Bayesian Optimization over Bounded Domains with the Beta Product Kernel (Supplementary Material)

Table S1: Training details of different models.

Model	Training Steps	Batch Size	Time per Evaluation	Num of Training Samples
GPT-2	512	25	55 mins	12,800
BERT	256	100	40 mins	25,600
DeBERTa-v3	256	100	30 mins	25,600
ViT	1 epoch	200	7 mins	Full training set

A UPPER BOUND OF $K_\beta(\mathbf{x}, \mathbf{x})$

A.1 PROOF OF LEMMA 1

Lemma 1. *For gamma function $\Gamma(\cdot)$, we have that*

$$\frac{\Gamma(2x+1)}{\Gamma^2(x+1)} = \frac{2^{2x}\Gamma(x+\frac{1}{2})}{\sqrt{\pi}\Gamma(x+1)} \tag{1}$$

Proof. We start by utilizing the duplication formula for the Gamma function, which states:

$$\Gamma(z)\Gamma\left(z+\frac{1}{2}\right) = 2^{1-2z}\sqrt{\pi}\Gamma(2z)$$

Applying the duplication formula to our specific case by setting $z = x + \frac{1}{2}$, we get:

$$\Gamma\left(x+\frac{1}{2}\right)\Gamma(x+1) = 2^{-2x}\sqrt{\pi}\Gamma(2x+1).$$

Dividing both sides by $\Gamma^2(x+1)$, we obtain:

$$\frac{\Gamma(2x+1)}{\Gamma^2(x+1)} = \frac{2^{2x}\Gamma\left(x+\frac{1}{2}\right)}{\sqrt{\pi}\Gamma(x+1)}.$$

which completes the proof. $\square$

A.2 PROOF OF LEMMA 2

Lemma 2. *For $x \geq 0$ and $0 < s < 1$, it holds that:*

$$\left(\frac{2}{2x+1}\right)^{\frac{1}{2}} \leq \frac{\Gamma(x+\frac{1}{2})}{\Gamma(x+1)} \leq 2.$$

Proof. The Wendel's inequality is stated as

$$\left(\frac{z}{z+s}\right)^{1-s} \leq \frac{1}{z^s} \cdot \frac{\Gamma(z+s)}{\Gamma(z)} \leq 1, \tag{2}$$

where $z > 0$ and $s \in (0,1)$. When $s = \frac{1}{2}$, it is equivalent to

$$1 \leq z^{\frac{1}{2}} \frac{\Gamma(z)}{\Gamma(z+\frac{1}{2})} \leq \left(\frac{z+\frac{1}{2}}{z}\right)^{\frac{1}{2}} \tag{3}$$

$$z^{-\frac{1}{2}} \leq \frac{\Gamma(z)}{\Gamma(z+\frac{1}{2})} \leq z^{-\frac{1}{2}} \left(\frac{1}{2z}+1\right)^{\frac{1}{2}}. \tag{4}$$

Apply the inequality with $z = x + \frac{1}{2}$ and $s = \frac{1}{2}$, we have that

$$\left(\frac{2}{2x+1}\right)^{\frac{1}{2}} \leq \frac{\Gamma\left(x+\frac{1}{2}\right)}{\Gamma\left(x+1\right)} \leq \left(x+\frac{1}{2}\right)^{-\frac{1}{2}} \left(\frac{1}{2x+1}+1\right)^{\frac{1}{2}} \tag{5}$$

$$= \left[\frac{2}{2x+1}\left(\frac{1}{2x+1}+1\right)\right]^{\frac{1}{2}} =: g(x). \tag{6}$$

As $g(x)$ is a decreasing function on $[0,\infty)$, thus $g(0) = \max_{x\geq 0} g(x) = 2$, which concludes the proof. □

A.3 PROOF OF PROPOSITION 1

Proposition 2. $K_\beta(\mathbf{x},\mathbf{x}) = \mathcal{O}(2^{2d-\frac{2d}{h}} h^{-\frac{3d}{2}}), \forall \mathbf{x} \in [0,1]^d$.

Proof. For any $\mathbf{x} = (x_1,\ldots,x_d) \in [0,1]^d$, $K_\beta(\mathbf{x},\mathbf{x})$ is expressed as

$$K_\beta(\mathbf{x},\mathbf{x}) = C \prod_{i=1}^{d} \frac{\Gamma(2\frac{x_i}{h_i}+1)\Gamma(2\frac{1-x_i}{h_i}+1)}{\Gamma^2(\frac{x_i}{h_i}+1)\Gamma^2(\frac{1-x_i}{h_i}+1)},$$

where

$$C = \frac{\Gamma^2(\frac{1}{h_i}+2)}{\Gamma(\frac{2}{h_i}+2)}. \tag{7}$$

By utilizing Lemma 1 with $\frac{x_i}{h_i}$ and $\frac{1-x_i}{h_i}$, we have that

$$K_\beta(\mathbf{x},\mathbf{x}) = C \prod_{i=1}^{d} \frac{2^{2\frac{x_i}{h_i}+2(1-\frac{x_i}{h_i})}\Gamma(\frac{x_i}{h_i}+\frac{1}{2})\Gamma(\frac{1-x_i}{h_i}+\frac{1}{2})}{\pi\Gamma(\frac{x_i}{h_i}+1)\Gamma(\frac{1-x_i}{h_i}+1)} \tag{8}$$

$$= C \prod_{i=1}^{d} \frac{4}{\pi} \frac{\Gamma(\frac{x_i}{h_i}+\frac{1}{2})\Gamma(\frac{1-x_i}{h_i}+\frac{1}{2})}{\Gamma(\frac{x_i}{h_i}+1)\Gamma(\frac{1-x_i}{h_i}+1)} \tag{9}$$

When applying Lemma 2, we have that

$$\frac{\Gamma(\frac{x_i}{h_i}+\frac{1}{2})\Gamma(\frac{1-x_i}{h_i}+\frac{1}{2})}{\Gamma(\frac{x_i}{h_i}+1)\Gamma(\frac{1-x_i}{h_i}+1)} \leq 4 \tag{10}$$

Therefore, we can derive that

$$
\begin{aligned}
K_\beta(\mathbf{x}, \mathbf{x}) &\le \frac{16^d}{\pi^d} \prod_{i=1}^{d} \frac{\Gamma^2(\frac{1}{h_i}+2)}{\Gamma(\frac{2}{h_i}+2)} && && (11)\\
&= \frac{16^d}{\pi^d} \prod_{i=1}^{d} \frac{(\frac{2}{h_i}+2)\Gamma^2(\frac{1}{h_i}+2)}{\Gamma(\frac{2}{h_i}+2+1)} && \text{by } \Gamma(x+1) = x\Gamma(x) && (12)\\
&= \frac{16^d}{\pi^d} \prod_{i=1}^{d} \frac{(\frac{2}{h_i}+2)\sqrt{\pi}\Gamma(\frac{1}{h_i}+2)}{2^{2(\frac{1}{h_i}+1)}\Gamma(\frac{1}{h_i}+\frac{3}{2})} && \text{by Lemma 1 with } x = \frac{1}{h_i}+1 && (13)\\
&= \frac{2^{2d}}{\pi^{\frac{d}{2}}} \prod_{i=1}^{d} \frac{(\frac{2}{h_i}+2)\Gamma(\frac{1}{h_i}+2)}{2^{\frac{2}{h_i}}\Gamma(\frac{1}{h_i}+\frac{3}{2})} && && (14)\\
&\le \frac{2^{3d}}{\pi^{\frac{d}{2}}} \prod_{i=1}^{d} \frac{(\frac{1}{h_i}+1)(\frac{1}{h_i}+\frac{3}{2})^{\frac{1}{2}}}{2^{\frac{2}{h_i}}} && \text{by Lemma 2 } \frac{\Gamma(\frac{1}{h_i}+2)}{\Gamma(\frac{1}{h_i}+\frac{3}{2})} \le \left(\frac{1}{h_i}+\frac{3}{2}\right)^{\frac{1}{2}} && (15)\\
&= 2^{3d-\frac{2d}{h}} \left(\frac{1}{h}+1\right)^d \left(\frac{1}{h\pi}+\frac{3}{2\pi}\right)^{\frac{d}{2}} && && (16)
\end{aligned}
$$

Therefore, we conclude the proof. □