Online Appendix to "Technical Note—Knowledge Gradient for Selection with Covariates: Consistency and Computation" by Ding, Hong, Shen and Zhang

A. Proof of Lemma 1

Before proving Lemma 1, we first establish the following Lemma 2.

Lemma 2. *Let $g(s,t) := t\phi(s/t) - s\Phi(-s/t)$, where Φ is the standard normal distribution function and ϕ is its density function. Then,*

(i) $g(s,t) > 0$ *for all* $s \geq 0$ *and* $t > 0$;

(ii) $g(s,t)$ *is strictly decreasing in* $s \in [0,\infty)$ *and strictly increasing in* $t \in (0,\infty)$;

(iii) $g(s,t) \to 0$ *as* $s \to \infty$ *or as* $t \to 0$.

Proof of Lemma 2. Let $h(u) := \phi(u) - u\Phi(-u)$ for $u \geq 0$, then $g(s,t) = th(s/t)$. Note that

$$h'(u) = \phi'(u) + u\phi(-u) - \Phi(-u) = -u\phi(u) + u\phi(u) - \Phi(-u) = -\Phi(-u) < 0,$$

Hence, $h(u)$ is strictly decreasing in $u \in [0,\infty)$. Note that $\lim_{u\to\infty} \phi(u) = 0$ and

$$\lim_{u\to\infty} u\Phi(-u) = \lim_{u\to\infty} \frac{\Phi(-u)}{u^{-1}} = \lim_{u\to\infty} \frac{\phi(u)}{u^{-2}} = \lim_{u\to\infty} \frac{u^2}{\sqrt{2\pi} e^{u^2/2}} = 0,$$

hence $\lim_{u\to\infty} h(u) = 0$. Then we must have $h(u) > 0$ for all $u \in [0,\infty)$, from which part (i) follows immediately.

For part (ii), the strict decreasing monotonicity of $g(s,t)$ in $s \in [0,\infty)$ and the strict increasing monotonicity of $g(s,t)$ in $t \in (0,\infty)$ follow immediately from the strict decreasing monotonicity of $h(u)$ in u and $g(s,t) = th(s/t)$.

Part (iii) is due to that $\lim_{u\to\infty} h(u) = 0$ and $g(s,t) = th(s/t)$. □

Now we are ready to prove Lemma 1

Proof of Lemma 1. By eqs. (5) and (7),

$$\begin{aligned} f(i,\boldsymbol{x},\boldsymbol{v}) &:= \mathbb{E}\left[\max_{1\leq a\leq M} \mu_a^{n+1}(\boldsymbol{v}) \,\middle|\, \mathcal{F}^n, a^n = i, \boldsymbol{v}^n = \boldsymbol{x}\right] \\ &= \mathbb{E}\left[\max_{1\leq a\leq M} \left(\mu_a^n(\boldsymbol{v}) + \sigma_a^n(\boldsymbol{v},\boldsymbol{x})Z^{n+1}\right)\right] \\ &= \mathbb{E}\left[\max\left\{\mu_i^n(\boldsymbol{v}) + \tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})Z^{n+1},\ \max_{a\neq i} \mu_a^n(\boldsymbol{v})\right\}\right] \\ &= \mathbb{E}\left[\max\left\{\mu_i^n(\boldsymbol{v}) + |\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})|Z^{n+1},\ \max_{a\neq i} \mu_a^n(\boldsymbol{v})\right\}\right]. \end{aligned} \tag{20}$$

For notational simplicity, let $\alpha := \mu_i^n(\boldsymbol{v})$, $\beta := \tilde{\sigma}_i^n(\boldsymbol{v}, \boldsymbol{x})$, $\gamma := \max_{a\neq i} \mu_a^n(\boldsymbol{v})$, and $\delta := \alpha - \gamma$.

If $\beta \neq 0$, then

$$\begin{aligned} f(i, \boldsymbol{x}, \boldsymbol{v}) = & \int_{-\infty}^{-\delta/|\beta|} \gamma\phi(z)\,\mathrm{d}z + \int_{-\delta/|\beta|}^{\infty} (\alpha + |\beta|z)\phi(z)\,\mathrm{d}z \\ = & \gamma\Phi(-\delta/|\beta|) + \alpha[1 - \Phi(-\delta/|\beta|)] + \beta\phi(-\delta/|\beta|), \end{aligned}$$

where the second equality follows from the identity $\int_t^\infty z\phi(z)\,\mathrm{d}z = \phi(t)$ for all $t \in \mathbb{R}$. Next, we calculate the integrand in eq. (12). By noting that $\phi(z) = \phi(-z)$ and $\Phi(-z) = 1 - \Phi(z)$ for all $z \in \mathbb{R}$,

$$\begin{aligned} f(i, \boldsymbol{x}, \boldsymbol{v}) - \max_{1\leq a\leq M} \mu_a^n(\boldsymbol{v}) = f(i, \boldsymbol{x}, \boldsymbol{v}) - \max(\alpha, \gamma) = & \begin{cases} |\beta|\phi(\delta/|\beta|) - \delta\Phi(-\delta/|\beta|), & \text{if } \alpha \geq \gamma \\ |\beta|\phi(\delta/|\beta|) + \delta\Phi(\delta/|\beta|), & \text{if } \alpha < \gamma \end{cases} \\ = & |\beta|\phi(|\delta/\beta|) - |\delta|\Phi(-|\delta/\beta|). \end{aligned} \quad (21)$$

If $\beta = 0$, then it is straightforward from eq. (20) to see that $f(i, \boldsymbol{x}, \boldsymbol{v}) - \max_{1\leq a\leq M} \mu_a^n(\boldsymbol{v}) = 0$. On the other hand, by Lemma 2 (iii), we can set the right-hand side of eq. (21) to be zero for $\beta = 0$. Hence, eq. (21) holds for $\beta = 0$ as well.

Replacing the integrand in eq. (12) with eq. (21) yields the expression of $\mathrm{IKG}^n(i, \boldsymbol{x})$ in Lemma 1. □

B. Proof of Proposition 1

To simplify notation, in this subsection we assume $M = 1$ and suppress the subscript i unless otherwise specified, but the results can be generalized to the case of $M > 1$ without essential difficulty. In particular, we use κ to denote a generic covariance function, k^0 the prior covariance function of a Gaussian process, and k^n the posterior covariance function. We will collect below several basic results on reproducing kernel Hilbert space (RKHS) and refer to Berlinet and Thomas-Agnan (2004) for an extensive treatment on the subject.

Definition 2. Let $\mathcal{X}$ be a nonempty set and κ be a covariance function on $\mathcal{X}$. A Hilbert space $\mathcal{H}_\kappa$ of functions on $\mathcal{X}$ equipped with an inner-product $\langle\cdot,\cdot\rangle_{\mathcal{H}_\kappa}$ is called a RKHS with reproducing kernel κ, if (i) $\kappa(\boldsymbol{x},\cdot) \in \mathcal{H}_\kappa$ for all $\boldsymbol{x} \in \mathcal{X}$, and (ii) $f(\boldsymbol{x}) = \langle f, \kappa(\boldsymbol{x},\cdot)\rangle_{\mathcal{H}_\kappa}$ for all $\boldsymbol{x} \in \mathcal{X}$ and $f \in \mathcal{H}_\kappa$. Furthermore, the norm of $\mathcal{H}_\kappa$ is induced by the inner-product, i.e., $\|f\|_{\mathcal{H}_\kappa}^2 = \langle f, f\rangle_{\mathcal{H}_\kappa}$ for all $f \in \mathcal{H}_\kappa$.

Remark 4. In Definition 2, for a fixed $\boldsymbol{x}$, $\kappa(\boldsymbol{x},\cdot)$ is understood as a function mapping $\mathcal{X}$ to $\mathbb{R}$ such that $\boldsymbol{y} \mapsto k(\boldsymbol{x}, \boldsymbol{y})$ for $\boldsymbol{y} \in \mathcal{X}$. Moreover, condition (ii) is called the *reproducing property*. In particular, it implies that $\kappa(\boldsymbol{x}, \boldsymbol{x}') = \langle \kappa(\boldsymbol{x},\cdot), \kappa(\boldsymbol{x}',\cdot)\rangle_{\mathcal{H}_\kappa}$ and $\kappa(\boldsymbol{x}, \boldsymbol{x}) = \|\kappa(\boldsymbol{x},\cdot)\|_{\mathcal{H}_\kappa}^2$ for all $\boldsymbol{x}, \boldsymbol{x}' \in \mathcal{X}$.

Remark 5. By Moore-Aronszajn theorem (Berlinet and Thomas-Agnan 2004, Theorem 3), for each covariance function κ there exists a unique RKHS $\mathcal{H}_\kappa$ for which κ is its reproducing kernel. Specifically,

$$\mathcal{H}_\kappa = \left\{ f = \sum_{i=1}^\infty c_i\kappa(\boldsymbol{x}_i,\cdot) : c_i \in \mathbb{R}, \boldsymbol{x}_i \in \mathcal{X},\ i = 1, 2, \ldots,\ \text{such that } \|f\|_{\mathcal{H}_\kappa}^2 < \infty \right\},$$

where $\|f\|^2_{\mathcal{H}_\kappa} := \sum_{i,j=1}^\infty c_i c_j \kappa(\boldsymbol{x}_i, \boldsymbol{x}_j)$. Moreover, the inner-product is defined by

$$\langle f, g\rangle_{\mathcal{H}_\kappa} = \sum_{i,j=1}^\infty a_i b_j \kappa(\boldsymbol{x}_i, \boldsymbol{x}'_j),$$

for any $f = \sum_{i=1}^\infty a_i \kappa(\boldsymbol{x}_i, \cdot) \in \mathcal{H}_\kappa$ and $g = \sum_{j=1}^\infty b_j \kappa(\boldsymbol{x}'_j, \cdot) \in \mathcal{H}_\kappa$.

The following lemma asserts that convergence in norm in a RKHS implies *uniform* pointwise convergence, provided that the covariance function κ is stationary.

Lemma 3. *Let $\mathcal{X}$ be a nonempty set and κ be a covariance function on $\mathcal{X}$. Suppose that a sequence of functions $\{f_n \in \mathcal{H}_\kappa : n = 1, 2, \dots\}$ converges in norm $\|\cdot\|_{\mathcal{H}_\kappa}$ as $n \to \infty$. Then the limit, denoted by f, is in $\mathcal{H}_\kappa$. Moreover, if κ is stationary, then $f_n(\boldsymbol{x}) \to f(\boldsymbol{x})$ as $n \to \infty$ uniformly in $\boldsymbol{x} \in \mathcal{X}$.*

Proof of Lemma 3. First of all, $f \in \mathcal{H}_\kappa$ is guaranteed as a Hilbert space is a complete metric space. A basic property of RKHS is that convergence in norm implies pointwise convergence to the same limit; see, e.g., Corollary 1 of Berlinet and Thomas-Agnan (2004, page 10). Namely, $f_n(\boldsymbol{x}) \to f(\boldsymbol{x})$ as $n \to \infty$ for all $\boldsymbol{x} \in \mathcal{X}$.

To show the pointwise convergence is uniform, note that since κ is stationary, there exists a function $\varphi : \mathbb{R}^d \mapsto \mathbb{R}$ such that $\kappa(\boldsymbol{x}, \boldsymbol{x}') = \varphi(\boldsymbol{x} - \boldsymbol{x}')$. Hence, $\|\kappa(\boldsymbol{x}, \cdot)\|^2_{\mathcal{H}_\kappa} = \kappa(\boldsymbol{x}, \boldsymbol{x}) = \varphi(\boldsymbol{0})$. It follows that

$$\begin{aligned} |f_{n+m}(\boldsymbol{x}) - f_n(\boldsymbol{x})| &= |\langle f_{n+m} - f_n, \kappa(\boldsymbol{x}, \cdot)\rangle_{\mathcal{H}_\kappa}| \\ &\le \|f_{n+m} - f_n\|_{\mathcal{H}_\kappa} \|\kappa(\boldsymbol{x}, \cdot)\|_{\mathcal{H}_\kappa} = \|f_{n+m} - f_n\|_{\mathcal{H}_\kappa} \sqrt{\varphi(\boldsymbol{0})}, \end{aligned} \tag{22}$$

for all n and m, where the first equality follows from the reproducing property.

Since a Hilbert space is a complete metric space, the $\|\cdot\|_{\mathcal{H}_\kappa}$-converging sequence $\{f_n\}$ is a Cauchy sequence in $\mathcal{H}_\kappa$, meaning that $\|f_{n+m} - f_n\|_{\mathcal{H}_\kappa} \to 0$ as $n \to \infty$ for all m. Since this convergence to zero is independent of $\boldsymbol{x}$, it follows from eq. (22) that $\{f_n\}$ is a uniform Cauchy sequence of functions, thereby converging to f uniformly in $\boldsymbol{x} \in \mathcal{X}$. □

In the light of Lemma 3, in order to establish the uniform convergence of $k^n(\boldsymbol{x}, \boldsymbol{x}')$ as a function of $\boldsymbol{x}'$, it suffices to prove the norm convergence of $k^n(\boldsymbol{x}, \cdot)$ in the RKHS induced by k^0. We first establish this result for a more general case in the following Lemma 4, where k^0 is not required to be stationary.

Lemma 4. *Let $\mathcal{H}_{k^0}$ be the RKHS induced by k^0. If $k^0(\boldsymbol{x}, \boldsymbol{x}) > 0$ for all $\boldsymbol{x} \in \mathcal{X}$, then for any $\boldsymbol{x} \in \mathcal{X}$, $k^n(\boldsymbol{x}, \cdot)$ converges in norm $\|\cdot\|_{\mathcal{H}_{k^0}}$ as $n \to \infty$.*

Proof of Lemma 4. Fix $\boldsymbol{x} \in \mathcal{X}$. The fact that $k^n(\boldsymbol{x}, \cdot) \in \mathcal{H}_{k^0}$ is due to eq. (4). It follows from eq. (8) that $\{k^n(\boldsymbol{x}, \boldsymbol{x}) : n \ge 1\}$ form a non-increasing sequence bounded below by zero. The monotone convergence theorem implies that $k^n(\boldsymbol{x}, \boldsymbol{x})$ converges as $n \to \infty$. Hence, for all $m \ge 1$,

$$\lim_{n\to\infty} \left|k^{n+m}(\boldsymbol{x}, \boldsymbol{x}) - k^n(\boldsymbol{x}, \boldsymbol{x})\right| = 0. \tag{23}$$

Let $\boldsymbol{V}^n := \{\boldsymbol{v}^\ell : \ell = 0, \dots, n-1\}$ and $\boldsymbol{V}_n^{n+m} := \{\boldsymbol{v}^\ell : \ell = n, \dots, n+m-1\}$. Then, by eq. (4),

$$k^{n+m}(\boldsymbol{x}, \cdot) - k^n(\boldsymbol{x}, \cdot) = -k^n(\boldsymbol{x}, \boldsymbol{V}_n^{n+m})[k^n(\boldsymbol{V}_n^{n+m}, \boldsymbol{V}_n^{n+m}) + \lambda(\boldsymbol{V}_n^{n+m})]^{-1} k^n(\boldsymbol{V}_n^{n+m}, \cdot). \tag{24}$$

For notational simplicity, let $\mathbf{\Sigma}_n^{n+m} := k^n(\boldsymbol{V}_n^{n+m}, \boldsymbol{V}_n^{n+m}) + \lambda(\boldsymbol{V}_n^{n+m})$. Then,

$$
\begin{aligned}
&\left\|k^{n+m}(\boldsymbol{x},\cdot) - k^n(\boldsymbol{x},\cdot)\right\|^2_{\mathcal{H}_{k^0}} \\
=\ &\langle k^n(\boldsymbol{x}, \boldsymbol{V}_n^{n+m})[\mathbf{\Sigma}_n^{n+m}]^{-1}k^n(\boldsymbol{V}_n^{n+m},\cdot), k^n(\boldsymbol{x}, \boldsymbol{V}_n^{n+m})[\mathbf{\Sigma}_n^{n+m}]^{-1}k^n(\boldsymbol{V}_n^{n+m},\cdot)\rangle_{\mathcal{H}_{k^0}} \\
=\ &k^n(\boldsymbol{x}, \boldsymbol{V}_n^{n+m})[\mathbf{\Sigma}_n^{n+m}]^{-1}\langle k^n(\boldsymbol{V}_n^{n+m},\cdot), k^n(\boldsymbol{V}_n^{n+m},\cdot)\rangle_{\mathcal{H}_{k^0}}[\mathbf{\Sigma}_n^{n+m}]^{-1}k^n(\boldsymbol{V}_n^{n+m},\boldsymbol{x}),
\end{aligned} \tag{25}
$$

where

$$
\langle k^n(\boldsymbol{V}_n^{n+m},\cdot), k^n(\boldsymbol{V}_n^{n+m},\cdot)\rangle_{\mathcal{H}_{k^0}} = \left(\langle k^n(\boldsymbol{v}^{n+i},\cdot), k^n(\boldsymbol{v}^{n+j},\cdot)\rangle_{\mathcal{H}_{k^0}}\right)_{0\le i,j\le m-1}.
$$

Moreover, note that by eq. (4),

$$
k^n(\boldsymbol{V}_n^{n+m},\cdot) = k^0(\boldsymbol{V}_n^{n+m},\cdot) - k^0(\boldsymbol{V}_n^{n+m},\boldsymbol{V}^n)[k^0(\boldsymbol{V}^n,\boldsymbol{V}^n) + \lambda(\boldsymbol{V}^n)]^{-1}k^0(\boldsymbol{V}^n,\cdot). \tag{26}
$$

Let $\mathbf{\Sigma}^n := k^0(\boldsymbol{V}^n,\boldsymbol{V}^n) + \lambda(\boldsymbol{V}^n)$. Then, it follows from eq. (26) and the reproducing property that

$$
\begin{aligned}
&\langle k^n(\boldsymbol{V}_n^{n+m},\cdot), k^n(\boldsymbol{V}_n^{n+m},\cdot)\rangle_{\mathcal{H}_{k^0}} \\
=\ &k^0(\boldsymbol{V}_n^{n+m},\boldsymbol{V}_n^{n+m}) - 2k^0(\boldsymbol{V}_n^{n+m},\boldsymbol{V}^n)[\mathbf{\Sigma}_n]^{-1}k^0(\boldsymbol{V}^n,\boldsymbol{V}_n^{n+m}) \\
&+ k^0(\boldsymbol{V}_n^{n+m},\boldsymbol{V}^n)[\mathbf{\Sigma}_n]^{-1}k^0(\boldsymbol{V}^n,\boldsymbol{V}^n)[\mathbf{\Sigma}_n]^{-1}k^0(\boldsymbol{V}^n,\boldsymbol{V}_n^{n+m}) \\
=\ &k^0(\boldsymbol{V}_n^{n+m},\boldsymbol{V}_n^{n+m}) - k^0(\boldsymbol{V}_n^{n+m},\boldsymbol{V}^n)[\mathbf{\Sigma}_n]^{-1}k^0(\boldsymbol{V}^n,\boldsymbol{V}_n^{n+m}) \\
&- k^0(\boldsymbol{V}_n^{n+m},\boldsymbol{V}^n)[\mathbf{\Sigma}_n]^{-1}\{\boldsymbol{I} - k^0(\boldsymbol{V}^n,\boldsymbol{V}^n)[\mathbf{\Sigma}_n]^{-1}\}k^0(\boldsymbol{V}^n,\boldsymbol{V}_n^{n+m}) \\
=\ &k^n(\boldsymbol{V}_n^{n+m},\boldsymbol{V}_n^{n+m}) - k^0(\boldsymbol{V}_n^{n+m},\boldsymbol{V}^n)[\mathbf{\Sigma}_n]^{-1}\{\boldsymbol{I} - k^0(\boldsymbol{V}^n,\boldsymbol{V}^n)[\mathbf{\Sigma}_n]^{-1}\}k^0(\boldsymbol{V}^n,\boldsymbol{V}_n^{n+m}),
\end{aligned} \tag{27}
$$

where $\boldsymbol{I}$ denotes the identity matrix of a compatible size. Furthermore, note that

$$
\begin{aligned}
\boldsymbol{I} - k^0(\boldsymbol{V}^n,\boldsymbol{V}^n)[\mathbf{\Sigma}_n]^{-1} &= \boldsymbol{I} - [k^0(\boldsymbol{V}^n,\boldsymbol{V}^n) + \lambda(\boldsymbol{V}^n) - \lambda(\boldsymbol{V}^n)][k^0(\boldsymbol{V}^n,\boldsymbol{V}^n) + \lambda(\boldsymbol{V}^n)]^{-1} \\
&= \boldsymbol{I} - \boldsymbol{I} + \lambda(\boldsymbol{V}^n)[k^0(\boldsymbol{V}^n,\boldsymbol{V}^n) + \lambda(\boldsymbol{V}^n)]^{-1} \\
&= \lambda(\boldsymbol{V}^n)[\mathbf{\Sigma}^n]^{-1}.
\end{aligned} \tag{28}
$$

We now combine eqs. (27) and (28) to have

$$
\begin{aligned}
&\langle k^n(\boldsymbol{V}_n^{n+m},\cdot), k^n(\boldsymbol{V}_n^{n+m},\cdot)\rangle_{\mathcal{H}_{k^0}} \\
=\ &k^n(\boldsymbol{V}_n^{n+m},\boldsymbol{V}_n^{n+m}) - k^0(\boldsymbol{V}_n^{n+m},\boldsymbol{V}^n)[\mathbf{\Sigma}_n]^{-1}\lambda(\boldsymbol{V}^n)[\mathbf{\Sigma}^n]^{-1}k^0(\boldsymbol{V}^n,\boldsymbol{V}_n^{n+m}),
\end{aligned}
$$

which is the difference between two positive semi-definite matrices. Therefore, by eq. (25),

$$
\begin{aligned}
\left\|k^{n+m}(\boldsymbol{x},\cdot) - k^n(\boldsymbol{x},\cdot)\right\|^2_{\mathcal{H}_{k^0}} &\le k^n(\boldsymbol{x},\boldsymbol{V}_n^{n+m})[\mathbf{\Sigma}_n^{n+m}]^{-1}k^n(\boldsymbol{V}_n^{n+m},\boldsymbol{V}_n^{n+m})[\mathbf{\Sigma}_n^{n+m}]^{-1}k^n(\boldsymbol{V}_n^{n+m},\boldsymbol{x}) \\
&\le k^n(\boldsymbol{x},\boldsymbol{V}_n^{n+m})[\mathbf{\Sigma}_n^{n+m}]^{-1}\mathbf{\Sigma}_n^{n+m}[\mathbf{\Sigma}_n^{n+m}]^{-1}k^n(\boldsymbol{V}_n^{n+m},\boldsymbol{x}) \\
&= k^n(\boldsymbol{x},\boldsymbol{x}) - k^{n+m}(\boldsymbol{x},\boldsymbol{x}),
\end{aligned}
$$

where the second inequality follows from the definition of $\boldsymbol{\Sigma}_n^{n+m}$ and the equality follows from eq. (24). Then, we apply eq. (23) to conclude that $\|k^{n+m}(\boldsymbol{x},\cdot) - k^n(\boldsymbol{x},\cdot)\|_{\mathcal{H}_{k^0}} \to 0$ as $n \to \infty$ for all $m \geq 1$. Therefore, $k^n(\boldsymbol{x},\cdot)$ converges in norm $\|\cdot\|_{\mathcal{H}_{k^0}}$ as $n \to \infty$. □

With Lemmas 3 and 4, we are ready to prove Proposition 1.

Proof of Proposition 1. Fix $i = 1,\ldots,M$. Since k_i^0 is stationary, $k_i^0(\boldsymbol{x},\boldsymbol{x}) > 0$ for all $\boldsymbol{x} \in \mathcal{X}$. Then by Lemma 4, for any $\boldsymbol{x} \in \mathcal{X}$, $k_i^n(\boldsymbol{x},\cdot)$ converges in norm $\|\cdot\|_{\mathcal{H}_{k^0}}$ as $n \to \infty$. Then by Lemma 3, for the $\|\cdot\|_{\mathcal{H}_{k^0}}$-converging limit $k_i^\infty(\boldsymbol{x},\cdot)$, $k_i^n(\boldsymbol{x},\boldsymbol{x}') \to k_i^\infty(\boldsymbol{x},\boldsymbol{x}')$ uniformly in $\boldsymbol{x}' \in \mathcal{X}$ as $n \to \infty$. □

C. Proof of Proposition 2

Notice that if $\eta_i^\infty = \infty$ under a sampling policy π, then due to the compactness of $\mathcal{X}$, $\{\boldsymbol{v}^n : a^n = i, n = 0,1,\ldots\}$ (i.e., the sampling locations associated with alternative i) must have an accumulation point $\boldsymbol{x}_i^{\mathsf{acc}} \in \mathcal{X}$. Namely, there exists a subsequence of $\{n : a^n = i, n = 0,1,\ldots\}$, say $\{\ell_{i,n}\}_{n=0}^\infty$, such that $\ell_{i,n} \to \infty$ and $\boldsymbol{v}^{\ell_{i,n}} \to \boldsymbol{x}_i^{\mathsf{acc}}$ as $n \to \infty$. For any $\epsilon > 0$, let $\mathcal{B}(\boldsymbol{x}_i^{\mathsf{acc}},\epsilon) := \{\boldsymbol{x} : \|\boldsymbol{x}_i^{\mathsf{acc}} - \boldsymbol{x}\| \leq \epsilon\}$ be the closed ball centered at $\boldsymbol{x}_i^{\mathsf{acc}}$ with radius ϵ. Let $\mathrm{Var}^{\pi,n}[\cdot]$ denote the posterior variance conditioned on $\mathcal{F}^n$ that is induced by π.

The proof of Proposition 2 is preceded by four technical results, i.e., Lemmas 5–8. In Lemmas 5 and 6, we establish an upper bound on $\mathrm{Var}^{\pi,n}[\theta_i(\boldsymbol{x})]$ for $\boldsymbol{x} \in \mathcal{B}(\boldsymbol{x}_i^{\mathsf{acc}},\epsilon)$. This result does not rely on the IKG policy *per se*, but is implied by the existence of the accumulation point $\boldsymbol{x}_i^{\mathsf{acc}}$ instead. In particular, the upper bound which depends on ϵ can be made arbitrarily small as $\epsilon \to 0$. This basically means that in the light of an unlimited number of samples of alternative i that are taken in proximity to $\boldsymbol{x}_i^{\mathsf{acc}}$, the uncertainty about $\theta_i(\boldsymbol{x}_i^{\mathsf{acc}})$ will eventually be eliminated, thanks to the correlation between $\theta_i(\boldsymbol{x}_i^{\mathsf{acc}})$ and $\theta_i(\boldsymbol{x})$ for $\boldsymbol{x}$ near $\boldsymbol{x}_i^{\mathsf{acc}}$.

Lemma 7 asserts that $\mathrm{IKG}^n(i,\boldsymbol{x})$ is bounded by a multiple of the posterior standard deviation of $\theta_i(\boldsymbol{x})$. This implies that when the posterior variance approaches to zero, the IKG factor does too.

Following the last three lemmas, Lemma 8 asserts that the limit inferior of the IKG factor is zero. The reasoning is as follows. By Lemmas 5 and 6, the posterior variance at those sampling locations that fall inside $\mathcal{B}(\boldsymbol{x}_i^{\mathsf{acc}},\epsilon)$ is small. Then, by Lemma 7, the IKG factor at these locations are also small, so does the limit superior. Since the sampling locations inside $\mathcal{B}(\boldsymbol{x}_i^{\mathsf{acc}},\epsilon)$ is a subsequence of the entire sampling locations, the limit inferior of the IKG factor over all sampling locations is even smaller.

At last, Proposition 2 is proved by contradiction — if there is a location that the posterior variance does not approach zero, then the limit inferior of the IKG factor at the same location must be positive as well.

Lemma 5. *Fix $i = 1,\ldots,M$, $n \geq 1$, and a compact set $\mathcal{S} \subseteq \mathcal{X}$. Suppose that the sampling decisions satisfy $a^0 = \cdots = a^{n-1} = i$ and $\boldsymbol{v}^0,\ldots,\boldsymbol{v}^{n-1} \in \mathcal{S}$. If Assumptions 1–3 hold, then for all $\boldsymbol{x} \in \mathcal{S}$,*

$$\mathrm{Var}^n[\theta_i(\boldsymbol{x})] \leq \tau_i^2 - \frac{n \min_{\boldsymbol{x}' \in \mathcal{S}} \left[k_i^0(\boldsymbol{x},\boldsymbol{x}')\right]^2}{n\tau_i^2 + \lambda_i^{\max}},$$

where $\lambda_i^{\max} := \max_{\boldsymbol{x} \in \mathcal{X}} \lambda_i(\boldsymbol{x}) \in (0,\infty)$.

Proof of Lemma 5. Fix $\boldsymbol{x} \in \mathcal{S}$. First note that $\lambda_i^{\max}$ is well defined under Assumptions 2 and 3. Let $\boldsymbol{V}_i^n$ be the set of the locations of the samples taken from θ_i up to time n. Under Assumption 1, eq. (4) reads

$$\mathrm{Var}^n[\theta_i(\boldsymbol{x})] = \tau_i^2 - k_i^0(\boldsymbol{x}, \boldsymbol{V}_i^n)[k_i^0(\boldsymbol{V}_i^n, \boldsymbol{V}_i^n) + \lambda_i(\boldsymbol{V}_i^n)]^{-1} k_i^0(\boldsymbol{V}_i^n, \boldsymbol{x}),$$

where $\boldsymbol{V}_i^n = \{\boldsymbol{v}^0, \ldots, \boldsymbol{v}^{n-1}\}$ due to the assumption that $a^0 = \cdots = a^{n-1} = i$.

For notational simplicity, let $\boldsymbol{A} := k_i^0(\boldsymbol{V}_i^n, \boldsymbol{V}_i^n) + \lambda_i(\boldsymbol{V}_i^n)$ and $\boldsymbol{B} := k_i^0(\boldsymbol{V}_i^n, \boldsymbol{V}_i^n) + \lambda_i^{\max}\boldsymbol{I}$. Note that $\boldsymbol{B} - \boldsymbol{A} = \lambda_i^{\max}\boldsymbol{I} - \lambda_i(\boldsymbol{V}_i^n)$ is a diagonal matrix with nonnegative elements, so it is positive semi-definite. Since $\boldsymbol{A}$ and $\boldsymbol{B}$ are both positive definite, by Horn and Johnson (2012, Corollary 7.7.4), $\boldsymbol{A}^{-1} - \boldsymbol{B}^{-1}$ is positive semi-definite. Therefore,

$$\begin{aligned} & k_i^0(\boldsymbol{x}, \boldsymbol{V}_i^n)[k_i^0(\boldsymbol{V}_i^n, \boldsymbol{V}_i^n) + \lambda_i(\boldsymbol{V}_i^n)]^{-1} k_i^0(\boldsymbol{V}_i^n, \boldsymbol{x}) - k_i^0(\boldsymbol{x}, \boldsymbol{V}_i^n)[k_i^0(\boldsymbol{V}_i^n, \boldsymbol{V}_i^n) + \lambda_i^{\max}\boldsymbol{I}]^{-1} k_i^0(\boldsymbol{V}_i^n, \boldsymbol{x}) \\ &= k_i^0(\boldsymbol{x}, \boldsymbol{V}_i^n)(\boldsymbol{A}^{-1} - \boldsymbol{B}^{-1}) k_i^0(\boldsymbol{V}_i^n, \boldsymbol{x}) \geq 0. \end{aligned} \tag{29}$$

It then follows from eqs. (4) and (29) that

$$\mathrm{Var}^n[\theta_i(\boldsymbol{x})] \leq \tau_i^2 - k_i^0(\boldsymbol{x}, \boldsymbol{V}_i^n)[k_i^0(\boldsymbol{V}_i^n, \boldsymbol{V}_i^n) + \lambda_i^{\max}\boldsymbol{I}]^{-1} k_i^0(\boldsymbol{V}_i^n, \boldsymbol{x}).$$

Thus, it suffices to prove that

$$f(\boldsymbol{v}^0, \ldots, \boldsymbol{v}^{n-1}) := k_i^0(\boldsymbol{x}, \boldsymbol{V}_i^n)[k_i^0(\boldsymbol{V}_i^n, \boldsymbol{V}_i^n) + \lambda_i^{\max}\boldsymbol{I}]^{-1} k_i^0(\boldsymbol{V}_i^n, \boldsymbol{x}) \geq \frac{n \min_{\boldsymbol{x}' \in \mathcal{S}} \left[k_i^0(\boldsymbol{x}, \boldsymbol{x}')\right]^2}{n\tau_i^2 + \lambda_i^{\max}}, \tag{30}$$

for all $\boldsymbol{v}^0, \ldots, \boldsymbol{v}^{n-1} \in \mathcal{S}$.

Since $k_i^0(\boldsymbol{V}_i^n, \boldsymbol{V}_i^n)$ is symmetric, we can always write $k_i^0(\boldsymbol{V}_i^n, \boldsymbol{V}_i^n) = \boldsymbol{Q}\mathrm{diag}\{\alpha_1, \ldots, \alpha_n\}\boldsymbol{Q}^\intercal$, where $\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_n \geq 0$ are the eigenvalues of $k_i^0(\boldsymbol{V}_i^n, \boldsymbol{V}_i^n)$, and $\boldsymbol{Q}$ is an orthogonal matrix, i.e., $\boldsymbol{Q}\boldsymbol{Q}^\intercal = \boldsymbol{I}$. Therefore,

$$k_i^0(\boldsymbol{V}_i^n, \boldsymbol{V}_i^n) + \lambda_i^{\max}\boldsymbol{I} = \boldsymbol{Q}\mathrm{diag}\big\{(\alpha_1 + \lambda_i^{\max}), \ldots, (\alpha_n + \lambda_i^{\max})\big\}\boldsymbol{Q}^\intercal.$$

and

$$[k_i^0(\boldsymbol{V}_i^n, \boldsymbol{V}_i^n) + \lambda_i^{\max}\boldsymbol{I}]^{-1} = \boldsymbol{Q}\mathrm{diag}\big\{(\alpha_1 + \lambda_i^{\max})^{-1}, \ldots, (\alpha_n + \lambda_i^{\max})^{-1}\big\}\boldsymbol{Q}^\intercal.$$

If we let β_j be the j-th element of the row vector $k_i^0(\boldsymbol{x}, \boldsymbol{V}_i^n)\boldsymbol{Q}$, i.e., $k_i^0(\boldsymbol{x}, \boldsymbol{V}_i^n)\boldsymbol{Q} = [\beta_1, \ldots, \beta_n]$, then

$$f(\boldsymbol{v}^0, \ldots, \boldsymbol{v}^{n-1}) = \frac{\beta_1^2}{\alpha_1 + \lambda_i^{\max}} + \cdots + \frac{\beta_n^2}{\alpha_n + \lambda_i^{\max}}.$$

Here, α_j and β_j clearly both depend on $\boldsymbol{v}^0, \ldots, \boldsymbol{v}^{n-1}$, for $j = 1, \ldots, n$. Moreover, they satisfy the following two conditions. First, $\sum_{j=1}^n \alpha_j = \mathrm{tr}(k_i^0(\boldsymbol{V}_i^n, \boldsymbol{V}_i^n)) = n\tau_i^2$, where the first equality is a straightforward fact that the trace of a matrix equals the sum of its eigenvalues, and the second equality is from Assumption 1.

Second,

$$\sum_{j=1}^{n}\beta_j^2 = k_i^0(\boldsymbol{x},\boldsymbol{V}_i^n)\boldsymbol{Q}\boldsymbol{Q}^\intercal k_i^0(\boldsymbol{V}_i^n,\boldsymbol{x}) = k_i^0(\boldsymbol{x},\boldsymbol{V}_i^n)k_i^0(\boldsymbol{V}_i^n,\boldsymbol{x}) = \sum_{\ell=0}^{n-1}[k_i^0(\boldsymbol{x},\boldsymbol{v}^\ell)]^2 \geq n\min_{\boldsymbol{x}'\in\mathcal{S}}[k_i^0(\boldsymbol{x},\boldsymbol{x}')]^2.$$

If we define $g:\mathbb{R}^{2n}\mapsto\mathbb{R}$ as follows

$$g(a_1,\ldots,a_n,b_1,\ldots,b_n) := \frac{b_1}{a_1+\lambda_i^{\max}}+\cdots+\frac{b_n}{a_n+\lambda_i^{\max}},$$

then $f(\boldsymbol{v}^0,\ldots,\boldsymbol{v}^{n-1}) = g(\alpha_1,\ldots,\alpha_n,\beta_1^2,\ldots,\beta_n^2)$. It follows that

$$\min_{\boldsymbol{v}^0,\ldots,\boldsymbol{v}^{n-1}\in\mathcal{S}} f(\boldsymbol{v}^0,\ldots,\boldsymbol{v}^{n-1}) \geq \min_{\substack{(a_1,\ldots,a_n)\in\mathcal{C}_1\\(b_1,\ldots,b_n)\in\mathcal{C}_2}} g(a_1,\ldots,a_n,b_1,\ldots,b_n), \tag{31}$$

where

$$\mathcal{C}_1 := \left\{(a_1,\ldots,a_n)\in\mathbb{R}^n : a_1\geq\cdots\geq a_n\geq 0 \quad\text{and}\quad \sum_{j=1}^{n}a_j = n\tau_i^2\right\},$$
$$\mathcal{C}_2 := \left\{(b_1,\ldots,b_n)\in\mathbb{R}^n : b_1\geq 0,\ldots,b_n\geq 0 \quad\text{and}\quad \sum_{j=1}^{n}b_j \geq n\min_{\boldsymbol{x}'\in\mathcal{S}}[k_i^0(\boldsymbol{x},\boldsymbol{x}')]^2\right\}.$$

The reason for the inequality in eq. (31) is that the two minimization problems have the same objective function while the one in left-hand side has smaller feasible region.

We now solve the minimization problem on the right-hand side of eq. (31). Note that for any $(a_1,\ldots,a_n)\in\mathcal{C}_1$, $\min_{(b_1,\ldots,b_n)\in\mathcal{C}_2} g(a_1,\ldots,a_n,b_1,\ldots,b_n)$ is a linear programming problem, and it is easy to see that its optimal solution is $b_1^* = n\min_{\boldsymbol{x}'\in\mathcal{S}}[k_i^0(\boldsymbol{x},\boldsymbol{x}')]^2$ and $b_2^*=\cdots=b_n^*=0$. Hence,

$$\min_{\substack{(a_1,\ldots,a_n)\in\mathcal{C}_1\\(b_1,\ldots,b_n)\in\mathcal{C}_2}} g(a_1,\ldots,a_n,b_1,\ldots,b_n) = \min_{(a_1,\ldots,a_n)\in\mathcal{C}_1}\frac{n\min_{\boldsymbol{x}'\in\mathcal{S}}[k_i^0(\boldsymbol{x},\boldsymbol{x}')]^2}{a_1+\lambda_i^{\max}} = \frac{n\min_{\boldsymbol{x}'\in\mathcal{S}}[k_i^0(\boldsymbol{x},\boldsymbol{x}')]^2}{n\tau_i^2+\lambda_i^{\max}}. \tag{32}$$

Then, we can apply eqs. (31) and (32) to show eq. (30), completing the proof of Lemma 5. □

Lemma 6. *Fix $i=1,\ldots,M$ and a sampling policy π. Suppose that the sequence of sampling locations $\{\boldsymbol{v}^n : a^n = i, n=0,1,\ldots\}$ under π has an accumulation point $\boldsymbol{x}_i^{\mathsf{acc}}$. If Assumptions 1–3 hold, then for any $\epsilon>0$,*

$$\limsup_{n\to\infty}\max_{\boldsymbol{x}\in\mathcal{B}(\boldsymbol{x}_i^{\mathsf{acc}},\epsilon)}\mathrm{Var}^{\pi,n}[\theta_i(\boldsymbol{x})] \leq \tau_i^2\left[1-\rho_i^2(2\epsilon\mathbf{1})\right],$$

where $\mathbf{1}$ is the vector of all ones with size $d\times 1$.

Proof of Lemma 6. It follows from eq. (8) that $\{\mathrm{Var}^{\pi,n}[\theta_i(\boldsymbol{x})]\}_{n=0}^{\infty}$ is a non-increasing sequence bounded below by zero. Hence, $\mathrm{Var}^{\pi,n}[\theta_i(\boldsymbol{x})]$ converges as $n\to\infty$ and its limit is well defined.

Fix $\epsilon>0$. Let $s_{i,n} := \left|\{\boldsymbol{v}^\ell\in\mathcal{B}(\boldsymbol{x}_i^{\mathsf{acc}},\epsilon) : a^\ell = i, \ell=0,\ldots,n-1\}\right|$ be the number of times that alternative i is sampled at a point in $\mathcal{B}(\boldsymbol{x}_i^{\mathsf{acc}}, \epsilon)$ under π among the total n samples. Then, we must have $s_{i,n} \to \infty$ since $\boldsymbol{x}_i^{\mathsf{acc}}$ is an accumulation point. Note that reordering the sampling decision-observation pairs $((a^0, \boldsymbol{v}^0), y^1), \ldots, ((a^{n-1}, \boldsymbol{v}^{n-1}), y^n)$ does not alter the conditional variance of $\theta_i(\boldsymbol{x})$. Hence, we may assume without loss of generality that the first $s_{i,n}$ samples are all taken from alternative i at locations that belong to $\mathcal{B}(\boldsymbol{x}_i^{\mathsf{acc}}, \epsilon)$. Since the posterior variance decreases in the number of samples by eq. (8), we conclude that for all $\boldsymbol{x} \in \mathcal{B}(\boldsymbol{x}_i^{\mathsf{acc}}, \epsilon)$,

$$\mathrm{Var}^{\pi,n}[\theta_i(\boldsymbol{x})] \le \mathrm{Var}^{\pi,s_{i,n}}[\theta_i(\boldsymbol{x})] \le \tau_i^2 - \frac{s_{i,n} \min_{\boldsymbol{x}' \in \mathcal{B}(\boldsymbol{x}_i^{\mathsf{acc}}, \epsilon)} [k_i^0(\boldsymbol{x}, \boldsymbol{x}')]^2}{s_{i,n}\tau_i^2 + \lambda_i^{\max}}, \tag{33}$$

where the second inequality follows from Lemma 5.

Note that $[k^0(\boldsymbol{x}, \boldsymbol{x}')]^2 = \tau_i^4 \rho_i^2(|\boldsymbol{x} - \boldsymbol{x}'|)$, and that $\|\boldsymbol{x} - \boldsymbol{x}'\| \le \|\boldsymbol{x} - \boldsymbol{x}_i^{\mathsf{acc}}\| + \|\boldsymbol{x}_i^{\mathsf{acc}} - \boldsymbol{x}'\| \le 2\epsilon$ for all $\boldsymbol{x}, \boldsymbol{x}' \in \mathcal{B}(\boldsymbol{x}_i^{\mathsf{acc}}, \epsilon)$. Hence, each component of $|\boldsymbol{x} - \boldsymbol{x}'|$ is no greater than 2ϵ. Since $\rho_i(\boldsymbol{\delta})$ is decreasing in $\boldsymbol{\delta}$ component-wise for $\boldsymbol{\delta} > 0$ (see Assumption 1), $\rho_i(|\boldsymbol{x} - \boldsymbol{x}'|) \ge \rho_i(2\epsilon\mathbf{1})$ for all $\boldsymbol{x}, \boldsymbol{x}' \in \mathcal{B}(\boldsymbol{x}_i^{\mathsf{acc}}, \epsilon)$. It then follows from eq. (33) that

$$\max_{\boldsymbol{x} \in \mathcal{B}(\boldsymbol{x}_i^{\mathsf{acc}}, \epsilon)} \mathrm{Var}^{\pi,n}[\theta_i(\boldsymbol{x})] \le \tau_i^2 - \frac{s_{i,n}\tau_i^4 \rho_i^2(2\epsilon\mathbf{1})}{s_{i,n}\tau_i^2 + \lambda_i^{\max}}.$$

Sending $n \to \infty$ completes the proof. □

Lemma 7. *Fix $i = 1, \ldots, M$. If Assumptions 1–3 hold, then for all $\boldsymbol{x} \in \mathcal{X}$,*

$$\mathrm{IKG}^n(i, \boldsymbol{x}) \le \sqrt{\frac{\tau_i^2 \, \mathrm{Var}^n[\theta_i(\boldsymbol{x})]}{2\pi\lambda_i(\boldsymbol{x}) c_i^2(\boldsymbol{x})}}.$$

Proof of Lemma 7. Notice that

$$\begin{aligned}
&\int_{\mathcal{X}} \mathbb{E}\left[\max_{1 \le a \le M} \mu_a^{n+1}(\boldsymbol{v}) \,\Big|\, \mathcal{F}^n, a^n = i, \boldsymbol{v}^n = \boldsymbol{x}\right] \gamma(\boldsymbol{v}) \,\mathrm{d}\boldsymbol{v} \\
= &\int_{\mathcal{X}} \mathbb{E}^n\left[\max_{1 \le a \le M} \left(\mu_a^n(\boldsymbol{v}) + \sigma_a^n(\boldsymbol{v}, \boldsymbol{v}^n) Z^{n+1}\right) \,\Big|\, a^n = i, \boldsymbol{v}^n = \boldsymbol{x}\right] \gamma(\boldsymbol{v}) \,\mathrm{d}\boldsymbol{v} \\
\le &\int_{\mathcal{X}} \max_{1 \le a \le M} \mu_a^n(\boldsymbol{v}) \gamma(\boldsymbol{v}) \,\mathrm{d}\boldsymbol{v} + \int_{\mathcal{X}} \mathbb{E}^n\left[\max_{1 \le a \le M} \left(\sigma_a^n(\boldsymbol{v}, \boldsymbol{v}^n) Z^{n+1}\right) \,\Big|\, a^n = i, \boldsymbol{v}^n = \boldsymbol{x}\right] \gamma(\boldsymbol{v}) \,\mathrm{d}\boldsymbol{v}\,.
\end{aligned} \tag{34}$$

Since $k_i^0(\boldsymbol{x}, \boldsymbol{x}')$ is a continuous function by Assumption 1, it follows from Assumption 3 and the updating eq. (3) that $\mu_i^n(\boldsymbol{x})$ is a continuous function for any n. Hence, $\mu_i^n(\boldsymbol{x})$ is bounded on $\mathcal{X}$ by Assumption 2. This implies that the first integral in eq. (34) is finite and can be subtracted from both sides of the inequality. Then, by the definition eq. (12),

$$\mathrm{IKG}^n(i, \boldsymbol{x}) \le \frac{1}{c_i(\boldsymbol{x})} \int_{\mathcal{X}} \mathbb{E}^n\left[\max_{1 \le a \le M} \left(\sigma_a^n(\boldsymbol{v}, \boldsymbol{v}^n) Z^{n+1}\right) \,\Big|\, a^n = i, \boldsymbol{v}^n = \boldsymbol{x}\right] \gamma(\boldsymbol{v}) \,\mathrm{d}\boldsymbol{v} := I. \tag{35}$$

It follows from eq. (7) that

$$I = \frac{1}{c_i(\boldsymbol{x})} \int_{\mathcal{X}} \mathbb{E}^n\left[\max\left\{\sigma_{a^n}^n(\boldsymbol{v}, \boldsymbol{v}^n) Z^{n+1}, 0\right\} \,\Big|\, a^n = i, \boldsymbol{v}^n = \boldsymbol{x}\right] \gamma(\boldsymbol{v}) \,\mathrm{d}\boldsymbol{v}$$

$$
\begin{aligned}
&= \frac{1}{c_i(\boldsymbol{x})} \int_{\mathcal{X}} \mathbb{E}^n \left[\max\left\{|\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})| Z^{n+1}, 0\right\}\right] \gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v} \\
&= \frac{1}{c_i(\boldsymbol{x})} \int_{\mathcal{X}} \mathbb{E}^n \left[|\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})| Z^{n+1}\, \mathbb{I}_{\{|\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})| Z^{n+1}>0\}}\right] \gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v} \\
&= \frac{1}{c_i(\boldsymbol{x})} \int_{\mathcal{X}} |\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})| \left[\int_0^\infty z\phi(z)\,\mathrm{d}z\right] \gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v} \\
&= \frac{1}{\sqrt{2\pi} c_i(\boldsymbol{x})} \int_{\mathcal{X}} |\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})| \gamma(\boldsymbol{v}) \mathrm{d}\boldsymbol{v}. \qquad (36)
\end{aligned}
$$

Moreover, by eq. (7),

$$
|\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})| = \left|\frac{\operatorname{Cov}^n[\theta_i(\boldsymbol{v}),\theta_i(\boldsymbol{x})]}{\sqrt{\operatorname{Var}^n[\theta_i(\boldsymbol{x})]+\lambda_i(\boldsymbol{x})}}\right| \le \sqrt{\frac{\operatorname{Var}^n[\theta_i(\boldsymbol{v})]\operatorname{Var}^n[\theta_i(\boldsymbol{x})]}{\operatorname{Var}^n[\theta_i(\boldsymbol{x})]+\lambda_i(\boldsymbol{x})}} \le \sqrt{\frac{\tau_i^2 \operatorname{Var}^n[\theta_i(\boldsymbol{x})]}{\lambda_i(\boldsymbol{x})}}, \qquad (37)
$$

where the last inequality follows because $0 \le \operatorname{Var}^n[\theta_i(\boldsymbol{v})] \le \operatorname{Var}[\theta_i(\boldsymbol{v})] = \tau_i^2$ for all $\boldsymbol{v} \in \mathcal{X}$ by eq. (8). The proof is completed by combining eqs. (35)–(37). □

Lemma 8. *Fix $i = 1,\ldots,M$. If Assumptions 1–3 hold, and $\eta_i^\infty = \infty$ under the IKG policy, then for any $\boldsymbol{x} \in \mathcal{X}$,*

$$
\liminf_{n\to\infty} \operatorname{IKG}^n(i,\boldsymbol{x}) = 0.
$$

Proof of Lemma 8. Since $\mathcal{X}$ is compact by Assumption 2, the sequence $\{\boldsymbol{v}^n \in \mathcal{X} : a^n = i, n = 0,1,\ldots,\}$ is bounded, and it is of length $\eta_i^\infty = \infty$. Hence, it has an accumulation point $\boldsymbol{x}_i^{\mathsf{acc}}$. Let $\{\ell_{i,n}\}_{n=0}^\infty$ be the subsequence of $\{n : a^n = i, n = 0,1,\ldots\}$ such that $\ell_{i,n} \to \infty$ and $\boldsymbol{v}^{\ell_{i,n}} \to \boldsymbol{x}_i^{\mathsf{acc}}$ as $n \to \infty$. Fix $\epsilon > 0$. Then, by Lemma 6,

$$
\limsup_{n\to\infty} \operatorname{Var}^n[\theta_i(\boldsymbol{v}^{\ell_{i,n}})] \le \tau_i^2[1-\rho_i^2(2\epsilon\mathbf{1})].
$$

It then follows from Lemma 7 that

$$
\limsup_{n\to\infty} \operatorname{IKG}^{\ell_{i,n}}(i,\boldsymbol{v}^{\ell_{i,n}}) \le \limsup_{n\to\infty} \sqrt{\frac{\tau_i^2 \operatorname{Var}^{\ell_{i,n}}[\theta_i(\boldsymbol{v}^{\ell_{i,n}})]}{2\pi\lambda_i(\boldsymbol{x})c_i^2(\boldsymbol{x})}} \le \sqrt{\frac{\tau_i^4[1-\rho_i^2(2\epsilon\mathbf{1})]}{2\pi\lambda_i(\boldsymbol{x})c_i^2(\boldsymbol{x})}}.
$$

By sending $\epsilon \to 0$, we have $\rho_i(2\epsilon\mathbf{1}) \to 1$ and thus, $\limsup_{n\to\infty} \operatorname{IKG}^{\ell_{i,n}}(i,\boldsymbol{v}^{\ell_{i,n}}) \le 0$. Since the limit inferior of a sequence is no greater than that of its subsequence,

$$
\liminf_{n\to\infty} \operatorname{IKG}^n(i,\boldsymbol{v}^n) \le \liminf_{n\to\infty} \operatorname{IKG}^{\ell_{i,n}}(i,\boldsymbol{v}^{\ell_{i,n}}) \le \limsup_{n\to\infty} \operatorname{IKG}^{\ell_{i,n}}(i,\boldsymbol{v}^{\ell_{i,n}}) \le 0. \qquad (38)
$$

Moreover, by the definition of IKG eq. (12) and Jensen's inequality,

$$
\operatorname{IKG}^n(i,\boldsymbol{x}) \ge \frac{1}{c_i(\boldsymbol{x})} \int_{\mathcal{X}} \left\{\max_{1\le a\le M} \mathbb{E}\left[\mu_a^{n+1}(\boldsymbol{v}) \,\middle|\, \mathcal{F}^n, a^n = i, \boldsymbol{v}^n = \boldsymbol{x}\right] - \max_{1\le a\le M} \mu_a^n(\boldsymbol{v})\right\} \gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v} = 0,
$$

for each $i = 1,\ldots,M$ and $\boldsymbol{x} \in \mathcal{X}$, where the equality follows immediately from the updating eq. (5). This, in conjunction with eq. (38), implies that $\liminf_{n\to\infty} \operatorname{IKG}^n(i,\boldsymbol{v}^n) = 0$. By the definition of the sampling location $\boldsymbol{v}^n$ in eq. (13), $\mathrm{IKG}^n(i,\boldsymbol{v}^n) = \max_{\boldsymbol{x}\in\mathcal{X}} \mathrm{IKG}^n(i,\boldsymbol{x})$. Hence, for any $\boldsymbol{x}\in\mathcal{X}$,

$$0 \le \liminf_{n\to\infty} \mathrm{IKG}^n(i,\boldsymbol{x}) \le \liminf_{n\to\infty} \mathrm{IKG}^n(i,\boldsymbol{v}^n) = 0, \tag{39}$$

which completes the proof. □

Before we prove Proposition 2, we need one more technical result about the almost sure convergence of μ_i^n, which is stated in the following Lemma 9. A similar result is also given in Bect et al. (2019, Proposition 2.9), and the proof there directly applies here.

Lemma 9. *If Assumptions 1–3 hold, then for all* $i = 1,\ldots,M$, $\mu_i^n(\boldsymbol{x})$ *converges to* $\mu_i^\infty(\boldsymbol{x}) := \mathbb{E}[\theta_i(\boldsymbol{x})|\mathcal{F}^\infty]$ *uniformly in* $\boldsymbol{x}\in\mathcal{X}$ *a.s. as* $n\to\infty$. *That is,*

$$\mathbb{P}\left\{\omega : \sup_{\boldsymbol{x}\in\mathcal{X}} |\mu_i^n(\boldsymbol{x};\omega) - \mu_i^\infty(\boldsymbol{x};\omega)| \to 0\right\} = 1.$$

Proof of Lemma 9. Fix $i = 1,\ldots,M$. Note that θ_i is a Gaussian process under the prior. It follows from Assumptions 1 and 3 and Theorem 1.4.1 of Adler and Taylor (2007) that the sample paths of θ_i are continuous a.s.. The proof is then completed by directly following the arguments in the proof of Proposition 2.9 in Bect et al. (2019). □

We are now ready to prove Proposition 2.

Proof of Proposition 2. Let $\mu^n := (\mu_1^n,\ldots,\mu_M^n)$ denote the posterior mean of $(\theta_1,\ldots,\theta_M)$ conditioned on $\mathcal{F}^n$. Let ω denote a generic sample path. Fix $i = 1,\ldots,M$. Define

$$\Omega_0 = \{\omega : \eta_i^\infty(\omega) = \infty,\ \mu^n(\boldsymbol{x};\omega) \to \mu^\infty(\boldsymbol{x};\omega) \text{ uniformly in } \boldsymbol{x}\in\mathcal{X} \text{ as } n\to\infty\}.$$

Then, $\mathbb{P}(\Omega_0) = 1$ by the assumption of Proposition 2 and Lemma 9. Fix an arbitrary $\boldsymbol{x}\in\mathcal{X}$. We now prove that, under the IKG policy,

$$k_i^\infty(\boldsymbol{x},\boldsymbol{x};\omega) = 0, \text{ for any } \omega\in\Omega_0, \tag{40}$$

which establishes Proposition 2. We prove eq. (40) by contraction and assume that there exists some $\omega_0\in\Omega_0$ such that $k_i^\infty(\boldsymbol{x},\boldsymbol{x};\omega) > 0$. In the remaining proof, we suppress the sample path ω_0 to simplify notation.

It follows from the continuity of $k_i^0(\boldsymbol{x},\cdot)$ assumed in Assumption 1 and the updating eq. (4) that $k_i^n(\boldsymbol{x},\cdot)$ is continuous. The uniform convergence of $k_i^n(\boldsymbol{x},\cdot)$ by Proposition 1 then implies that $k_i^\infty(\boldsymbol{x},\cdot)$ is also continuous. Hence, there exist $\epsilon > 0$ such that $\min_{\boldsymbol{v}\in\mathcal{B}(\boldsymbol{x},\epsilon)} k_i^\infty(\boldsymbol{x},\boldsymbol{v}) > 0$. The uniform convergence of $k_i^n(\boldsymbol{x},\cdot)$ further implies that there exists $\delta > 0$ such that $k_i^n(\boldsymbol{x},\boldsymbol{v}) \ge \delta$ for all $\boldsymbol{v}\in\mathcal{B}(\boldsymbol{x},\epsilon)$ and $n\ge 1$. By eq. (7),

$$\begin{aligned}\inf_{\boldsymbol{v}\in\mathcal{B}(\boldsymbol{x},\epsilon),n\ge1} \tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x}) &= [k_i^n(\boldsymbol{x},\boldsymbol{x}) + \lambda_i(\boldsymbol{x})]^{-1/2} \inf_{\boldsymbol{v}\in\mathcal{B}(\boldsymbol{x},\epsilon),n\ge1} k_i^n(\boldsymbol{v},\boldsymbol{x}) \\ &\ge \delta[k_i^0(\boldsymbol{x},\boldsymbol{x}) + \lambda_i(\boldsymbol{x})]^{-1/2} := \alpha_1 > 0.\end{aligned}$$

Let $g(s,t) := t\phi(s/t) - s\Phi(-s/t)$; see Lemma 2 for properties of $g(s,t)$, including positivity and monotonicity. Then,

$$|\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})|\phi\left(\left|\frac{\Delta_i^n(\boldsymbol{v})}{\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})}\right|\right) - |\Delta_i^n(\boldsymbol{v})|\Phi\left(-\left|\frac{\Delta_i^n(\boldsymbol{v})}{\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})}\right|\right) = g(|\Delta_i^n(\boldsymbol{v})|, |\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})|) \geq 0,$$

for all $\boldsymbol{v} \in \mathcal{X}$. Consequently, Lemma 1 implies that

$$\mathrm{IKG}^n(i,\boldsymbol{x}) \geq \frac{1}{c_i(\boldsymbol{x})}\int_{\mathcal{B}(\boldsymbol{x},\epsilon)} g(|\Delta_i^n(\boldsymbol{v})|, |\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})|)\gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v} \geq \frac{1}{c_i(\boldsymbol{x})}\int_{\mathcal{B}(\boldsymbol{x},\epsilon)} g(|\Delta_i^n(\boldsymbol{v})|, \alpha_1)\gamma(\boldsymbol{v})\mathrm{d}\boldsymbol{v},$$

for all $n \geq 1$, where the second inequality holds because $g(s,t)$ is strictly increasing in $t \in (0,\infty)$. Note that $\liminf_{n\to\infty} \mathrm{IKG}^n(i,\boldsymbol{x}) = 0$ by Lemma 8. Hence,

$$0 \geq \liminf_{n\to\infty} \frac{1}{c_i(\boldsymbol{x})}\int_{\mathcal{B}(\boldsymbol{x},\epsilon)} g(|\Delta_i^n(\boldsymbol{v})|, \alpha_1)\gamma(\boldsymbol{v})\mathrm{d}\boldsymbol{v} \geq \frac{1}{c_i(\boldsymbol{x})}\int_{\mathcal{B}(\boldsymbol{x},\epsilon)} \liminf_{n\to\infty} g(|\Delta_i^n(\boldsymbol{v})|, \alpha_1)\gamma(\boldsymbol{v})\mathrm{d}\boldsymbol{v}, \quad (41)$$

where the second inequality holds due to Fatou's lemma. Furthermore, since for any $\boldsymbol{v} \in \mathcal{X}$, $\Delta_i^n(\boldsymbol{v}) = \mu_i^n(\boldsymbol{v}) - \max_{a\neq i}\mu_a^n(\boldsymbol{v})$, and $\mu_a^n(\boldsymbol{v}) \to \mu_a^\infty(\boldsymbol{v})$ for $a = 1,\ldots,M$, where $|\mu_a^\infty(\boldsymbol{v})| < \infty$. then

$$\limsup_{n\to\infty} |\Delta_i^n(\boldsymbol{v})| \leq \limsup_{n\to\infty}[2\max_a |\mu_a^n(\boldsymbol{v})|] = 2\max_a |\mu_a^\infty(\boldsymbol{v})| := \alpha_2(\boldsymbol{v}) < \infty,$$

for all $\boldsymbol{v} \in \mathcal{B}(\boldsymbol{x},\epsilon)$. Then, in the light of eq. (41) and the fact that $g(s,t)$ is strictly decreasing in $s \in [0,\infty)$,

$$0 \geq \frac{1}{c_i(\boldsymbol{x})}\int_{\mathcal{B}(\boldsymbol{x},\epsilon)} \liminf_{n\to\infty} g(|\Delta_i^n(\boldsymbol{v})|, \alpha_1)\gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v} \geq \frac{1}{c_i(\boldsymbol{x})}\int_{\mathcal{B}(\boldsymbol{x},\epsilon)} g(\alpha_2(\boldsymbol{v}), \alpha_1)\gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v}\,.$$

This contracts the fact that $g(s,t) > 0$ for all $s \in [0,\infty)$ and $t \in (0,\infty)$. Therefore, eq. (40) is proved. □

D. Proof of Proposition 3

Let $S^n := (\mu_1^n,\ldots,\mu_M^n,k_1^n,\ldots,k_M^n)$ denote the state at time n, which fully determines the posterior distribution of $(\theta_1,\ldots,\theta_M)$ conditioned on $\mathcal{F}^n$. The state transition $S^n \to S^{n+1}$ is governed by eqs. (5) and (6), which is determined by the sampling decision $(a^n,\boldsymbol{v}^n)$.

Let $s := (\mu_1,\ldots,\mu_M,k_1,\ldots,k_M) \in \mathbb{S}$ be a generic state and $\mathbb{S}$ denote the set of states for which μ_i is a continuous function and k_i is a continuous covariance function for each $i = 1,\ldots,M$. For $s \in \mathbb{S}$, define

$$V(s) := \int_{\mathcal{X}} \max_{1\leq a\leq M} \mu_a(\boldsymbol{v})\gamma(\boldsymbol{v})\mathrm{d}\boldsymbol{v},$$

and

$$Q(s,i,\boldsymbol{x}) := \mathbb{E}[V(S^{n+1}) \,|\, S^n = s, a^n = i, \boldsymbol{v}^n = \boldsymbol{x}].$$

By the following Lemma 10, it is easy to see that at time n, the IKG policy (13) chooses

$$\operatorname*{argmax}_{1\le i\le M, \boldsymbol{x}\in\mathcal{X}} [c_i(\boldsymbol{x})]^{-1}[Q(S^n, i, \boldsymbol{x}) - V(S^n)]. \tag{42}$$

Lemma 10. *Fix $s \in \mathbb{S}$, $i = 1, \dots, M$, and $\boldsymbol{x} \in \mathcal{X}$ where $\mathcal{X}$ is compact,*

$$Q(s, i, \boldsymbol{x}) = \int_{\mathcal{X}} \mathbb{E}\left[\max_{1\le a\le M} \mu_a^{n+1}(\boldsymbol{v}) \,\Big|\, S^n = s, a^n = i, \boldsymbol{v}^n = \boldsymbol{x}\right]\gamma(\boldsymbol{v})\mathrm{d}\boldsymbol{v}.$$

Proof of Lemma 10. Notice that by the updating eq. (5), given $S^n = s$, $a^n = i$, $\boldsymbol{v}^n = \boldsymbol{x}$ and Z^{n+1},

$$\max_{1\le a\le M} \mu_a^{n+1}(\boldsymbol{v}) = \max\left\{\mu_i(\boldsymbol{v}) + \tilde{\sigma}_i(\boldsymbol{v}, \boldsymbol{x})Z^{n+1}, \max_{a\ne i} \mu_a(\boldsymbol{v})\right\}.$$

Let $f\big(s, i, \boldsymbol{x}, \boldsymbol{v}, Z^{n+1}\big) = \max_{1\le a\le M} \mu_a^{n+1}(\boldsymbol{v}) - \max_{a\ne i} \mu_a(\boldsymbol{v})$. Then $f\big(s, i, \boldsymbol{x}, \boldsymbol{v}, Z^{n+1}\big) \ge 0$, for all $\boldsymbol{v} \in \mathcal{X}$ and Z^{n+1}. Hence,

$$\begin{aligned}
Q(s, i, \boldsymbol{x}) &= \mathbb{E}\left[\int_{\mathcal{X}} \max_{1\le a\le M} \mu_a^{n+1}(\boldsymbol{v})\gamma(\boldsymbol{v})\mathrm{d}\boldsymbol{v} \,\Big|\, S^n = s, a^n = i, \boldsymbol{v}^n = \boldsymbol{x}\right] \\
&= \mathbb{E}\left[\int_{\mathcal{X}} \Big(f\big(s, i, \boldsymbol{x}, \boldsymbol{v}, Z^{n+1}\big) + \max_{a\ne i} \mu_a(\boldsymbol{v})\Big)\gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v}\right] \\
&= \mathbb{E}\left[\int_{\mathcal{X}} f\big(s, i, \boldsymbol{x}, \boldsymbol{v}, Z^{n+1}\big)\gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v}\right] + \int_{\mathcal{X}} \max_{a\ne i} \mu_a(\boldsymbol{v})\gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v} \\
&= \int_{\mathcal{X}} \mathbb{E}\left[f\big(s, i, \boldsymbol{x}, \boldsymbol{v}, Z^{n+1}\big)\right]\gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v} + \int_{\mathcal{X}} \max_{a\ne i} \mu_a(\boldsymbol{v})\gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v}\,,
\end{aligned}$$

where the interchange of integral and expectation is justified by Tonelli's theorem for nonnegative functions, and $\int_{\mathcal{X}} \max_{a\ne i} \mu_a(\boldsymbol{v})\gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v}$ is finite since $\mu_i(\boldsymbol{v})$ is continuous on the compact set $\mathcal{X}$ for $i = 1, \dots, M$. Thus the result in Lemma 10 follows immediately. □

Lemma 11. *Fix $s \in \mathbb{S}$, $i = 1, \dots, M$, and $\boldsymbol{x} \in \mathcal{X}$ where $\mathcal{X}$ is compact and $\alpha(\cdot) > 0$ on $\mathcal{X}$. Then, $Q(s, i, \boldsymbol{x}) \ge V(s)$ and the equality holds if and only if $k_i(\boldsymbol{x}, \boldsymbol{x}) = 0$.*

Proof of Lemma 11. Applying Lemma 10 and the updating eq. (5),

$$\begin{aligned}
Q(s, i, \boldsymbol{x}) &= \int_{\mathcal{X}} \mathbb{E}\left[\max\left\{\mu_i(\boldsymbol{v}) + \tilde{\sigma}_i(\boldsymbol{v}, \boldsymbol{x})Z^{n+1}, \max_{a\ne i} \mu_a(\boldsymbol{v})\right\}\right]\gamma(\boldsymbol{v})\,\mathrm{d}\boldsymbol{v} \\
&\ge \int_{\mathcal{X}} \max\left\{\mathbb{E}\left[\mu_i(\boldsymbol{v}) + \tilde{\sigma}_i(\boldsymbol{v}, \boldsymbol{x})Z^{n+1}\right], \max_{a\ne i} \mu_a(\boldsymbol{v})\right\}\gamma(\boldsymbol{v})\mathrm{d}\boldsymbol{v} \qquad (43) \\
&= \int_{\mathcal{X}} \max_{1\le a\le M} \mu_a(\boldsymbol{v})\gamma(\boldsymbol{v})\mathrm{d}\boldsymbol{v} = V(s),
\end{aligned}$$

where eq. (43) follows from Jensen's inequality since $\max(\cdot, \cdot)$ is a strictly convex function.

If $k_i(\boldsymbol{x},\boldsymbol{x})=0$, then in the light of the fact that k_i is a covariance function, we must have that

$$|k_i(\boldsymbol{v},\boldsymbol{x})| \le \sqrt{k_i(\boldsymbol{v},\boldsymbol{v})k_i(\boldsymbol{x},\boldsymbol{x})}=0,$$

so $k_i(\boldsymbol{v},\boldsymbol{x})=0$ for all $\boldsymbol{v}\in\mathcal{X}$. Hence, $\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})=0$ by eq. (7), so $\mu_a^{n+1}(\boldsymbol{v})=\mu_a^n(\boldsymbol{v})$ for all $a=1,\dots,M$ and $\boldsymbol{v}\in\mathcal{X}$. Hence, $\mu_a^{n+1}(\boldsymbol{v})$ is deterministic given S^n for all $a=1,\dots,M$ and $\boldsymbol{v}\in\mathcal{X}$. Thus, the inequality eq. (43) holds with equality.

Next, assume conversely that $Q(s,i,\boldsymbol{x})=V(s)$. If $k_i(\boldsymbol{x},\boldsymbol{x})\neq 0$, then the continuity of k_i implies that $k_i(\boldsymbol{v},\boldsymbol{x})\neq 0$ for all $\boldsymbol{v}\in\tilde{\mathcal{X}}$, where $\tilde{\mathcal{X}}\subset\mathcal{X}$ is an open neighborhood of $\boldsymbol{x}$. Without loss of generality, we assume that for all $\boldsymbol{v}\in\tilde{\mathcal{X}}$, $k_i(\boldsymbol{v},\boldsymbol{x})>0$ and thus, $\tilde{\sigma}_i(\boldsymbol{v},\boldsymbol{x})=k_i(\boldsymbol{v},\boldsymbol{x})/\sqrt{k_i(\boldsymbol{x},\boldsymbol{x})+\lambda_i(\boldsymbol{x})}>0$. By the strict convexity of $\max(\cdot,\cdot)$ and Jensen's inequality,

$$\mathbb{E}\left[\max\left\{\mu_i(\boldsymbol{v})+\tilde{\sigma}_i(\boldsymbol{v},\boldsymbol{x})Z^{n+1},\max_{a\neq i}\mu_a(\boldsymbol{v})\right\}\right]>\max\left\{\mathbb{E}\left[\mu_i(\boldsymbol{v})+\tilde{\sigma}_i(\boldsymbol{v},\boldsymbol{x})Z^{n+1}\right],\max_{a\neq i}\mu_a(\boldsymbol{v})\right\},$$

for $\boldsymbol{v}\in\tilde{\mathcal{X}}$. Hence, eq. (43) becomes a strict inequality since $\gamma(\boldsymbol{v})>0$ for all $\boldsymbol{v}\in\mathcal{X}$. This contradicts $Q(s,i,\boldsymbol{x})=V(s)$, so $k_i(\boldsymbol{x},\boldsymbol{x})=0$. □

Lemma 12. *Fix $i=1,\dots,M$. If Assumptions 1 and 3 hold, and $k_i^\infty(\boldsymbol{x},\boldsymbol{x})=0$ for some $\boldsymbol{x}\in\mathcal{X}$, then $\eta_i^\infty=\infty$.*

Proof of Lemma 12. We prove by contradiction and assume that $\eta_i^\infty<\infty$. Then, $N_i:=\min\{n:\eta_i^n=\eta_i^\infty\}<\infty$ and $a^n\neq i$ for all $n\ge N_i$. Due to the mutual independence between the alternatives, it follows that the posterior distribution of θ_i remains the same for $n\ge N_i$. In particular, $k_i^n(\boldsymbol{x},\boldsymbol{x})=k_i^{N_i}(\boldsymbol{x},\boldsymbol{x})$ for all $n>N_i$. Hence, $k_i^{N_i}(\boldsymbol{x},\boldsymbol{x})=k_i^\infty(\boldsymbol{x},\boldsymbol{x})=0$. It follows from eq. (6) that

$$k_i^{N_i-1}(\boldsymbol{x},\boldsymbol{x})=k_i^{N_i}(\boldsymbol{x},\boldsymbol{x})+\left[\sigma_i^{N_i-1}(\boldsymbol{x},\boldsymbol{v}^{N_i-1})\right]^2=\left[\sigma_i^{N_i-1}(\boldsymbol{x},\boldsymbol{v}^{N_i-1})\right]^2.$$

By the definition of N_i, $a^{N_i-1}=i$. Then by eq. (7),

$$k_i^{N_i-1}(\boldsymbol{x},\boldsymbol{x})=\frac{\left[k_i^{N_i-1}(\boldsymbol{x},\boldsymbol{v}^{N_i-1})\right]^2}{k_i^{N_i-1}(\boldsymbol{v}^{N_i-1},\boldsymbol{v}^{N_i-1})+\lambda_i(\boldsymbol{v}^{N_i-1})}. \tag{44}$$

Notice that

$$\begin{aligned}
[k_i^{N_i-1}(\boldsymbol{x},\boldsymbol{v}^{N_i-1})]^2 &= \left\{\mathrm{Cov}^{N_i-1}\left[\theta_i(\boldsymbol{x}),\theta_i(\boldsymbol{v}^{N_i-1})\right]\right\}^2\\
&\le \mathrm{Var}^{N_i-1}[\theta_i(\boldsymbol{x})]\,\mathrm{Var}^{N_i-1}[\theta_i(\boldsymbol{v}^{N_i-1})]\\
&= k_i^{N_i-1}(\boldsymbol{x},\boldsymbol{x})k_i^{N_i-1}(\boldsymbol{v}^{N_i-1},\boldsymbol{v}^{N_i-1}).
\end{aligned} \tag{45}$$

It follows from eqs. (44) and (45) that $\lambda_i(\boldsymbol{v}^{N_i-1})k_i^{N_i-1}(\boldsymbol{x},\boldsymbol{x})\le 0$. Thus, $k_i^{N_i-1}(\boldsymbol{x},\boldsymbol{x})=0$, since $k_i^{N_i-1}(\boldsymbol{x},\boldsymbol{x})\ge 0$ and $\lambda_i(\boldsymbol{v}^{N_i-1})>0$ in Assumption 3. By induction, we can conclude that $k_i^0(\boldsymbol{x},\boldsymbol{x})=0$, which contracts the fact that $k_i^0(\boldsymbol{x},\boldsymbol{x})=\tau_i^2>0$ in Assumption 1. Therefore, we must have $\eta_i^\infty=\infty$. □

We are now ready to prove Proposition 3.

Proof of Proposition 3. Define $\Omega_1 := \{\omega : S^n(\omega) \to S^\infty(\omega) \text{ pointwise as } n \to \infty\}$. By Lemma 9 and Proposition 1, $\mathbb{P}(\Omega_1) = 1$. For any $i = 1, \dots, M$, define the event $\mathsf{H}_i := \{\omega : \eta_i^\infty(\omega) < \infty\}$. Then, $k_i^\infty(\boldsymbol{x}, \boldsymbol{x}; \omega) > 0$ for all $\boldsymbol{x} \in \mathcal{X}$ and $\omega \in \mathsf{H}_i$ by Lemma 12. On the other hand, Proposition 2 implies that $k_i^\infty(\boldsymbol{x}, \boldsymbol{x}; \omega) = 0$ for all $\boldsymbol{x} \in \mathcal{X}$ and $\omega \in \mathsf{H}_i^\mathsf{c} \cap \Omega_1$, where H_i^c is the complement of H_i. Thus, by Lemma 11,

$$\begin{aligned} Q(S^\infty(\omega), i, \boldsymbol{x}) &> V(S^\infty(\omega)), \quad \text{for all } \omega \in \mathsf{H}_i \cap \Omega_1, \\ Q(S^\infty(\omega), i, \boldsymbol{x}) &= V(S^\infty(\omega)), \quad \text{for all } \omega \in \mathsf{H}_i^\mathsf{c} \cap \Omega_1. \end{aligned} \tag{46}$$

Further, for any subset $A \subseteq \{1, \dots, M\}$, define the event

$$\mathsf{H}_A := \{\cap_{i \in A} \mathsf{H}_i\} \cap \{\cap_{i \notin A} \mathsf{H}_i^\mathsf{c}\}.$$

Choose any $A \neq \emptyset$. When $A = \{1, \dots, M\}$, $\mathsf{H}_A = \emptyset$, because it is impossible that all alternative have finite samples while $n \to \infty$. So $\mathsf{H}_A \cap \Omega_1 = \emptyset$. When $A \neq \{1, \dots, M\}$, we prove $\mathsf{H}_A \cap \Omega_1 = \emptyset$ by contradiction. Suppose that $\mathsf{H}_A \cap \Omega_1 \neq \emptyset$ so that we can choose and fix a sample path $\omega_0 \in \mathsf{H}_A \cap \Omega_1$. Then, $\eta_i^\infty(\omega_0) < \infty$ for all $i \in A$. Hence, there exists $T_i(\omega_0) < \infty$ for all $i \in A$ such that the IKG policy does not choose alternative i for $n > T_i(\omega_0)$. Let $T(\omega_0) := \max_{i \in A} T_i(\omega_0)$. Then, $T(\omega_0) < \infty$ and the IKG policy does not choose $i \in A$ for $n > T(\omega_0)$. On the other hand, it follows from eq. (46) that for all $i \in A$, $i' \notin A$, and $\boldsymbol{x} \in \mathcal{X}$,

$$Q(S^\infty(\omega_0), i, \boldsymbol{x}) - V(S^\infty(\omega_0)) > Q(S^\infty(\omega_0), i', \boldsymbol{x}) - V(S^\infty(\omega_0)) = 0.$$

Let $Q^\dagger(s, i, \boldsymbol{x}) := Q(s, i, \boldsymbol{x}) - V(s)$ for simplicity. Then, by virtue of the compactness of $\mathcal{X}$ and the positivity of $c_i(\boldsymbol{x})$,

$$\max_{\boldsymbol{x} \in \mathcal{X}} [c_i(\boldsymbol{x})]^{-1} Q^\dagger(S^\infty(\omega_0), i, \boldsymbol{x}) > \max_{\boldsymbol{x} \in \mathcal{X}} [c_{i'}(\boldsymbol{x})]^{-1} Q^\dagger(S^\infty(\omega_0), i', \boldsymbol{x}) = 0,$$

for all $i \in A$ and $i' \notin A$. Hence,

$$\min_{i \in A} \max_{\boldsymbol{x} \in \mathcal{X}} [c_i(\boldsymbol{x})]^{-1} Q^\dagger(S^\infty(\omega_0), i, \boldsymbol{x}) > \max_{i' \notin A} \max_{\boldsymbol{x} \in \mathcal{X}} [c_{i'}(\boldsymbol{x})]^{-1} Q^\dagger(S^\infty(\omega_0), i', \boldsymbol{x}) = 0. \tag{47}$$

Notice that $S^n(\omega_0) \to S^\infty(\omega_0)$ pointwise as $n \to \infty$ since $\omega_0 \in \Omega_1$. Hence, there exists a finite number $\tilde{n}(\omega_0) > T(\omega_0)$ such that

$$\min_{i \in A} \max_{\boldsymbol{x} \in \mathcal{X}} [c_i(\boldsymbol{x})]^{-1} Q^\dagger(S^{\tilde{n}(\omega_0)}(\omega_0), i, \boldsymbol{x}) > \max_{i' \notin A} \max_{\boldsymbol{x} \in \mathcal{X}} [c_{i'}(\boldsymbol{x})]^{-1} Q^\dagger(S^{\tilde{n}(\omega_0)}(\omega_0), i', \boldsymbol{x}),$$

which implies that IKG policy must choose alternative $i \in A$ at time $\tilde{n}(\omega_0)$ by eq. (42). This contradicts the definition of $T(\omega_0)$. Therefore, the event $\mathsf{H}_A \cap \Omega_1$ must be empty for any nonempty $A \subseteq \{1, \dots, M\}$.

It then follows immediately that $\mathbb{P}(\mathsf{H}_A) = 0$ for any nonempty $A \subseteq \{1, \dots, M\}$, since $\mathbb{P}(\Omega_1) = 1$. Notice that the whole sample space $\Omega = \cup_{A \subseteq \{1, \dots, M\}} \mathsf{H}_A$. Hence,

$$1 = \mathbb{P}(\mathsf{H}_\emptyset) = \mathbb{P}\left(\cap_{i=1}^M \mathsf{H}_i^\mathsf{c}\right) = \mathbb{P}\left(\{\omega : \eta_i^\infty = \infty \text{ for all } i = 1, \dots, M\}\right),$$

which completes the proof. □

E. Proof of Theorem 2

Part (i) is an immediate consequence of Propositions 2 and 3. The other two parts follow closely the proof of similar results in Theorem 1 of Xie et al. (2016).

For part (ii), fix an arbitrary $\boldsymbol{x} \in \mathcal{X}$. Note that for each $i = 1, \ldots, M$,

$$\mathbb{E}[(\mu_i^n(\boldsymbol{x}) - \theta_i(\boldsymbol{x}))^2] = \mathbb{E}[\mathbb{E}^n[(\mu_i^n(\boldsymbol{x}) - \theta_i(\boldsymbol{x}))^2]] = \mathbb{E}[k_i^n(\boldsymbol{x}, \boldsymbol{x})] \to \mathbb{E}[k_i^\infty(\boldsymbol{x}, \boldsymbol{x})] = 0,$$

as $n \to \infty$, where the convergence holds due to the fact that $0 \le k_i^n(\boldsymbol{x}, \boldsymbol{x}) \le k_i^0(\boldsymbol{x}, \boldsymbol{x})$ from eq. (8) and the dominated convergence theorem. This asserts that $\mu_i^n(\boldsymbol{x}) \to \theta_i(\boldsymbol{x})$ in L^2. By Lemma 9, $\mu_i^n(\boldsymbol{x}) \to \mu_i^\infty(\boldsymbol{x})$ a.s., which implies that $\theta_i(\boldsymbol{x}) = \mu_i^\infty(\boldsymbol{x})$ a.s., due to the a.s. uniqueness of convergence in probability. Thus, $\mu_i^n(\boldsymbol{x}) \to \theta_i(\boldsymbol{x})$ a.s. as $n \to \infty$.

For part (iii), let us again fix $\boldsymbol{x} \in \mathcal{X}$. Let $i^*(\boldsymbol{x}) \in \operatorname{argmax}_i \theta_i(\boldsymbol{x})$. We now show that $\operatorname{argmax}_i \mu_i^n(\boldsymbol{x}) \to i^*(\boldsymbol{x})$ a.s. as $n \to \infty$. Again, we let ω denote a generic sample path and use notations like $i^*(\boldsymbol{x}; \omega)$ to emphasize the dependence on ω. Let $\epsilon(\boldsymbol{x}; \omega) := \theta_{i^*(\boldsymbol{x},\omega)}(\boldsymbol{x}; \omega) - \max_{a \ne i^*(\boldsymbol{x},\omega)} \theta_a(\boldsymbol{x}; \omega)$. Then, $\mathbb{P}(\{\omega : \epsilon(\boldsymbol{x}; \omega) > 0\}) = 1$ because $(\theta_1(\boldsymbol{x}; \omega), \ldots, \theta_M(\boldsymbol{x}; \omega))$ is a realization of a multivariate normal random variable under the prior distribution. Hence, the event $\tilde{\Omega} := \{\omega : \epsilon(\boldsymbol{x}; \omega) > 0$ and $\mu_i^n(\boldsymbol{x}; \omega) \to \theta_i(\boldsymbol{x}; \omega)$ for all $i = 1, \ldots, M\}$ occurs with probability 1. Fix an arbitrary $\tilde{\omega} \in \tilde{\Omega}$. To complete the proof, it suffices to show that $\operatorname{argmax}_i \mu_i^n(\boldsymbol{x}; \tilde{\omega}) \to i^*(\boldsymbol{x}; \tilde{\omega})$ as $n \to \infty$.

Clearly, there exists $N(\tilde{\omega}) < \infty$ such that $|\mu_i^n(\boldsymbol{x}; \tilde{\omega}) - \theta_i(\boldsymbol{x}; \tilde{\omega})| < \epsilon(\boldsymbol{x}; \tilde{\omega})/2$ for all $n > N(\tilde{\omega})$ and $i = 1, \ldots, M$. Hence, for all $i \ne i^*(\boldsymbol{x}; \tilde{\omega})$ and $n \ge N(\tilde{\omega})$,

$$\mu_{i^*(\boldsymbol{x};\tilde{\omega})}^n(\boldsymbol{x}; \tilde{\omega}) > \theta_{i^*(\boldsymbol{x};\tilde{\omega})}(\boldsymbol{x}; \tilde{\omega}) - \frac{\epsilon(\boldsymbol{x}; \tilde{\omega})}{2} \ge \theta_i(\boldsymbol{x}; \tilde{\omega}) + \frac{\epsilon(\boldsymbol{x}; \tilde{\omega})}{2} > \mu_i^n(\boldsymbol{x}; \tilde{\omega}).$$

This implies that $i^*(\boldsymbol{x}; \tilde{\omega}) = \operatorname{argmax}_i \mu_i^n(\boldsymbol{x}; \tilde{\omega})$ for all $n > N(\tilde{\omega})$, and thus $\operatorname{argmax}_i \mu_i^n(\boldsymbol{x}; \tilde{\omega}) \to i^*(\boldsymbol{x}; \tilde{\omega})$ as $n \to \infty$. □

F. Proof of Theorem 3

The steps to prove Theorem 3 are exactly the same to those for Theorem 2, and we only need to modify the arguments related to the actual sampling decision (which is $(a^n, \boldsymbol{v}^n)$ satisfies eq. (13) in the IKG policy, and $(\tilde{a}^n, \tilde{\boldsymbol{v}}^n)$ satisfies eq. (15) in the quasi-IKG policy). So, we will not repeat the entire proofs, but only point out the modification briefly. Specifically, the two main steps to prove Theorem 3 are summarized as the following Propositions 4 and 5, which are parallel to Propositions 2 and 3.

Proposition 4. *Fix $i = 1, \ldots, M$. If Assumptions 1–3 hold and $\eta_i^\infty = \infty$ a.s., then for any $\boldsymbol{x} \in \mathcal{X}$, $k_i^\infty(\boldsymbol{x}, \boldsymbol{x}) = 0$ a.s. under the quasi-IKG policy.*

Proof of Proposition 4. All the intermediate lemmas for Proposition 2 directly apply to Proposition 4, except for Lemma 8. Instead, we now need to show that under the quasi-IKG policy, for any $\boldsymbol{x} \in \mathcal{X}$,

$\liminf_{n\to\infty} \mathrm{IKG}^n(i, \boldsymbol{x}) = 0$. We first observe that, for the sequence $\{\tilde{\boldsymbol{v}}^n \in \mathcal{X} : \tilde{a}^n = i, n = 0, 1, \ldots, \}$, we can still show $\liminf_{n\to\infty} \mathrm{IKG}^n(i, \tilde{\boldsymbol{v}}^n) = 0$ with the same arguments. Then, by the definition of the quasi-IKG policy (15),

$$\mathrm{IKG}^n(i, \tilde{\boldsymbol{v}}^n) = \mathrm{IKG}^n(\tilde{a}^n, \tilde{\boldsymbol{v}}^n) \geq \mathrm{IKG}^n(a^n, \boldsymbol{v}^n) - \varepsilon_n \geq \mathrm{IKG}^n(i, \boldsymbol{v}^n) - \varepsilon_n.$$

On the other hand, since $\mathrm{IKG}^n(i, \boldsymbol{v}^n) = \max_{\boldsymbol{x}\in\mathcal{X}} \mathrm{IKG}^n(i, \boldsymbol{x})$, then for any $\boldsymbol{x} \in \mathcal{X}$, eq. (39) is replaced by

$$0 \leq \liminf_{n\to\infty} \mathrm{IKG}^n(i, \boldsymbol{x}) \leq \liminf_{n\to\infty} \mathrm{IKG}^n(i, \boldsymbol{v}^n) \leq \liminf_{n\to\infty} [\mathrm{IKG}^n(i, \tilde{\boldsymbol{v}}^n) + \varepsilon_n] = 0,$$

where the equality is due to $\liminf_{n\to\infty} \mathrm{IKG}^n(i, \tilde{\boldsymbol{v}}^n) = 0$ and $\varepsilon_n \to 0$. Finally, the proof of Proposition 4 follows the similar arguments as in the proof of Proposition 2. □

Proposition 5. *If Assumptions 1–3 hold, then $\eta_i^\infty = \infty$ a.s. for each $i = 1, \ldots, M$ under the quasi-IKG policy.*

Proof of Proposition 5. All the intermediate lemmas for Proposition 3 directly apply to Proposition 5. We then proceed by following the same arguments as in the proof Proposition 3, with $T_i(\omega_0)$ meaning that the quasi-IKG policy does not choose alternative i for $n > T_i(\omega_0)$. After we obtain eq. (47), we now want to show that quasi-IKG policy must choose alternative $i \in A$ at some time $\tilde{n}(\omega_0) > T(\omega_0)$, which leads to the contradiction.

Due to eq. (47), there exists some small $\Delta > 0$ such that

$$\min_{i\in A} \max_{\boldsymbol{x}\in\mathcal{X}} [c_i(\boldsymbol{x})]^{-1} Q^\dagger(S^\infty(\omega_0), i, \boldsymbol{x}) - \Delta > \max_{i'\notin A} \max_{\boldsymbol{x}\in\mathcal{X}} [c_{i'}(\boldsymbol{x})]^{-1} Q^\dagger(S^\infty(\omega_0), i', \boldsymbol{x}) = 0.$$

Notice that $S^n(\omega_0) \to S^\infty(\omega_0)$ pointwise as $n \to \infty$ since $\omega_0 \in \Omega_1$. Hence, there exists a finite number $\tilde{n}_1(\omega_0) > T(\omega_0)$ such that

$$\min_{i\in A} \max_{\boldsymbol{x}\in\mathcal{X}} [c_i(\boldsymbol{x})]^{-1} Q^\dagger(S^n, i, \boldsymbol{x}) - \Delta/2 > \max_{i'\notin A} \max_{\boldsymbol{x}\in\mathcal{X}} [c_{i'}(\boldsymbol{x})]^{-1} Q^\dagger(S^n, i', \boldsymbol{x}), \tag{48}$$

for all $n \geq \tilde{n}_1(\omega_0)$. Since $\varepsilon_n \to 0$ as $n \to \infty$, there exists a finite number $\tilde{n}_2(\omega_0) > T(\omega_0)$ such that $\varepsilon_n < \Delta/2$ for all $n \geq \tilde{n}_2(\omega_0)$. Then, we can conclude that at time $\tilde{n}(\omega_0) := \max(\tilde{n}_1(\omega_0), \tilde{n}_2(\omega_0)) > T(\omega_0)$, quasi-IKG policy must choose alternative $i \in A$. Otherwise, for $n = \tilde{n}(\omega_0)$, if $\tilde{a}^n \notin A$, then by eqs. (42) and (48),

$$\mathrm{IKG}^n(\tilde{a}^n, \tilde{\boldsymbol{v}}^n) < \mathrm{IKG}^n(a^n, \boldsymbol{v}^n) - \Delta/2 < \mathrm{IKG}^n(a^n, \boldsymbol{v}^n) - \varepsilon_n,$$

which violates the definition of quasi-IKG policy defined in eq. (15). □

G. Gradient Calculation

It is easy to see that

$$g_i^n(\boldsymbol{v}, \boldsymbol{x}) = \frac{\partial[h_i^n(\boldsymbol{v}, \boldsymbol{x})/c_i(\boldsymbol{x})]}{\partial \boldsymbol{x}} = \frac{\frac{\partial h_i^n(\boldsymbol{v},\boldsymbol{x})}{\partial \boldsymbol{x}} c_i(\boldsymbol{x}) - h_i^n(\boldsymbol{v}, \boldsymbol{x}) \frac{\mathrm{d}c_i(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}}}{[c_i(\boldsymbol{x})]^2},$$

$$\frac{\partial h_i^n(\boldsymbol{v},\boldsymbol{x})}{\partial \boldsymbol{x}} = \begin{cases} \phi\left(\left|\frac{\Delta_i^n(\boldsymbol{v})}{\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})}\right|\right)\frac{\partial \tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})}{\partial \boldsymbol{x}}, & \text{if } \tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x}) > 0,\\ 0, & \text{if } \tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x}) = 0,\\ -\phi\left(\left|\frac{\Delta_i^n(\boldsymbol{v})}{\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})}\right|\right)\frac{\partial \tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})}{\partial \boldsymbol{x}}, & \text{if } \tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x}) < 0, \end{cases}$$

and that, by the definition of $\tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})$ in eq. (7) and Assumptions 1 and 3,

$$\frac{\partial \tilde{\sigma}_i^n(\boldsymbol{v},\boldsymbol{x})}{\partial \boldsymbol{x}} = [k_i^n(\boldsymbol{x},\boldsymbol{x})+\lambda_i(\boldsymbol{x})]^{-\frac{1}{2}}\frac{\partial k_i^n(\boldsymbol{v},\boldsymbol{x})}{\partial \boldsymbol{x}} - \frac{[k_i^n(\boldsymbol{x},\boldsymbol{x})+\lambda_i(\boldsymbol{x})]^{-\frac{3}{2}}k_i^n(\boldsymbol{v},\boldsymbol{x})}{2}\left[\frac{\mathrm{d}k_i^n(\boldsymbol{x},\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}} + \frac{\mathrm{d}\lambda_i(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}}\right], \tag{49}$$

provided that the prior correlation function ρ_i and the cost function c_i are both differentiable. Assuming ρ_i to be differentiable excludes some covariance functions that satisfy Assumption 1 such as the Matérn(ν) type with $\nu = 1/2$, but many others including both the Matérn(ν) type with $\nu > 1$ and the SE type do have the desired differentiability. We next calculate analytically the derivatives of $k_i^n(\cdot,\cdot)$ in eq. (49) for several common covariance functions. The calculation is a routine exercise so we omit the details.

Throughout the subsequent Examples 1–3, we use the following notation. For $i = 1,\dots,M$,

$$\boldsymbol{\alpha}_i := (\alpha_{i,1},\dots,\alpha_{i,d})^\intercal \quad \text{and} \quad r_i(\boldsymbol{x},\boldsymbol{x}') := \sqrt{\sum_{j=1}^d \alpha_{i,j}(x_j - x_j')^2}.$$

Recall that $\boldsymbol{V}_i^n$ denotes the set of locations of the samples taken from θ_i up to time n. With slight abuse of notation, here we treat $\boldsymbol{V}_i^n$ as a matrix wherein the columns are corresponding to the points in the set and arranged in the order of appearance. Moreover, for notational simplicity, let $\boldsymbol{V}_i^n := (\boldsymbol{v}_1,\dots,\boldsymbol{v}_{m_i^n})$, where m_i^n is the number of columns of $\boldsymbol{V}_i^n$. Let $\boldsymbol{X}$ be a matrix with the same dimension as $\boldsymbol{V}_i^n$ and all columns are identically $\boldsymbol{x}$. We adopt the denominator layout for matrix calculus. For the following Examples 1–3, it can be shown that

$$\frac{\partial k_i^n(\boldsymbol{v},\boldsymbol{x})}{\partial \boldsymbol{x}} = \operatorname{diag}(\boldsymbol{\alpha}_i)(\boldsymbol{x}-\boldsymbol{v})a_0 - \boldsymbol{A}k_i^0(\boldsymbol{V}_i^n,\boldsymbol{v}), \tag{50}$$

$$\frac{\mathrm{d}k_i^n(\boldsymbol{x},\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}} = -2\boldsymbol{A}k_i^0(\boldsymbol{V}_i^n,\boldsymbol{x}), \tag{51}$$

where

$$\boldsymbol{A} := \operatorname{diag}(\boldsymbol{\alpha}_i)(\boldsymbol{X}-\boldsymbol{V}_i^n)\operatorname{diag}\{a_1,\dots,a_{m_i^n}\}[k_i^0(\boldsymbol{V}_i^n,\boldsymbol{V}_i^n)+\lambda_i\boldsymbol{I}]^{-1},$$

while the values of $a_0, a_1,\dots,a_{m_i^n}$ depend on the choice of the covariance function.

Example 1 (SE). Let $k_i^0(\boldsymbol{x},\boldsymbol{x}') = \tau_i^2\exp\left(-r_i^2(\boldsymbol{x},\boldsymbol{x}')\right)$. Then, in eqs. (50) and (51), $a_0 := -2k_i^0(\boldsymbol{v},\boldsymbol{x})$ and $a_\ell := -2k_i^0(\boldsymbol{v}_\ell,\boldsymbol{x})$, for $\ell = 1,\dots,m_i^n$.

Example 2 (Matérn(3/2)). Let $k_i^0(\boldsymbol{x},\boldsymbol{x}') = \tau_i^2\left(1+\sqrt{3}r_i(\boldsymbol{x},\boldsymbol{x}')\right)\exp\left(-\sqrt{3}r_i(\boldsymbol{x},\boldsymbol{x}')\right)$. Then, in eqs. (50) and (51),

$$a_\ell := \sqrt{3}r_i^{-1}(\boldsymbol{v}_\ell,\boldsymbol{x})\Big[\tau_i^2\exp\Big(-\sqrt{3}r_i(\boldsymbol{v}_\ell,\boldsymbol{x})\Big) - k_i^0(\boldsymbol{v}_\ell,\boldsymbol{x})\Big],$$

for $\ell = 0,1,\dots,m_i^n$ and $\boldsymbol{v}_0 = \boldsymbol{v}$.

Example 3 (Matérn(5/2)). Let $k_i^0(\boldsymbol{x},\boldsymbol{x}') = \tau_i^2\big(1+\sqrt{5}r_i(\boldsymbol{x},\boldsymbol{x}')+\frac{5}{3}r_i^2(\boldsymbol{x},\boldsymbol{x}')\big)\exp\big(-\sqrt{5}r_i(\boldsymbol{x},\boldsymbol{x}')\big)$. Then, in eqs. (50) and (51),

$$a_\ell := \left(\sqrt{5}r_i^{-1}(\boldsymbol{v}_\ell,\boldsymbol{x})+\tfrac{10}{3}\right)\tau_i^2\exp\left(-\sqrt{5}r_i(\boldsymbol{v}_\ell,\boldsymbol{x})\right) - \sqrt{5}r_i^{-1}(\boldsymbol{v}_\ell,\boldsymbol{x})k_i^0(\boldsymbol{v}_\ell,\boldsymbol{x}),$$

for $\ell = 0,1,\ldots,m_i^n$ and $\boldsymbol{v}_0=\boldsymbol{v}$.

H. Implementation Issues

A plain-vanilla implementation of $\widehat{\mathrm{IKG}}^n(i,\boldsymbol{x})$ in eq. (18) may encounter rounding errors, since $h_i^n(\boldsymbol{\xi}_j,\boldsymbol{x})$ may be rounded to zero when evaluated via eq. (16); see Frazier et al. (2009) for discussion on a similar issue. To enhance numerical stability, we first evaluate the logarithm of the summand and then do exponentiation. For notational simplicity, we set

$$u_j := |\Delta_i^n(\boldsymbol{\xi}_j)/\tilde{\sigma}_i^n(\boldsymbol{\xi}_j,\boldsymbol{x})| \quad \text{and} \quad h_i^n(\boldsymbol{\xi}_j,\boldsymbol{x}) = |\tilde{\sigma}_i^n(\boldsymbol{\xi}_j,\boldsymbol{x})|[\phi(u_j)-u_j\Phi(-u_j)].$$

If $\tilde{\sigma}_i^n(\boldsymbol{\xi}_j,\boldsymbol{x})\neq 0$, we compute

$$g_j := \log\left(\frac{h_i^n(\boldsymbol{\xi}_j,\boldsymbol{x})}{J}\right) = \log\left(\frac{|\tilde{\sigma}_i^n(\boldsymbol{\xi}_j,\boldsymbol{x})|}{\sqrt{2\pi}J}\right) - \frac{1}{2}u_j^2 + \log\left(1-u_j\frac{\Phi(-u_j)}{\phi(u_j)}\right),$$

where $\Phi(-u_j)/\phi(u_j)$ is known as the Mills ratio, and can be asymptotically approximated by $u_j/(u_j^2+1)$ for large u_j. Moreover, $\log(1+x)$ can be accurately computed by `log1p` function available in most numerical software packages. At last, we compute

$$\log\widehat{\mathrm{IKG}}^n(i,\boldsymbol{x}) = \log\sum_{j\in\mathcal{J}}e^{g_j} - \log(c_i(\boldsymbol{x})) = g^* + \log\sum_{j\in\mathcal{J}}e^{g_j-g^*} - \log(c_i(\boldsymbol{x})),$$

where $\mathcal{J}:=\{j:\tilde{\sigma}_i^n(\boldsymbol{\xi}_j,\boldsymbol{x})\neq 0,\ j=1,\ldots,J\}$, and $g^*=\max_{j\in\mathcal{J}} g_j$; we set $\log\widehat{\mathrm{IKG}}_\gamma^n(i,\boldsymbol{x})=-\infty$ if $\mathcal{J}$ is empty. The above procedure is summarized in Algorithm 1.

In the implementation of SGA, we adopt two well-known modifications.

(i) We use *mini-batch* SGA to have more productive iterations. Specifically, in each iteration eq. (19), instead of using a single $g_i^n(\boldsymbol{\xi}_k,\boldsymbol{x}_k)$ as the gradient estimate, we use the average of m independent estimates $g_i^n(\boldsymbol{\xi}_{k1},\boldsymbol{x}_k),\ldots,g_i^n(\boldsymbol{\xi}_{km},\boldsymbol{x}_k)$, which is denoted as $\bar{g}_i^n(\boldsymbol{\xi}_{k1},\ldots,\boldsymbol{\xi}_{km},\boldsymbol{x}_k)$.

(ii) We adopt the *Polyak-Ruppert averaging* (Polyak and Juditsky 1992) to mitigate of the algorithm's sensitivity on the choice of the step size. Specifically, when K iterations are completed, we report $\frac{1}{K+2-K_0}\sum_{k=K_0}^{K+1}\boldsymbol{x}_k$, instead of $\boldsymbol{x}_{K+1}$, as the approximated solution of $\boldsymbol{v}_i^n$, where $1\le K_0\le K$ is a pre-specified integer.

Upon computing $\hat{\boldsymbol{v}}_i^n \approx \mathrm{argmax}_{\boldsymbol{x}}\,\mathrm{IKG}^n(i,\boldsymbol{x})$ with SGA for each i, we set

$$\hat{a}^n = \underset{1\le i\le M}{\mathrm{argmax}}\log\widehat{\mathrm{IKG}}^n(i,\hat{\boldsymbol{v}}_i^n) \quad \text{and} \quad \hat{\boldsymbol{v}}^n = \hat{\boldsymbol{v}}_{\hat{a}^n}^n,$$

Algorithm 1 Computing $\log \widehat{\mathrm{IKG}}^n(i, \boldsymbol{x})$.

Inputs: $\mu_1^n, \ldots, \mu_M^n, k_1^n, \ldots, k_M^n, \lambda_1, \ldots, \lambda_M, \boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_J, i, \boldsymbol{x}, c_i(\boldsymbol{x})$
Outputs: *log_IKG*

$\mathcal{J} \leftarrow \emptyset$, *log_IKG* $\leftarrow -\infty$
for $j = 1$ to J **do**
  if $|\tilde{\sigma}_i^n(\boldsymbol{\xi}_j, \boldsymbol{x})| > 0$ **then**
    $u \leftarrow |\Delta_i^n(\boldsymbol{\xi}_j)| / |\tilde{\sigma}_i^n(\boldsymbol{\xi}_j, \boldsymbol{x})|$
    if $u < 20$ **then**
      $r \leftarrow \Phi(-u)/\phi(u)$
    else
      $r \leftarrow u/(u^2 + 1)$
    end if
    $g_j \leftarrow \log\left(\frac{|\tilde{\sigma}_i^n(\boldsymbol{\xi}_j, \boldsymbol{x})|}{\sqrt{2\pi} J}\right) - \frac{1}{2}u^2 + \texttt{log1p}(-ur)$ ▷ $\texttt{log1p}(x) = \log(1 + x)$.
    $\mathcal{J} \leftarrow \{\mathcal{J}, j\}$
  end if
end for
if $\mathcal{J} \neq \emptyset$ **then**
  $g^* \leftarrow \max_{j \in \mathcal{J}} g_j$
  log_IKG $\leftarrow g^* + \log \sum_{j \in \mathcal{J}} e^{g_j - g^*} - \log(c_i(\boldsymbol{x}))$
end if

Algorithm 2 Approximately Computing $(a^n, \boldsymbol{v}^n)$ Using SGA.

Inputs: $\mu_1^n, \ldots, \mu_M^n, k_1^n, \ldots, k_M^n, \lambda_1, \ldots, \lambda_M, \boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_J, c_1, \ldots, c_M$
Outputs: $\hat{a}^n, \hat{\boldsymbol{v}}^n$

for $i = 1$ to M **do**
  $\boldsymbol{x}_1 \leftarrow$ initial value
  for $k = 1$ to K **do**
    Generate independent sample $\{\boldsymbol{\xi}_{k1}, \ldots, \boldsymbol{\xi}_{km}\}$ from density $\gamma(\cdot)$
    $\boldsymbol{x}_{k+1} \leftarrow \Pi_{\mathcal{X}}[\boldsymbol{x}_k + b_k \bar{g}_i^n(\boldsymbol{\xi}_{k1}, \ldots, \boldsymbol{\xi}_{km}, \boldsymbol{x}_k)]$ ▷ Mini-batch SGA.
  end for
  $\hat{\boldsymbol{v}}_i^n \leftarrow \frac{1}{K+2-K_0} \sum_{k=K_0}^{K+1} \boldsymbol{x}_k$ ▷ Polyak-Ruppert averaging.
  log_IKG$_i \leftarrow \log \widehat{\mathrm{IKG}}^n(i, \hat{\boldsymbol{v}}_i^n)$ ▷ Call Algorithm 1.
end for
$\hat{a}^n \leftarrow \mathrm{argmax}_i$ *log_IKG*$_i$
$\hat{\boldsymbol{v}}^n \leftarrow \hat{\boldsymbol{v}}_{\hat{a}^n}^n$

to be the sampling decision at time n, i.e., let $(\hat{a}^n, \hat{\boldsymbol{v}}^n)$ be the computed solution for $(a^n, \boldsymbol{v}^n)$ under the IKG policy. The complete procedure is summarized in Algorithm 2.

I. Additional Numerical Experiments

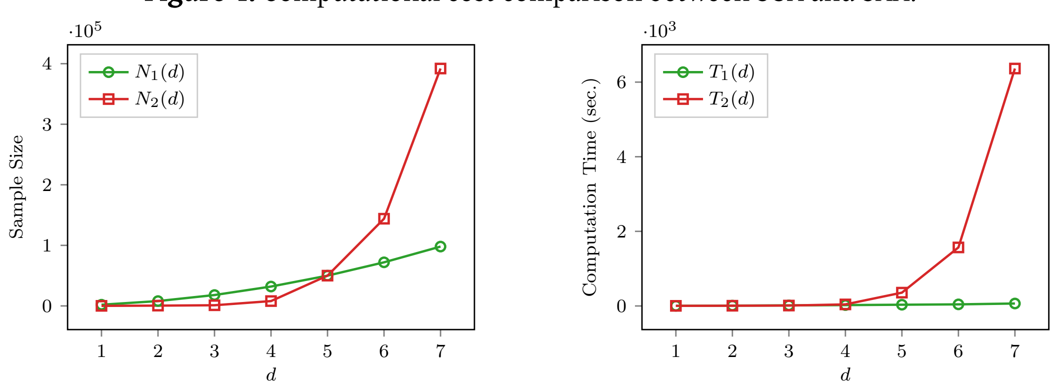
Computational cost comparison

We conduct simple experiment to compare the computational cost when the IKG sampling policy defined in eq. (13), i.e., $(a^n, \boldsymbol{v}^n) \in \mathrm{argmax}_{1 \le i \le M, \boldsymbol{x} \in \mathcal{X}} \mathrm{IKG}^n(i, \boldsymbol{x})$, is solved purely using sample average approximation (SAA) method or our proposed SGA (together with SAA). For IKG with SGA, here refer to as method 1, as described in Section 5, the computation of eq. (13) consists of two steps. Step (i) is to solve $\boldsymbol{v}_i^n = \max_{\boldsymbol{x} \in \mathcal{X}} \mathrm{IKG}^n(i, \boldsymbol{x})$ for all $i = 1, \ldots, M$ with SGA, and step (ii) is to solve $a^n = \mathrm{argmax}_{1 \le i \le M} \mathrm{IKG}^n(i, \boldsymbol{v}_i^n)$ with SAA. For IKG with pure SAA, here refer to as method 2, the problems in the above two steps are both solved with SAA. In particular, the problem in step (i) is converted into a continuous deterministic optimization after applying SAA, which is solved directly using the `fmincon` solver in MATLAB. It is expected that for either method, the computational cost will increase as the dimensionality d increases. But to evaluate the exact value of the computational cost, one needs to know the true optimal solution of eq. (13) and control the optimality gap when a specific method is used. Here we simply compare the relative computational cost of two methods by roughly controlling the resulting OC at the same level.

The same problem in Section 5 is considered and we let the dimensionality d increase from 1 to 7. The density function of covariates is the uniform distribution and the cost function is constantly 1. All the parameters for the problem, the IKG with SGA (i.e., method 1) and the evaluation of OC are the same as before. For each d, the sampling policy under the two methods is carried out respectively until the budget $B = 100$ is exhausted, and the $\widehat{\text{OC}}(B)$ curves are obtained. For fair comparison, we let the step (ii) of method 2 be exactly the same (i.e., same sample used) as that of method 1, and tune the sample size in step (i) of method 2 as follows. We gradually increase the sample size of random covariates used in SAA (not the number of samples from alternatives), until the resulting $\widehat{\text{OC}}(B)$ curve from method 2 is roughly comparable to that from method 1. Note that for either method the computation time needs to solve eq. (13) depends on the number of samples allocated to each alternative so far, and will increase as the samples accumulate. So, we report the total computation time spent on solving eq. (13) during the entire sampling process (until the budget $B = 100$ is exhausted, which means eq. (13) is solved for 100 times), averaged on $L = 30$ replications, for the two methods, which are denoted as $T_1(d)$ and $T_2(d)$ respectively.

The following Figure 4 shows the comparison between methods 1 and 2. Left panel of Figure 4 shows the sample sizes of random covariates used to approximately solve $\boldsymbol{v}_i^n = \max_{\boldsymbol{x}\in\mathcal{X}} \text{IKG}^n(i, \boldsymbol{x})$ for each i in step (i) by the two methods, which are denoted as $N_1(d)$ and $N_2(d)$ respectively. Note that $N_1(d) = mK = 20d \times 100d = 2000d^2$ as specified, and $N_2(d)$ is tuned so that the performance of method 2 matches that of method 1. Right panel of Figure 4 shows the computation times $T_1(d)$ and $T_2(d)$ (in MATLAB, Windows 10 OS, 3.60 GHz CPU, 16 GB RAM). It can be seen that IKG with SGA (i.e., method 1) scales much better in dimensionality d than IKG with pure SAA (i.e., method 2). Recall that for each method, the sample size of covariates in step (ii) is set as $500d^2$. So, even consider the fact that in method 2 the function approximation in step (i) can be directly used in step (ii), which saves the sample of covariates and the relevant computation in step (ii), the entire sample size and the computation time of method 2 still grows much faster than method 1.

Figure 4: Computational cost comparison between SGA and SAA.



Estimated sampling variance

In practice, the sampling variance $\lambda_i(\boldsymbol{x})$ is usually unknown and needs to be estimated. We suggest to follow the approach in Ankenman et al. (2010). Specifically, for each alternative i, at some predetermined design points $\boldsymbol{x}^1, \ldots, \boldsymbol{x}^m$, multiple simulations are run and the sample variances are computed, which are denoted as $s_i^2(\boldsymbol{x}^1), \ldots, s_i^2(\boldsymbol{x}^m)$. Then ordinary kriging (i.e., Gaussian process interpolation) is used to fit the entire surface of $\lambda_i(\boldsymbol{x})$. Under the Bayesian viewpoint, it is equivalent to impose a Gaussian process with constant mean function $\mu_i^0(\boldsymbol{x}) \equiv \mu_i^0$ and covariance function $k_i^0(\boldsymbol{x}, \boldsymbol{x}')$ as prior of $\lambda_i(\boldsymbol{x})$, and compute the posterior mean function by ignoring the sampling variance at the design points, i.e.,

$$\mu_i^m(\boldsymbol{x}) = \mu_i^0 + k_i^0(\boldsymbol{x}, \boldsymbol{X}_i) k_i^0(\boldsymbol{X}_i, \boldsymbol{X}_i)^{-1} [\boldsymbol{y}_i - \mu_i^0 \boldsymbol{I}],$$

where $\boldsymbol{X}_i := (\boldsymbol{x}^1, \ldots, \boldsymbol{x}^m)$ and $\boldsymbol{y}_i := (s_i^2(\boldsymbol{x}^1), \ldots, s_i^2(\boldsymbol{x}^m))^\intercal$. Then, $\mu_i^m(\boldsymbol{x})$ is used as estimate of $\lambda_i(\boldsymbol{x})$, and the IKG policy is applied as if $\lambda_i(\boldsymbol{x})$ was known. In ordinary kriging, μ_i^0 and the parameters in $k_i^0(\boldsymbol{x}, \boldsymbol{x}')$ are usually optimized via maximum likelihood estimation (MLE).

We again consider the problem in Section 5. To better investigate the effect of estimating $\lambda_i(\boldsymbol{x})$, we consider two sampling variance: (1) $\lambda_i(\boldsymbol{x}) \equiv 0.01$, as before; (2) $\lambda_i(\boldsymbol{x}) = 0.01 \times (1.5^{d-1} + \theta_i(\boldsymbol{x}))$. The density function of covariates is the uniform distribution and the cost function is constantly 1. All the other parameters for the problem are the same as before. The prior for estimating $\lambda_i(\boldsymbol{x})$ is directly set as $\mu_i^0 = 0$, and $k_i^0(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(-\frac{1}{d}\|\boldsymbol{x} - \boldsymbol{x}'\|^2\right)$, without invoking the MLE. The design points are generated by Latin hypercube sampling and the same design points are used for each i. All the parameters for the IKG policy and the evaluation of OC are the same as before. The following Figure 5 shows the estimated opportunity cost when the sampling variance is known or estimated using the above approach, for the case of $d = 1$ or 3 and sampling variance (1) or (2). Numerical results show that the effect of estimating the sampling variance is minor for this problem, which agrees with the observation in Ankenman et al. (2010).

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Figure 5: Estimated opportunity cost (vertical axis) as a function of the sampling budget (horizontal axis).