s)}(k_{1:n},\ell_{1:m})},$$

the posterior probability of $\{v_j[\ell]=1\}$ conditional on $\boldsymbol{y}$ and given $\widehat{\theta}^{(s)}$ is

$$\widehat{v}_j^{(s)}[\ell]=\frac{\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L},\ell_j=\ell}f_\tau^{(s)}(k_{1:n})f_\omega^{(s)}(\ell_{1:m})f_{\boldsymbol{y}}^{(s)}(k_{1:n},\ell_{1:m})}{\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L}}f_\tau^{(s)}(k_{1:n})f_\omega^{(s)}(\ell_{1:m})f_{\boldsymbol{y}}^{(s)}(k_{1:n},\ell_{1:m})},$$

where $f_\tau^{(s)}(k_{1:n})\triangleq\prod_{i=1}^{n}\widehat{\tau}_{k_i}^{(s)}$, $f_\omega^{(s)}(\ell_{1:m})\triangleq\prod_{j=1}^{m}\widehat{\omega}_{\ell_j}^{(s)}$, and $f_{\boldsymbol{y}}^{(s)}(k_{1:n},\ell_{1:m})\triangleq\prod_{i=1}^{n}\prod_{j=1}^{m}\phi\left(y_i(\boldsymbol{x}_j)|\widehat{\Lambda}_{k_i,\ell_j}^{(s)},(\widehat{\Xi}^2_{k_i,\ell_j})^{(s)}\right)$. The estimates of the parameters in the $(s+1)$-th iteration of the EM algorithm are given by

$$\widehat{\tau}_k^{(s+1)}=\frac{\sum_{i=1}^{n}\widehat{z}_i^{(s)}[k]}{n},\ \widehat{\omega}_\ell^{(s+1)}=\frac{\sum_{j=1}^{m}\widehat{v}_j^{(s)}[\ell]}{m},$$

$$\widehat{\Lambda}_{k,\ell}^{(s+1)}=\frac{\sum_{i=1}^{n}\sum_{j=1}^{m}\widehat{z}_i^{(s)}[k]\widehat{v}_j^{(s)}[\ell]y_i(\boldsymbol{x}_j)}{\sum_{i=1}^{n}\sum_{j=1}^{m}\widehat{z}_i^{(s)}[k]\widehat{v}_j^{(s)}[\ell]},$$

and

$$(\widehat{\Xi}^2_{k,\ell})^{(s+1)}=\frac{\sum_{i=1}^{n}\sum_{j=1}^{m}\widehat{z}_i^{(s)}[k]\widehat{v}_j^{(s)}[\ell]\left(y_i(\boldsymbol{x}_j)-\widehat{\Lambda}_{k,\ell}^{(s+1)}\right)^2}{\sum_{i=1}^{n}\sum_{j=1}^{m}\widehat{z}_i^{(s)}[k]\widehat{v}_j^{(s)}[\ell]}.$$

PROPOSITION EC.2. *Suppose each design-context pair is sampled infinitely often as t goes to infinity. Then*

$$\lim_{t\to+\infty}\left[\frac{C_{i,j}^{(t,s)}[k_i,\ell_j]}{C_{i,j}^{(t,s)}[k,\ell]}-\frac{\phi\left(y_i(\boldsymbol{x}_j)|\widehat{\Lambda}_{k_i,\ell_j}^{(s)},(\widehat{\Xi}^2_{k_i,\ell_j})^{(s)}\right)}{\phi\left(y_i(\boldsymbol{x}_j)|\widehat{\Lambda}_{k,\ell}^{(s)},(\widehat{\Xi}^2_{k,\ell})^{(s)}\right)}\right]=0,\ a.s.$$

where

$$C_{i,j}^{(t,s)}[k,\ell]\triangleq\left(\frac{1}{2\pi\sigma_i^2(\boldsymbol{x}_j)}\right)^{\frac{t_{i,j}}{2}}\sqrt{\frac{(\sigma^2_{i,j})^{(t,s)}[k,\ell]}{(\widehat{\Xi}^2_{k,\ell})^{(t,s)}}}\exp\left\{\frac{1}{2}\left[\frac{(\mu_{i,j}^{(t,s)}[k,\ell])^2}{(\sigma^2_{i,j})^{(t,s)}[k,\ell]}-\frac{\sum_{h=1}^{t_{i,j}}Y_{i,h}^2(\boldsymbol{x}_j)}{\sigma_i^2(\boldsymbol{x}_j)}-\frac{(\widehat{\Lambda}_{k,\ell}^{(t,s)})^2}{(\widehat{\Xi}^2_{k,\ell})^{(t,s)}}\right]\right\}.$$

Proof of Proposition EC.2 We have

$$\begin{aligned}
&\frac{(\mu_{i,j}^{(t,s)}[k_i,\ell_j])^2}{(\sigma_{i,j}^2)^{(t,s)}[k_i,\ell_j]}\\
&=(\sigma_{i,j}^2)^{(t,s)}[k_i,\ell_j]\left[\frac{\sum_{h=1}^{t_{i,j}}Y_{i,h}(\boldsymbol{x}_j)}{\sigma_i^2(\boldsymbol{x}_j)}+\frac{\widehat{\Lambda}_{k_i,\ell_j}^{(t,s)}}{(\widehat{\Xi}_{k_i,\ell_j}^2)^{(t,s)}}\right]^2\\
&=\frac{t_{i,j}\left[\frac{1}{t_{i,j}}\sum_{h=1}^{t_{i,j}}Y_{i,h}(\boldsymbol{x}_j)\right]^2}{\sigma_i^2(\boldsymbol{x}_j)}-\frac{\left[\frac{1}{t_{i,j}}\sum_{h=1}^{t_{i,j}}Y_{i,h}(\boldsymbol{x}_j)\right]^2}{(\widehat{\Xi}_{k_i,\ell_j}^2)^{(t,s)}}+2\frac{\left[\frac{1}{t_{i,j}}\sum_{h=1}^{t_{i,j}}Y_{i,h}(\boldsymbol{x}_j)\right]\widehat{\Lambda}_{k_i,\ell_j}^{(t,s)}}{(\widehat{\Xi}_{k_i,\ell_j}^2)^{(t,s)}}+o_{a.s.}(1),
\end{aligned}$$

where $o_{a.s.}(1)$ means a term that goes to zero as t goes to infinity a.s., by observing $\lim_{t\to+\infty}t_{i,j}(\sigma_{i,j}^2)^{(t,s)}[k_i,\ell_j]=\sigma_i^2(\boldsymbol{x}_j)$, a.s. Therefore, the conclusion of the proposition can be obtained straightforwardly by observing $\lim_{t\to+\infty}\frac{1}{t_{i,j}}\sum_{h=1}^{t_{i,j}}Y_{i,h}(\boldsymbol{x}_j)=y_i(\boldsymbol{x}_j)$, a.s., and canceling the terms independent of k_i and ℓ_j in $C_{i,j}^{(t,s)}[k_i,\ell_j]$. □

The above proposition implies $C_{i,j}^{(t,s)}[k_i,\ell_j]$ corresponds to $\phi\left(y_i(\boldsymbol{x}_j)|\widehat{\Lambda}_{k_i,\ell_j}^{(s)},(\widehat{\Xi}_{k_i,\ell_j}^2)^{(s)}\right)$. Further, $f_Y^{(t,s)}(\mathcal{E}_t|k_{1:n},\ell_{1:m})$ corresponds to $f_{\boldsymbol{y}}^{(s)}(k_{1:n},\ell_{1:m})$ in the classic results. Therefore, Corollary EC.1 is a direct conclusion from Proposition EC.2.

Corollary EC.1. *Suppose each design-context pair is sampled infinitely often as t goes to infinity. Then*

$$\lim_{t\to+\infty}\left[\widehat{z}_i^{(t,s)}[k]-\widehat{z}_i^{(s)}[k]\right]=0 \textit{ and } \lim_{t\to+\infty}\left[\widehat{v}_j^{(t,s)}[\ell]-\widehat{v}_j^{(s)}[\ell]\right]=0,\ a.s.$$

EC.4. Proof of Propositions 1 and 2

Proof of Proposition 1 Notice that we have $\lim_{t\to+\infty}\widehat{\Lambda}_{k_i,\ell_j}^{(t,s)}=\Lambda_{k_i,\ell_j}^{(s)}$ and $\lim_{t\to+\infty}(\widehat{\Xi}_{k_i,\ell_j}^2)^{(t,s)}=(\Xi_{k_i,\ell_j}^2)^{(s)}>0$. Therefore, when $2e\pi\sigma_i^2(x_j)\geq 1$,

$$\begin{aligned}
&\lim_{t_{i,j}\to+\infty}C_{i,j}^{(t,s)}[k_i,\ell_j]\\
&=\lim_{t_{i,j}\to+\infty}\left(\frac{1}{2\pi\sigma_i^2(\boldsymbol{x}_j)}\right)^{\frac{t_{i,j}}{2}}\sqrt{\frac{(\sigma_{i,j}^2)^{(t,s)}[k_i,\ell_j]}{(\widehat{\Xi}_{k_i,\ell_j}^2)^{(t,s)}}}\exp\left\{\frac{1}{2}\left[\frac{(\mu_{i,j}^{(t,s)}[k_i,\ell_j])^2}{(\sigma_{i,j}^2)^{(t,s)}[k_i,\ell_j]}-\frac{\sum_{h=1}^{t_{i,j}}Y_{i,h}^2(\boldsymbol{x}_j)}{\sigma_i^2(\boldsymbol{x}_j)}-\frac{(\widehat{\Lambda}_{k_i,\ell_j}^{(t,s)})^2}{(\widehat{\Xi}_{k_i,\ell_j}^2)^{(t,s)}}\right]\right\}\\
&=\lim_{t_{i,j}\to+\infty}\left(\frac{1}{2\pi\sigma_i^2(\boldsymbol{x}_j)}\right)^{\frac{t_{i,j}}{2}}\sqrt{\frac{\sigma_i^2(x_j)}{t_{i,j}(\Xi_{k_i,\ell_j}^2)^{(s)}}}\exp\left\{\frac{1}{2}\left[\frac{t_{i,j}\left(\mathbb{E}[Y_{i,h}(\boldsymbol{x}_j)]\right)^2}{\sigma_i^2(\boldsymbol{x}_j)}-\frac{t_{i,j}\mathbb{E}[Y_{i,h}^2(\boldsymbol{x}_j)]}{\sigma_i^2(\boldsymbol{x}_j)}-o(t_{i,j})\right]\right\}\\
&=\lim_{t_{i,j}\to+\infty}\left(\frac{1}{2\pi\sigma_i^2(\boldsymbol{x}_j)}\right)^{\frac{t_{i,j}}{2}}\sqrt{\frac{\sigma_i^2(x_j)}{t_{i,j}(\Xi_{k_i,\ell_j}^2)^{(s)}}}\exp\left\{\frac{1}{2}\left[-t_{i,j}-o(t_{i,j})\right]\right\}\\
&=0,
\end{aligned}$$

where the second equation follows from the law of large numbers and the last equation is a result of $2e\pi\sigma_i^2(x_j)\geq 1$. Similarly, when $2e\pi\sigma_i^2(x_j)<1$, $\lim_{t_{i,j}\to+\infty}C_{i,j}^{(t,s)}[k_i,\ell_j]=+\infty$ since the exponential function grows faster than any power function. □

Proof of Proposition 2 In (6) and (7), $f_\tau^{(t,s)}(k_{1:n})$ requires $(n-1)$ multiplications, $f_\omega^{(t,s)}(\ell_{1:m})$ requires $(m-1)$ multiplications, and $f_Y^{(t,s)}(\mathcal{E}_t|k_{1:n},\ell_{1:m})$ requires $(mn-1)$ multiplications and mn function evaluations. Therefore, the number of basic operations in $f_\tau^{(t,s)}(k_{1:n})f_\omega^{(t,s)}(\ell_{1:m})f_Y^{(t,s)}(\mathcal{E}_t|k_{1:n},\ell_{1:m})$ is in an order of $O(mn)$. Note that (6) requires $(K^nL^m + K^{n-1}L^m - 2)$ additions, 1 division, and $(K^nL^m + K^{n-1}L^m)$ calls of $f_\tau^{(t,s)}(k_{1:n})f_\omega^{(t,s)}(\ell_{1:m})f_Y^{(t,s)}(\mathcal{E}_t|k_{1:n},\ell_{1:m})$. Therefore, the number of basic operations in (6) is in an order of $O(mnK^nL^m)$, and (7) follows the same manner as (6). □

EC.5. Algorithm EC.1 and Proof of Proposition 3

Algorithm EC.1: Equivalent transformation for $\widehat{z}_i^{(t,s)}[k]$ and $\widehat{v}_j^{(t,s)}[\ell]$

Log transformation: For each $k_{1:n}\in\mathcal{K},\ell_{1:m}\in\mathcal{L}$,

$$\log f^{(t,s)}(k_{1:n},\ell_{1:m}) \triangleq \sum_{i=1}^{n}\log\widehat{\tau}_{k_i}^{(t,s)} + \sum_{j=1}^{m}\log\widehat{\omega}_{\ell_j}^{(t,s)} + \sum_{i=1}^{n}\sum_{j=1}^{m}\log C_{i,j}^{(t,s)}[k_i,\ell_j].$$

Magnification:

$$g^{(t,s)}(k_{1:n},\ell_{1:m}) \triangleq \log f^{(t,s)}(k_{1:n},\ell_{1:m}) - \max_{k_{1:n}\in\mathcal{K},\ell_{1:m}\in\mathcal{L}}\log f^{(t,s)}(k_{1:n},\ell_{1:m}).$$

Equivalent transformation:

$$\widehat{z}_i^{(t,s)}[k] = \frac{\sum_{k_{1:n}\in\mathcal{K},k_i=k}\sum_{\ell_{1:m}\in\mathcal{L}}\exp(g^{(t,s)}(k_{1:n},\ell_{1:m}))}{\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L}}\exp(g^{(t,s)}(k_{1:n},\ell_{1:m}))},$$

$$\widehat{v}_j^{(t,s)}[\ell] = \frac{\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L},\ell_j=\ell}\exp(g^{(t,s)}(k_{1:n},\ell_{1:m}))}{\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L}}\exp(g^{(t,s)}(k_{1:n},\ell_{1:m}))}.$$

return $\widehat{z}_i^{(t,s)}[k]$ and $\widehat{v}_j^{(t,s)}[\ell]$.

Proof of Proposition 3 Given by Algorithm EC.1, the denominator of $\widehat{z}_i^{(t,s)}[k]$ and $\widehat{v}_j^{(t,s)}[\ell]$ is $\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L}}\exp(g^{(t,s)}(k_{1:n},\ell_{1:m}))$. Note that each $g^{(t,s)}(k_{1:n},\ell_{1:m})$ is not greater than zero, and there must exist a clustering situation $(k_{1:n},\ell_{1:m})$ such that $g^{(t,s)}(k_{1:n},\ell_{1:m})=0$. Therefore, the denominator $\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L}}\exp(g^{(t,s)}(k_{1:n},\ell_{1:m}))$ is not less than one and is bounded by $K^n\times L^m$. □

EC.6. Approximations of $\widehat{z}_i^{(t;(r,q)_E)}[k]$ and $\widehat{v}_j^{(t;(r,q)_E)}[\ell]$

In order to reduce the complexity of

$$\widehat{z}_i^{(t;(r,q)_E)}[k] = \frac{\sum_{k_{1:n}\in\mathcal{K},k_i=k}\sum_{\ell_{1:m}\in\mathcal{L}} f_\tau^{(t;(r,q)_E)}(k_{1:n})f_\omega^{(t;(r,q)_E)}(\ell_{1:m})f_Y^{(t;(r,q)_E)}(\mathcal{E}_t|k_{1:n},\ell_{1:m})}{\sum_{k_{1:n}\in\mathcal{K}}\sum_{\ell_{1:m}\in\mathcal{L}} f_\tau^{(t;(r,q)_E)}(k_{1:n})f_\omega^{(t;(r,q)_E)}(\ell_{1:m})f_Y^{(t;(r,q)_E)}(\mathcal{E}_t|k_{1:n},\ell_{1:m})},$$

we focus on the change in the numerator of $\widehat{z}_i^{(t;(r,q)_E)}[k]$ and make the following approximation by considering the denominators of $\widehat{z}_i^{(t;(r,q)_E)}[k]$ and $\widehat{z}_i^{(t)}[k]$ as a same constant:

$$\frac{\widehat{z}_i^{(t;(r,q)_E)}[k]}{\widehat{z}_i^{(t)}[k]} \approx \frac{\sum_{k_{1:n}\in\mathcal{K},k_i=k}\sum_{\ell_{1:m}\in\mathcal{L}} f_\tau^{(t;(r,q)_E)}(k_{1:n}) f_\omega^{(t;(r,q)_E)}(\ell_{1:m}) f_Y^{(t;(r,q)_E)}(\mathcal{E}_t|k_{1:n},\ell_{1:m})}{\sum_{k_{1:n}\in\mathcal{K},k_i=k}\sum_{\ell_{1:m}\in\mathcal{L}} f_\tau^{(t)}(k_{1:n}) f_\omega^{(t)}(\ell_{1:m}) f_Y^{(t)}(\mathcal{E}_t|k_{1:n},\ell_{1:m})}.$$

Note that $k_i^* = \arg\max_{k=1,\dots,K} \widehat{z}_i^{(t)}[k]$ and $\ell_j^* = \arg\max_{\ell=1,\dots,L} \widehat{v}_j^{(t)}[\ell]$ denote the indexes of the optimal posterior probabilities of clustering for each design and context. If there indeed exists obvious clustering phenomenon in designs and contexts, then we would tend to have $\phi\left(y_i(\boldsymbol{x}_j)|\widehat{\Lambda}_{k_i^*,\ell_j^*}^{(t,s)},(\widehat{\Xi}_{k_i^*,\ell_j^*}^2)^{(t,s)}\right) \gg \phi\left(y_i(\boldsymbol{x}_j)|\widehat{\Lambda}_{k,\ell}^{(t,s)},(\widehat{\Xi}_{k,\ell}^2)^{(t,s)}\right)$, $\forall (k,\ell)\neq(k_i^*,\ell_j^*)$. According to the results of Proposition EC.2, we have $C_{i,j}^{(t,s)}[k_i^*,\ell_j^*] \gg C_{i,j}^{(t,s)}[k,\ell]$ when t is relatively large. Therefore, by ignoring the events with non-optimal posterior probabilities of clustering, we have

$$\begin{aligned}
&\sum_{k_{1:n}\in\mathcal{K},k_i=k}\sum_{\ell_{1:m}\in\mathcal{L}} f_\tau^{(t)}(k_{1:n}) f_\omega^{(t)}(\ell_{1:m}) f_Y^{(t)}(\mathcal{E}_t|k_{1:n},\ell_{1:m}) \\
&\approx f_\tau^{(t)}([k^*_{1:(i-1)},k,k^*_{(i+1):n}]) f_\omega^{(t)}(\ell^*_{1:m}) f_Y^{(t)}(\mathcal{E}_t|[k^*_{1:(i-1)},k,k^*_{(i+1):n}],\ell^*_{1:m}) \\
&= \widehat{\tau}_k^{(t)}\left(\prod_{i'=1,i'\neq i}^n \widehat{\tau}_{k^*_{i'}}^{(t)}\right)\left(\prod_{j=1}^m \widehat{\omega}_{\ell_j^*}^{(t)}\right)\left(\prod_{j=1}^m C_{i,j}^{(t)}[k,\ell_j^*]\right)\left(\prod_{i'=1,i'\neq i}^n\prod_{j=1}^m C_{i',j}^{(t)}[k^*_{i'},\ell_j^*]\right),
\end{aligned}$$

and then

$$\frac{\widehat{z}_i^{(t;(r,q)_E)}[k]}{\widehat{z}_i^{(t)}[k]} \approx \frac{\left(\prod_{j=1}^m C_{i,j}^{(t;(r,q)_E)}[k,\ell_j^*]\right)\left(\prod_{i'=1,i'\neq i}^n\prod_{j=1}^m C_{i',j}^{(t;(r,q)_E)}[k^*_{i'},\ell_j^*]\right)}{\left(\prod_{j=1}^m C_{i,j}^{(t)}[k,\ell_j^*]\right)\left(\prod_{i'=1,i'\neq i}^n\prod_{j=1}^m C_{i',j}^{(t)}[k^*_{i'},\ell_j^*]\right)}.$$

EC.7. Proof of Propositions 4, 5, and 6

Proof of Proposition 4 Note that for $(i,j)\neq(r,q)$,

$$\begin{aligned}
\frac{C_{i,j}^{(t;(r,q)_E)}[k,\ell]}{C_{i,j}^{(t)}[k,\ell]} = &\sqrt{\frac{(\sigma_{i,j}^2)^{(t;(r,q)_E)}[k,\ell]}{(\widehat{\Xi}_{k,\ell}^2)^{(t;(r,q)_E)}}\frac{(\widehat{\Xi}_{k,\ell}^2)^{(t)}}{(\sigma_{i,j}^2)^{(t)}[k,\ell]}}\exp\left\{\frac{1}{2}\left[\left(\frac{(\mu_{i,j}^{(t)}[k,\ell])^2}{(\sigma_{i,j}^2)^{(t;(r,q)_E)}[k,\ell]} - \frac{(\mu_{i,j}^{(t)}[k,\ell])^2}{(\sigma_{i,j}^2)^{(t)}[k,\ell]}\right)\right.\right. \\
&\left.\left. - \left(\frac{(\widehat{\Lambda}_{k,\ell}^{(t)})^2}{(\widehat{\Xi}_{k,\ell}^2)^{(t;(r,q)_E)}} - \frac{(\widehat{\Lambda}_{k,\ell}^{(t)})^2}{(\widehat{\Xi}_{k,\ell}^2)^{(t)}}\right)\right]\right\}.
\end{aligned}$$

In addition,

$$\lim_{t\to+\infty}\frac{1}{(\sigma_{i,j}^2)^{(t;(r,q)_E)}[k,\ell]} - \frac{1}{(\sigma_{i,j}^2)^{(t)}[k,\ell]} = \lim_{t\to+\infty}\frac{1}{(\widehat{\Xi}_{k,\ell}^2)^{(t;(r,q)_E)}} - \frac{1}{(\widehat{\Xi}_{k,\ell}^2)^{(t)}} = 0 \ a.s.$$

where the first equation is due to $(i,j)\neq(r,q)$ and the second equation is due to that both $(\widehat{\Xi}_{k,\ell}^2)^{(t;(r,q)_E)}$ and $(\widehat{\Xi}_{k,\ell}^2)^{(t)}$ converge to a same positive value. Therefore, $\lim_{t\to+\infty}\frac{C_{i,j}^{(t;(r,q)_E)}[k,\ell]}{C_{i,j}^{(t)}[k,\ell]} = 1 \ a.s.$

□

Proof of Proposition 5 Note that

$$\frac{C_{r,q}^{(t;(r,q)_E)}[k,\ell_q^*]}{C_{r,q}^{(t)}[k,\ell_q^*]} = \sqrt{\frac{1}{2\pi\sigma_r^2(\boldsymbol{x}_q)}}\sqrt{\frac{(\sigma_{r,q}^2)^{(t;(r,q)_E)}[k,\ell_q^*]}{(\widehat{\Xi}_{k,\ell_q^*}^2)^{(t;(r,q)_E)}}\frac{(\widehat{\Xi}_{k,\ell_q^*}^2)^{(t)}}{(\sigma_{r,q}^2)^{(t)}[k,\ell_q^*]}}\exp\left\{\frac{1}{2}\left[-\frac{\left[\frac{\sum_{h=1}^{t_{r,q}} Y_{r,h}(\boldsymbol{x}_q)}{\sigma_r^2(\boldsymbol{x}_q)}+\frac{\widehat{\Lambda}_{k,\ell_q^*}^{(t)}}{(\widehat{\Xi}_{k,\ell_q^*}^2)^{(t)}}\right]^2}{\frac{t_{r,q}}{\sigma_r^2(\boldsymbol{x}_q)}+\frac{1}{\left(\widehat{\Xi}_{k,\ell_q^*}^2\right)^{(t)}}} + \frac{\left[\frac{\sum_{h=1}^{t_{r,q}} Y_{r,h}(\boldsymbol{x}_q)+\mu_{r,q}^{(t)}[k,\ell_q^*]}{\sigma_r^2(\boldsymbol{x}_q)}+\frac{\widehat{\Lambda}_{k,\ell_q^*}^{(t)}}{\left(\widehat{\Xi}_{k,\ell_q^*}^2\right)^{(t)}}\right]^2}{\frac{t_{r,q}+1}{\sigma_r^2(\boldsymbol{x}_q)}+\frac{1}{\left(\widehat{\Xi}_{k,\ell_q^*}^2\right)^{(t)}}} - \frac{\left(\mu_{r,q}^{(t)}[k,\ell_q^*]\right)^2}{\sigma_r^2(\boldsymbol{x}_q)}\right]\right\}.$$

In addition, $\lim_{t\to+\infty}\frac{(\sigma_{r,q}^2)^{(t;(r,q)_E)}[k,\ell_q^*]}{(\widehat{\Xi}_{k,\ell_q^*}^2)^{(t;(r,q)_E)}}\frac{(\widehat{\Xi}_{k,\ell_q^*}^2)^{(t)}}{(\sigma_{r,q}^2)^{(t)}[k,\ell_q^*]}=1$ *a.s.* and $\lim_{t\to+\infty}\frac{1}{t_{r,q}}\sum_{h=1}^{t_{r,q}} Y_{r,h}(\boldsymbol{x}_q)-\mu_{r,q}^{(t)}[k,\ell_q^*]=0$ *a.s.*, which means that the effect of prior information on the posterior estimate vanishes as the number of samples goes to infinity. Therefore, the conclusion of the proposition can be obtained. □

Proof of Proposition 6 In our proposed approximation method, (13) requires $(K-1)$ additions, K multiplications, 1 division, and K function evaluations. Note that the number of possible design-context pairs is mn. Therefore, the number of basic operations in (13) for traversing all possible design-context pairs (r,q) is in an order of $O(mnK)$. Similarly, the number of basic operations in (14) for traversing all possible design-context pairs (r,q) is in an order of $O(mnL)$. □

EC.8. Exponential decay of approximation error

PROPOSITION EC.3. *The error between the integral of multivariate standard normal density over a region Ω and that over the maximal tangent inner ball in Ω decreases to zero at least in an order of $O(t^{(n-1)/2}e^{-t/2})$ as $t\to+\infty$.*

Proof of Proposition EC.3 We have

$$\int\cdots\int_{\Omega}\frac{1}{\sqrt{(2\pi)^n}}\exp(-\frac{1}{2}\sum_{i=1}^n z_i^2)dz_1\dots dz_n - \int\cdots\int_{\sum_{i=1}^n z_i^2\le R^2}\frac{1}{\sqrt{(2\pi)^n}}\exp(-\frac{1}{2}\sum_{i=1}^n z_i^2)dz_1\dots dz_n$$
$$\le 1-\int\cdots\int_{\sum_{i=1}^n z_i^2\le R^2}\frac{1}{\sqrt{(2\pi)^n}}\exp(-\frac{1}{2}\sum_{i=1}^n z_i^2)dz_1\dots dz_n$$
$$=\int_R^{+\infty}\int_0^{\pi}\cdots\int_0^{\pi}\int_0^{2\pi}\frac{1}{\sqrt{(2\pi)^n}}\exp(-\frac{1}{2}r^2)r^{n-1}(\sin\varphi_1)^{n-2}(\sin\varphi_2)^{n-3}\cdots(\sin\varphi_{n-3})^2\sin\varphi_{n-2}\,drd\varphi_1\dots d\varphi_{n-1}$$
$$=C(n)\int_R^{+\infty}\exp(-\frac{1}{2}r^2)r^{n-1}\,dr$$

where R is the radius of the inner ball, and

$$C(n) = \frac{1}{\sqrt{(2\pi)^n}} \int_0^{\pi} \cdots \int_0^{\pi} \int_0^{2\pi} (\sin\varphi_1)^{n-2} (\sin\varphi_2)^{n-3} \cdots (\sin\varphi_{n-3})^2 \sin\varphi_{n-2} \; d\varphi_1 \dots d\varphi_{n-1}$$

is a constant depending only on n.

Given by integration by parts,

$$\int_R^{+\infty} \exp(-\frac{1}{2}r^2) r^{n-1} \; dr = \frac{1}{n}\left(\left[\exp(-\frac{1}{2}r^2) r^n \right]_R^{+\infty} - \int_R^{+\infty} \exp(-\frac{1}{2}r^2)(-r) r^{n-1} \; dr \right).$$

In addition, we have

$$\int_R^{+\infty} \exp(-\frac{1}{2}r^2) r^n \; dr \geq R \int_R^{+\infty} \exp(-\frac{1}{2}r^2) r^{n-1} \; dr.$$

Therefore,

$$\exp(-\frac{1}{2}R^2) R^n + n \int_R^{+\infty} \exp(-\frac{1}{2}r^2) r^{n-1} \; dr \geq R \int_R^{+\infty} \exp(-\frac{1}{2}r^2) r^{n-1} \; dr$$

which concludes

$$\int_R^{+\infty} \exp(-\frac{1}{2}r^2) r^{n-1} \; dr \leq \frac{1}{R-n} \exp(-\frac{1}{2}R^2) R^n.$$

Note that

$$R^2 = \min_{i \neq 1} \frac{\left(\mu^{(t)}_{\langle 1 \rangle_j^{(t)}, j} \left[k_{\langle 1 \rangle_j^{(t)}}, \ell_j \right] - \mu^{(t)}_{\langle i \rangle_j^{(t)}, j} \left[k_{\langle i \rangle_j^{(t)}}, \ell_j \right] \right)^2}{\left(\sigma^2_{\langle 1 \rangle_j^{(t)}, j} \right)^{(t)} \left[k_{\langle 1 \rangle_j^{(t)}}, \ell_j \right] + \left(\sigma^2_{\langle i \rangle_j^{(t)}, j} \right)^{(t)} \left[k_{\langle i \rangle_j^{(t)}}, \ell_j \right]} = O(t),$$

which concludes the proposition. □

EC.9. Proof of Theorem 1

Proof of Theorem 1 We only need to prove that each $y_i(\boldsymbol{x}_j)$ will be sampled infinitely often a.s. following DSCO policy, and the consistency will follow by the law of large numbers. Suppose $y_i(\boldsymbol{x}_j)$ is only sampled finitely often and $y_r(\boldsymbol{x}_q)$ is sampled infinitely often. Therefore, there exists a finite number N_0 such that $y_i(\boldsymbol{x}_j)$ will stop receiving replications after the sampling number t exceeds N_0. Thus we have

$$\lim_{t \to +\infty} (\sigma^2_{i,j})^{(t)}[k,\ell] > 0, \; \lim_{t \to +\infty} (\sigma^2_{r,q})^{(t)}[k,\ell] = 0, \; \forall k = 1, \dots, K, \; \ell = 1, \dots, L.$$

By noticing that

$$\lim_{t \to +\infty} \left[(\sigma^2_{r,q})^{(t)}[k,\ell] - (\sigma^2_{r,q})^{(t;(r,q)_E)}[k,\ell] \right] = 0,$$

$$\lim_{t \to +\infty} \left[(\Xi^2_{k,\ell})^{(t)} - (\Xi^2_{k,\ell})^{(t;(r,q)_E)} \right] = 0,$$

and

$$\lim_{t\to+\infty}\left[\widehat{z}_r^{(t)}[k]-\widehat{z}_r^{(t;(r,q)_E)}[k]\right]=0,$$

$$\lim_{t\to+\infty}\left[\widehat{v}_q^{(t)}[\ell]-\widehat{v}_{q,\ell}^{(t;(r,q)_E)}[\ell]\right]=0,$$

we have

$$\lim_{t\to+\infty}\left[V(\mathcal{E}_t;(r,q))-V(\mathcal{E}_t)\right]=0 \quad a.s.$$

If there exists a design-context pair (i,j) whose performance $y_i(\boldsymbol{x}_j)$ is only sampled finitely often such that

$$\lim_{t\to+\infty}\left[V(\mathcal{E}_t;(i,j))-V(\mathcal{E}_t)\right]>0 \quad a.s.,$$

then it contradicts with the sampling rule in equation (19) that the design-context pair with the largest $V(\mathcal{E}_t;(i,j))$ is sampled.

Therefore,

$$\lim_{t\to+\infty}\left[V(\mathcal{E}_t;(i,j))-V(\mathcal{E}_t)\right]\le 0$$

holds for all design-context pairs, and thus sample allocation is determined by the sampling rule in equation (22). By noticing that

$$\lim_{t\to+\infty}\left[(\sigma_{i,j}^2)^{(t)}[k,\ell]-(\sigma_{i,j}^2)^{(t;(i,j)_E)}[k,\ell]\right]>0,$$

and

$$\lim_{t\to+\infty}\left[(\Xi_{k_i^*,\ell_j^*}^2)^{(t)}-(\Xi_{k_i^*,\ell_j^*}^2)^{(t;(i,j)_E)}\right]>0,$$

there must exist a design-context pair (i,j) which is only sampled finitely often such that

$$\lim_{t\to+\infty}\left[W(\mathcal{E}_t;(i,j))-W(\mathcal{E}_t)\right]>0 \quad a.s.,$$

which contradicts with the sampling rule in equation (22) that the design-context pair with the largest $W(\mathcal{E}_t;(i,j))$ is sampled. Therefore, the proposed DSCO policy must be consistent.

By the law of large numbers, $\lim_{t\to+\infty}\mu_{i,j}^{(t)}[k,\ell]=y_i(\boldsymbol{x}_j)$. For simplicity of analysis, we can replace $\mu_{i,j}^{(t)}[k,\ell]$ and $(\sigma_{i,j}^2)^{(t)}[k,\ell]$ with $y_i(\boldsymbol{x}_j)$ and $\sigma_i^2(\boldsymbol{x}_j)/t_{i,j}$ in $V(\mathcal{E}_t;(r,q))$. Then when $t\to+\infty$, both $V(\mathcal{E}_t;(r,q))$ and $W(\mathcal{E}_t;(r,q))$ are reduced to

$$\min_{j=1,\dots,m}\min_{i\neq 1}\frac{\left(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\right)^2}{\dfrac{\sigma_{\langle 1\rangle_j}^2(\boldsymbol{x}_j)}{t_{\langle 1\rangle_j,j}+\mathbb{1}\{(\langle 1\rangle_j,j)=(r,q)\}}+\dfrac{\sigma_{\langle i\rangle_j}^2(\boldsymbol{x}_j)}{t_{\langle i\rangle_j,j}+\mathbb{1}\{(\langle i\rangle_j,j)=(r,q)\}}}.$$

Let $r_{i,j}^{(t)}\triangleq t_{i,j}/t,\ i=1,\dots,n,\ j=1,\dots,m$. By the Bolzano-Weierstrass theorem (Rudin et al. 1964), there exists a subsequence of $\{r_{i,j}^{(t)}\}$ converging to $\{r_{i,j}\}$ such that $\sum_{i=1}^n\sum_{j=1}^m r_{i,j}=1,\ r_{i,j}\ge 0$. Without loss of generality, we can assume $\{r_{i,j}^{(t)}\}$ converges to $\{r_{i,j}\}$; otherwise, the following argument is made over a subsequence. We claim $r_{i,j}>0,\ i=1,\ldots,n,\ j=1,\ldots,m$; otherwise, there exist $r_{\langle i\rangle_j,j}=0$ and $r_{\langle i'\rangle_{j'},j'}>0$. Notice that

$$\begin{aligned}
&\lim_{t\to+\infty}\left[\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/t_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/(t_{\langle i\rangle_j,j}+1)}-\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/t_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/t_{\langle i\rangle_j,j}}\right]\\
&=\lim_{t\to+\infty}t\left[\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/(r^{(t)}_{\langle i\rangle_j,j}+1/t)}-\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle i\rangle_j,j}}\right]\\
&=\lim_{t\to+\infty}\left(\frac{\sigma_{\langle i\rangle_j}(\boldsymbol{x}_j)}{r^{(t)}_{\langle i\rangle_j,j}}\right)^2\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\Big(\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle i\rangle_j,j}\Big)^2}
\end{aligned}$$

and

$$\begin{aligned}
&\lim_{t\to+\infty}\left[\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/(t_{\langle 1\rangle_j,j}+1)+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/t_{\langle i\rangle_j,j}}-\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/t_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/t_{\langle i\rangle_j,j}}\right]\\
&=\lim_{t\to+\infty}t\left[\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/(r^{(t)}_{\langle 1\rangle_j,j}+1/t)+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle i\rangle_j,j}}-\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle i\rangle_j,j}}\right]\\
&=\lim_{t\to+\infty}\left(\frac{\sigma_{\langle 1\rangle_j}(\boldsymbol{x}_j)}{r^{(t)}_{\langle 1\rangle_j,j}}\right)^2\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\Big(\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle i\rangle_j,j}\Big)^2}.
\end{aligned}$$

If $r_{\langle 1\rangle_j,j}=0$ and $r_{\langle i\rangle_j,j}>0$, then

$$\lim_{t\to+\infty}\left(\frac{\sigma_{\langle 1\rangle_j}(\boldsymbol{x}_j)}{r^{(t)}_{\langle 1\rangle_j,j}}\right)^2\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\Big(\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle i\rangle_j,j}\Big)^2}>0$$

and

$$\lim_{t\to+\infty}\left(\frac{\sigma_{\langle i\rangle_j}(\boldsymbol{x}_j)}{r^{(t)}_{\langle i\rangle_j,j}}\right)^2\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\Big(\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle i\rangle_j,j}\Big)^2}=0$$

which contradicts with the sampling rules in equations (19) and (22). If $r_{\langle 1\rangle_j,j}>0$ and $r_{\langle i\rangle_j,j}=0$, then

$$\lim_{t\to+\infty}\left(\frac{\sigma_{\langle 1\rangle_j}(\boldsymbol{x}_j)}{r^{(t)}_{\langle 1\rangle_j,j}}\right)^2\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\Big(\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle i\rangle_j,j}\Big)^2}=0$$

and

$$\lim_{t\to+\infty}\left(\frac{\sigma_{\langle i\rangle_j}(\boldsymbol{x}_j)}{r^{(t)}_{\langle i\rangle_j,j}}\right)^2\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\Big(\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/r^{(t)}_{\langle i\rangle_j,j}\Big)^2}>0$$

which contradicts with the sampling rules in equations (19) and (22). If $r_{\langle i\rangle_j,j}=0,\ i=1,\ldots,n$ and $r_{\langle i\rangle_{j'},j'}>0$, $i=1,\ldots,n$, then by replacing $\mu^{(t)}_{i,j}[k,\ell]$ and $(\sigma^2_{i,j})^{(t)}[k,\ell]$ with $y_i(\boldsymbol{x}_j)$ and $\sigma^2_i(\boldsymbol{x}_j)/t_{i,j}$ when $t\to+\infty$, we have

$$\lim_{t\to+\infty}\sum_{k_{1:n}\in\mathcal{K},\ell_j\in\mathcal{L}}p_z(k_{1:n},\mathcal{E}_t)p_v(\ell_j,\mathcal{E}_t)\mathrm{APCS}(k_{1:n},\ell_j,\mathcal{E}_t)-\min_{i\neq 1}\frac{\big(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\big)^2}{\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/t_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/t_{\langle i\rangle_j,j}}=0,$$

$$\min_{i\neq 1}\frac{\left(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\right)^2}{\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/t_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/t_{\langle i\rangle_j,j}}=o(t),$$

and

$$\lim_{t\to+\infty}\sum_{k_{1:n}\in\mathcal{K},\ell_{j'}\in\mathcal{L}}p_z(k_{1:n},\mathcal{E}_t)p_v(\ell_{j'},\mathcal{E}_t)\mathrm{APCS}(k_{1:n},\ell_{j'},\mathcal{E}_t)-\min_{i\neq 1}\frac{\left(y_{\langle 1\rangle_{j'}}(\boldsymbol{x}_{j'})-y_{\langle i\rangle_{j'}}(\boldsymbol{x}_{j'})\right)^2}{\sigma^2_{\langle 1\rangle_{j'}}(\boldsymbol{x}_{j'})/t_{\langle 1\rangle_{j'},j'}+\sigma^2_{\langle i\rangle_{j'}}(\boldsymbol{x}_{j'})/t_{\langle i\rangle_{j'},j'}}=0,$$

$$\min_{i\neq 1}\frac{\left(y_{\langle 1\rangle_{j'}}(\boldsymbol{x}_{j'})-y_{\langle i\rangle_{j'}}(\boldsymbol{x}_{j'})\right)^2}{\sigma^2_{\langle 1\rangle_{j'}}(\boldsymbol{x}_{j'})/t_{\langle 1\rangle_{j'},j'}+\sigma^2_{\langle i\rangle_{j'}}(\boldsymbol{x}_{j'})/t_{\langle i\rangle_{j'},j'}}=O(t),$$

which contradict with the definition of $\mathrm{PCS_W}$. Therefore, $r_{i,j}>0,\ i=1,\ldots,n,\ j=1,\ldots,m$.

Let $G_{i,j}(r_{\langle 1\rangle_j,j},r_{\langle i\rangle_j,j})\triangleq\dfrac{\left(y_{\langle 1\rangle_j}(\boldsymbol{x}_j)-y_{\langle i\rangle_j}(\boldsymbol{x}_j)\right)^2}{\sigma^2_{\langle 1\rangle_j}(\boldsymbol{x}_j)/r_{\langle 1\rangle_j,j}+\sigma^2_{\langle i\rangle_j}(\boldsymbol{x}_j)/r_{\langle i\rangle_j,j}},\ i=2,\ldots,n,\ j=1,\ldots,m$. If $\{r_{i,j}\}$ does not satisfy equation (25), there exist $i\neq i',\ i,i'=2,\ldots,n$ such that

$$G_{i,j}(r_{\langle 1\rangle_j,j},r_{\langle i\rangle_j,j})>G_{i',j}(r_{\langle 1\rangle_j,j},r_{\langle i'\rangle_j,j}).$$

If the inequality above holds, there exists $T_0>0$ such that $\forall t>T_0$,

$$G_{i,j}(r^{(t)}_{\langle 1\rangle_j,j},r^{(t)}_{\langle i\rangle_j,j})>G_{i',j}(r^{(t)}_{\langle 1\rangle_j,j},r^{(t)}_{\langle i'\rangle_j,j}),$$

due to continuity of $G_{i,j}$ on $(0,1)\times(0,1)$. By the sampling rules in equations (19) and (22), $y_{\langle i'\rangle_j}(\boldsymbol{x}_j)$ will be sampled and $y_{\langle i\rangle_j}(\boldsymbol{x}_j)$ will stop receiving replications before the inequality above reverses. This contradicts $\{r^{(t)}_{i,j}\}$ converging to $\{r_{i,j}\}$, so equation (25) must hold. If $\{r_{i,j}\}$ does not satisfy equation (26), there exist $i,i'=2,\ldots,n$ and $j\neq j',\ j,j'=1,\ldots,m$ such that

$$G_{i,j}(r_{\langle 1\rangle_j,j},r_{\langle i\rangle_j,j})>G_{i',j'}(r_{\langle 1\rangle_{j'},j'},r_{\langle i'\rangle_{j'},j'}).$$

If the inequality above holds, there exists $T_0>0$ such that $\forall t>T_0$,

$$G_{i,j}(r^{(t)}_{\langle 1\rangle_j,j},r^{(t)}_{\langle i\rangle_j,j})>G_{i',j'}(r^{(t)}_{\langle 1\rangle_{j'},j'},r^{(t)}_{\langle i'\rangle_{j'},j'}),$$

due to continuity of $G_{i,j}$ on $(0,1)\times(0,1)$. By the definition of $\mathrm{PCS_W}$, context j' will be sampled and context j will stop receiving replications before the inequality above reverses. This contradicts $\{r^{(t)}_{i,j}\}$ converging to $\{r_{i,j}\}$, so equation (26) must hold.

By the implicit function theorem (Rudin et al. 1964), equations (25), (26), and $\sum_{i=1}^n\sum_{j=1}^m r_{i,j}=1$ determine implicit functions $r_{\langle i\rangle_j,j}(x)\Big|_{x=(r_{\langle 1\rangle_1,1},\ldots,r_{\langle 1\rangle_m,m})},\ i=2,\ldots,n,\ j=1,\ldots,m$, because

$$\det(\Sigma)=\prod_{i=2}^n\prod_{j=1}^m\zeta_{i,j}\left(\sum_{i=2}^n\sum_{j=1}^m\zeta_{i,j}^{-1}\right)>0,$$

where

$$\zeta_{i,j} \triangleq \frac{\partial G_{i,j}(r_{\langle 1\rangle_j,j}, x)}{\partial x}\bigg|_{x=r_{\langle i\rangle_j,j}}, \ i=2,\dots,n, \ j=1,\dots,m,$$

$$\Sigma \triangleq \begin{pmatrix} \zeta_{2,1} & -\zeta_{3,1} & \cdots & 0 & 0 & \cdots & 0 & 0 \\ 0 & \zeta_{3,1} & \cdots & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & \zeta_{n,1} & -\zeta_{2,2} & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & \zeta_{2,2} & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots & \zeta_{n-1,m} & -\zeta_{n,m} \\ 1 & 1 & \cdots & 1 & 1 & \cdots & 1 & 1 \end{pmatrix},$$

and $\Sigma R = -\Upsilon$, where

$$R \triangleq \begin{pmatrix} \frac{\partial r_{\langle 2\rangle_1,1}(x)}{\partial x_1} & \cdots & \frac{\partial r_{\langle 2\rangle_1,1}(x)}{\partial x_m} \\ \frac{r_{\langle 3\rangle_1,1}(x)}{\partial x_1} & \cdots & \frac{\partial r_{\langle 3\rangle_1,1}(x)}{\partial x_m} \\ \vdots & \cdots & \vdots \\ \frac{r_{\langle n\rangle_1,1}(x)}{\partial x_1} & \cdots & \frac{\partial r_{\langle n\rangle_1,1}(x)}{\partial x_m} \\ \frac{r_{\langle 2\rangle_2,2}(x)}{\partial x_1} & \cdots & \frac{\partial r_{\langle 2\rangle_2,2}(x)}{\partial x_m} \\ \vdots & \cdots & \vdots \\ \frac{r_{\langle n\rangle_m,m}(x)}{\partial x_1} & \cdots & \frac{\partial r_{\langle n\rangle_m,m}(x)}{\partial x_m} \end{pmatrix}_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})},$$

$$\Upsilon \triangleq \begin{pmatrix} \frac{\partial G_{2,1}(x_1,r_{\langle 2\rangle_1,1})-G_{3,1}(x_1,r_{\langle 3\rangle_1,1})}{\partial x_1} & \cdots & 0 \\ \frac{\partial G_{3,1}(x_1,r_{\langle 3\rangle_1,1})-G_{4,1}(x_1,r_{\langle 4\rangle_1,1})}{\partial x_1} & \cdots & 0 \\ \vdots & \cdots & \vdots \\ \frac{\partial G_{n,1}(x_1,r_{\langle n\rangle_1,1})}{\partial x_1} & \cdots & 0 \\ 0 & \cdots & 0 \\ \vdots & \cdots & \vdots \\ 0 & \cdots & \frac{\partial G_{n-1,m}(x_m,r_{\langle n-1\rangle_m,m})-G_{n,m}(x_m,r_{\langle n\rangle_m,m})}{\partial x_m} \\ 1 & \cdots & 1 \end{pmatrix}_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})}.$$

In addition,

$$\frac{\partial G_{i,j}(x_j, r_{\langle i\rangle_j,j})}{\partial x_j}\bigg|_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})} + \zeta_{i,j}\frac{\partial r_{\langle i\rangle_j,j}(x)}{\partial x_j}\bigg|_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})} = 0, \ i=2,\dots,n, \ j=1,\dots,m;$$

otherwise, there exist $i' \neq 1$ and j' such that the equality above does not hold, say

$$\frac{\partial G_{i',j'}(x_{j'}, r_{\langle i'\rangle_{j'},j'})}{\partial x_{j'}}\bigg|_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})} + \zeta_{i',j'}\frac{\partial r_{\langle i'\rangle_{j'},j'}(x)}{\partial x_{j'}}\bigg|_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})} > 0.$$

Following the sampling rules in equations (19) and (22), $y_{\langle 1\rangle_{j'}}(\boldsymbol{x}_{j'})$ will be sampled and $y_{\langle i'\rangle_{j'}}(\boldsymbol{x}_{j'})$ will stop receiving replications before the inequality above reverses, which contradicts $\{r_{i,j}^{(t)}\}$ converging to $\{r_{i,j}\}$. Similarly,

$$\left.\frac{\partial G_{i,j}(x_j, r_{\langle i\rangle_j,j})}{\partial x_{j'}}\right|_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})} + \zeta_{i,j}\left.\frac{\partial r_{\langle i\rangle_j,j}(x)}{\partial x_{j'}}\right|_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})} = 0,\ i=2,\dots,n,\ j\neq j';$$

otherwise, there exist $i\neq 1$ and j' such that the equality above does not hold, say

$$\begin{aligned}&\left.\frac{\partial G_{i,j}(x_j, r_{\langle i\rangle_j,j})}{\partial x_{j'}}\right|_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})} + \zeta_{i,j}\left.\frac{\partial r_{\langle i\rangle_j,j}(x)}{\partial x_{j'}}\right|_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})}\\ > &\left.\frac{\partial G_{i,j}(x_j, r_{\langle i\rangle_j,j})}{\partial x_{j}}\right|_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})} + \zeta_{i,j}\left.\frac{\partial r_{\langle i\rangle_j,j}(x)}{\partial x_{j}}\right|_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})} = 0\end{aligned}$$

without loss of generality. Following the sampling rules in equations (19) and (22), context j' will be sampled and context j will stop receiving replications before the inequality above reverses, which contradicts $\{r_{i,j}^{(t)}\}$ converging to $\{r_{i,j}\}$. Further, note that

$$\left.\frac{\partial G_{i,j}(x_j, r_{\langle i\rangle_j,j})}{\partial x_{j'}}\right|_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})} = 0,\ i=2,\dots,n,\ j\neq j',$$

which is due to x_j and $x_{j'}$ are independent, then we have

$$\zeta_{i,j}\left.\frac{\partial r_{\langle i\rangle_j,j}(x)}{\partial x_{j'}}\right|_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})} = 0,\ i=2,\dots,n,\ j\neq j'.$$

Then, $HR=-G$, where

$$G \triangleq \left.\begin{pmatrix} \frac{\partial G_{2,1}(x_1,r_{\langle 2\rangle_1,1})}{\partial x_1} & \cdots & 0\\ \frac{\partial G_{3,1}(x_1,r_{\langle 3\rangle_1,1})}{\partial x_1} & \cdots & 0\\ \vdots & \cdots & \vdots\\ \frac{\partial G_{n,1}(x_1,r_{\langle n\rangle_1,1})}{\partial x_1} & \cdots & 0\\ 0 & \cdots & 0\\ 0 & \cdots & \frac{\partial G_{n,m}(x_m,r_{\langle n\rangle_m,m})}{\partial x_m}\end{pmatrix}\right|_{x=(r_{\langle 1\rangle_1,1},\dots,r_{\langle 1\rangle_m,m})}$$

and

$$H \triangleq \begin{pmatrix}\zeta_{2,1} & 0 & \cdots & 0\\ 0 & \zeta_{3,1} & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & \zeta_{n,m}\end{pmatrix}.$$

Summarizing the above, we have

$$\Upsilon = \Sigma H^{-1} G$$

which leads to

$$\sum_{i=2}^{n} \frac{\partial G_{i,j}(x_j, r_{\langle i \rangle_j, j})/\partial x_j\Big|_{x=(r_{\langle 1 \rangle_1,1},\ldots,r_{\langle 1 \rangle_m,m})}}{G_{i,j}(r_{\langle 1 \rangle_j,j}, x)/\partial x\Big|_{x=r_{\langle i \rangle_j,j}}} = 1,\ j = 1,\ldots,m \Leftrightarrow \text{Equation (24)}.$$

Therefore, $\{r_{i,j}^{(t)}\}$ converges to $\{r_{i,j}^{*}\}$. □

EC.10. Performance clustering phenomenon

Table EC.1 Results for design clustering.

	# of designs	Type of drugs	Mean of dosage	Standard deviation of dosage
Design Cluster 1	11	Aspirin	77.7275	16.5825
Design Cluster 2	9	Aspirin	127.7775	13.6925
Design Cluster 3	7	Statin	8.0858	1.3152
Design Cluster 4	13	Statin	14.1384	2.3432

Table EC.2 Results for context clustering.

	# of contexts	Parameter	Mean of parameter	Standard deviation of parameter
Context Cluster 1	12	x_1	48.8417	3.1575
		x_2	122.0083	7.2111
Context Cluster 2	9	x_1	51.2333	3.1535
		x_2	138.5667	11.3039
Context Cluster 3	10	x_1	61.5100	3.0277
		x_2	122.0100	6.0553
Context Cluster 4	13	x_1	64.6231	4.7000
		x_2	132.7000	13.7803
Context Cluster 5	9	x_1	73.6778	3.1623
		x_2	127.0111	5.4772
Context Cluster 6	7	x_1	75.0143	2.1602
		x_2	143.0143	4.3205