Information-Theoretic Regret Bounds for Gaussian Process Optimization in the Bandit Setting: Addendum

Matthias Seeger
mseeger@gmail.com

November 12, 2019

Abstract

This note contains some additional details, helping with the understanding of proofs in [1].

1 RKHS Norm corresponding to Posterior Kernel

In Appendix II of [1], it is stated that it "is easy to see that the RKHS norm corresponding to k_T is given by"

$$\|f\|_{k_T}^2 = \|f\|_k^2 + \sigma^{-2} \sum_{i=1}^{T} f(\boldsymbol{x}_i)^2. \tag{1}$$

Here, $\|\cdot\|_k$ denotes the norm of the RKHS corresponding to the kernel $k(\cdot, \cdot)$, and $\|\cdot\|_{k_T}$ respectively for k_T. Moreover, the posterior kernel is given by

$$k_T(\boldsymbol{x}_a, \boldsymbol{x}_b) = k(\boldsymbol{x}_a, \boldsymbol{x}_b) - \boldsymbol{k}(\boldsymbol{x}_a)^T (\boldsymbol{K} + \sigma^2 \boldsymbol{I})^{-1} \boldsymbol{k}(\boldsymbol{x}_b),$$
$$\boldsymbol{K} = [k(\boldsymbol{x}_i, \boldsymbol{x}_j)]_{i,j} \in \mathbb{R}^{T \times T}, \quad \boldsymbol{k}(\boldsymbol{x}_a) = [k(\boldsymbol{x}_i, \boldsymbol{x}_a)]_i \in \mathbb{R}^T.$$

In fact, we write

$$k_T(\boldsymbol{x}_a, \boldsymbol{x}_b) = k(\boldsymbol{x}_a, \boldsymbol{x}_b) - \boldsymbol{v}(\boldsymbol{x}_a)^T \boldsymbol{k}(\boldsymbol{x}_b), \quad \boldsymbol{v}(\boldsymbol{x}_a) = (\boldsymbol{K} + \sigma^2 \boldsymbol{I})^{-1} \boldsymbol{k}(\boldsymbol{x}_a).$$

Since this is maybe not all that "easy to see", we provide a simple proof here. All we need is the reproducing property of the respective kernel w.r.t. their RKHS inner product.

We only have to show (1) for finite kernel expansions

$$f(\boldsymbol{x}) = \sum_{j=1}^{n} \alpha_j k_T(\tilde{\boldsymbol{x}}_j, \boldsymbol{x}),$$

since limits of such form the RKHS $\mathcal{H}_{k_T}$. Also, since the expressions $\|f\|_{k_T}^2$, $\|f\|_k^2$, $f(\boldsymbol{x}_i)^2$ all admit quadratic expansions, for example

$$\left\| \sum_{j=1}^{n} \alpha_j k_T(\tilde{\boldsymbol{x}}_j, \cdot) \right\|_{k_T}^2 = \sum_{j,k=1}^{n} \alpha_j \alpha_k \langle k_T(\tilde{\boldsymbol{x}}_j, \cdot), k_T(\tilde{\boldsymbol{x}}_k, \cdot) \rangle_{k_T},$$

it is enough to show that

$$\langle k_T(\boldsymbol{x}_a, \cdot), k_T(\boldsymbol{x}_b, \cdot) \rangle_{k_T} = \langle k_T(\boldsymbol{x}_a, \cdot), k_T(\boldsymbol{x}_b, \cdot) \rangle_k + \sigma^{-2} \sum_{i=1}^{T} k_T(\boldsymbol{x}_a, \boldsymbol{x}_i) k_T(\boldsymbol{x}_b, \boldsymbol{x}_i). \tag{2}$$

First, by the reproducing property for $\mathcal{H}_{k_T}$:

$$\langle k_T(\boldsymbol{x}_a, \cdot), k_T(\boldsymbol{x}_b, \cdot)\rangle_{k_T} = k_T(\boldsymbol{x}_a, \boldsymbol{x}_b).$$

Second, using the reproducing property for $\mathcal{H}_k$:

$$\langle k_T(\boldsymbol{x}_a, \cdot), k_T(\boldsymbol{x}_b, \cdot)\rangle_k = \langle k_T(\boldsymbol{x}_a, \cdot), k(\boldsymbol{x}_b, \cdot) - \boldsymbol{v}(\boldsymbol{x}_b)^T \boldsymbol{k}(\cdot)\rangle_k = k_T(\boldsymbol{x}_a, \boldsymbol{x}_b) - \boldsymbol{v}(\boldsymbol{x}_b)^T [k_T(\boldsymbol{x}_a, \boldsymbol{x}_i)]_i.$$

Also,

$$[k_T(\boldsymbol{x}_a, \boldsymbol{x}_i)]_i = \boldsymbol{k}(\boldsymbol{x}_a) - \boldsymbol{K}\boldsymbol{v}(\boldsymbol{x}_a) = \boldsymbol{k}(\boldsymbol{x}_a) - (\boldsymbol{K} + \sigma^2 \boldsymbol{I} - \sigma^2 \boldsymbol{I})(\boldsymbol{K} + \sigma^2 \boldsymbol{I})^{-1} \boldsymbol{k}(\boldsymbol{x}_a) = \sigma^2 \boldsymbol{v}(\boldsymbol{x}_a). \tag{3}$$

Therefore:

$$\langle k_T(\boldsymbol{x}_a, \cdot), k_T(\boldsymbol{x}_b, \cdot)\rangle_{k_T} - \langle k_T(\boldsymbol{x}_a, \cdot), k_T(\boldsymbol{x}_b, \cdot)\rangle_k = \sigma^2 \boldsymbol{v}(\boldsymbol{x}_a)^T \boldsymbol{v}(\boldsymbol{x}_b). \tag{4}$$

Finally, using (3), we have

$$\sum_{i=1}^{T} k_T(\boldsymbol{x}_a, \boldsymbol{x}_i) k_T(\boldsymbol{x}_b, \boldsymbol{x}_i) = \sigma^4 \boldsymbol{v}(\boldsymbol{x}_a)^T \boldsymbol{v}(\boldsymbol{x}_b).$$

Together with (4), this establishes (2).

References

[1] N. Srinivas, A. Krause, S. Kakade, and M. Seeger. Information-theoretic regret bounds for Gaussian process optimization in the bandit setting. *IEEE Transactions on Information Theory*, 58:3250–3265, 2012.