A Boost to the Upper Bound on the Variance in Liang and Rakhlin [2020]

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Abstract

In this document, we provide a boost to the upper bound on the Variance, derived in Liang and Rakhlin [2020]. The boost to the upper bound provides easier interpretation, and further connects to the population eigenvalues of the covariance matrix.

Keywords— Minimum-norm interpolation, kernel rigeless regression.

In the Theorem 1 of Liang and Rakhlin [2020], the variance upper bound V can be boosted to

$$\mathbf{V} \le \frac{C\sigma^2}{\gamma} \cdot \inf_{0 \le k \le d} \left\{ \lambda_1(\Sigma) \frac{k}{n} + \lambda_k(\Sigma) \right\} , \tag{0.1}$$

where $\lambda_i(\Sigma)$, $1 \le i \le d$ are the population eigenvalues sorted in a non-increasing order. All the notations follow from the original paper.

To see this, let's only consider the case with $\alpha = 0$ and $\beta = 1$ (this can be done by centering and scaling the kernel). The full expression in **V** in Page 1339 of Liang and Rakhlin [2020] reads

$$\mathbf{V} \le 8\sigma^2 \cdot \mathbf{E}_{\mathbf{x} \sim \mu} \left\| \left(\gamma I + \frac{XX^*}{d} \right)^{-1} \frac{X\mathbf{x}}{d} \right\|^2 = 8\sigma^2 \cdot \text{Tr} \left(\left(d\gamma I + XX^* \right)^{-1} X \Sigma X^* \left(d\gamma I + XX^* \right)^{-1} \right)$$
(0.2)

Denote $\Sigma = \sum_{j=1}^d \lambda_j(\Sigma) \cdot u_j u_j^{\star}$ as the eigenvalue decomposition of the population covariance matrix. Take any $1 \le k \le d$. Denote $\Sigma_{>k} = \sum_{j>k} \lambda_j(\Sigma) \cdot u_j u_j^{\star}$, for this high frequency component we have

$$\operatorname{Tr}\left(\left(d\gamma I + XX^{\star}\right)^{-1} X\Sigma_{>k} X^{\star} \left(d\gamma I + XX^{\star}\right)^{-1}\right) \leq \lambda_{k}(\Sigma) \cdot \operatorname{Tr}\left(\left(d\gamma I + XX^{\star}\right)^{-1} XX^{\star} \left(d\gamma I + XX^{\star}\right)^{-1}\right) \tag{0.3}$$

$$\leq \lambda_k(\Sigma) \sum_{i=1}^n \frac{\lambda_i(XX^\top)}{(d\gamma + \lambda_i(XX^\top))^2} \tag{0.4}$$

$$\leq \lambda_k(\Sigma) n \frac{1}{4d\gamma} \leq \frac{C}{4\gamma} \cdot \lambda_k(\Sigma) \tag{0.5}$$

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where the last line uses Remark 5.1 in Liang and Rakhlin [2020], $\frac{t}{(r+t)^2} \le \frac{1}{4r}$ for all a, r > 0. This proof is identical to that in Liang and Rakhlin [2020]. The last step also uses the fact $d \times n$.

Now for the low frequency component, $\Sigma_{\leq k} = \sum_{j \leq k} \lambda_j(\Sigma) \cdot u_j u_j^*$. Denote $P_{u_j}^{\perp} := I - u_j u_j^* \in \mathbb{R}^{d \times d}$ the projection matrix to the orthogonal complement of u_j , we have

$$\operatorname{Tr}\left(\left(d\gamma I + XX^{\star}\right)^{-1} X\Sigma_{\leq k} X^{\star} \left(d\gamma I + XX^{\star}\right)^{-1}\right) \leq \sum_{j \leq k} \lambda_{j}(\Sigma) \cdot \|\left(d\gamma I + XX^{\star}\right)^{-1} X u_{j}\|^{2} \tag{0.6}$$

with the definition $v := Xu_j \in \mathbb{R}^n$, and $M := d\gamma I + XP_{u_i}^{\perp}X^{\star}$, we continue to bound

$$\left\| \left(d\gamma I + XX^{\star} \right)^{-1} X u_{j} \right\|^{2} = \left\| (M + vv^{\star})^{-1} v \right\|^{2} \tag{0.7}$$

$$= \left\| \left(M^{-1} - \frac{M^{-1}vv^{\star}M^{-1}}{1 + v^{\star}M^{-1}v} \right)v \right\|^2 \quad \text{Woodbury formula}$$
 (0.8)

$$= \frac{v^{\star}M^{-2}v}{\left(1 + v^{\star}M^{-1}v\right)^{2}} \le \frac{1}{d\gamma} \frac{v^{\star}M^{-1}v}{\left(1 + v^{\star}M^{-1}v\right)^{2}} \quad \text{recall } \lambda_{\min}(M) > d\gamma \tag{0.9}$$

$$\leq \frac{1}{4\nu} \frac{1}{d} , \qquad (0.10)$$

where the last line again uses Remark 5.1 in Liang and Rakhlin [2020]. Therefore recalling $d \times n$

$$\operatorname{Tr}\left(\left(d\gamma I + XX^{\star}\right)^{-1} X\Sigma_{\leq k} X^{\star} \left(d\gamma I + XX^{\star}\right)^{-1}\right) \leq \sum_{j \leq k} \lambda_{j}(\Sigma) \cdot \|\left(d\gamma I + XX^{\star}\right)^{-1} Xu_{j}\|^{2} \tag{0.11}$$

$$\leq k\lambda_1(\Sigma) \cdot \frac{1}{4\gamma d} \leq \frac{C}{4\gamma} \cdot \lambda_1(\Sigma) \frac{k}{n} . \tag{0.12}$$

The proof is now complete by combining Equations (0.5) and (0.12).

References

Tengyuan Liang and Alexander Rakhlin. Just interpolate: Kernel "Ridgeless" regression can generalize. *The Annals of Statistics*, 48(3):1329–1347, June 2020. doi: 10.1214/19-AOS1849.