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A Omitted Proofs

We list all the omitted proofs in the following section.

A.1 Proof of Theorem 3.2

Theorem 3.2. *Consider a kernel* $\mathrm{K} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ *and the associated objective with regularization parameter* $\lambda > 0$ *under mean squared loss. Define* $\boldsymbol{A} = \boldsymbol{K}\left(\boldsymbol{K} + \lambda \mathbf{1}_n\right)^{-1}$. *Then it holds that*

$$L_{LOO}\left(\mathcal{Q}_\lambda^{ERM}\right) = \frac{1}{n}\sum_{i=1}^{n}\sum_{k=1}^{K}\left(\Delta_{ik}^\lambda\right)^2, \qquad A_{LOO}\left(\mathcal{Q}_\lambda^{ERM}\right) = \frac{1}{n}\sum_{i=1}^{n}\mathbb{1}_{\left\{(\boldsymbol{y}_i - \Delta_{i\bullet})^* = \boldsymbol{y}_i^*\right\}}$$

where the residuals $\Delta_{ik}^\lambda \in \mathbb{R}$ *for* $i = 1, \ldots, n$, $k = 1, \ldots, K$ *is given by* $\Delta_{ik}^\lambda = \frac{Y_{ik} - \hat{f}_k^\lambda(\boldsymbol{x}_i)}{1 - A_{ii}}$.

Proof. Recall that $\hat{f}_{\mathcal{S}}^\lambda$ solves the optimization problem

$$\hat{f}_{\mathcal{S}}^\lambda = \mathrm{argmin}_{f\in\mathcal{F}}\, L_{\mathcal{S}}^\lambda(f) := \mathrm{argmin}_{f\in\mathcal{F}}\left\{\sum_{i=1}^{n}\sum_{k=1}^{K}\left(f_k(\boldsymbol{x}_i) - Y_{ik}\right)^2 + \lambda||f||_{\mathcal{H}}^2\right\}$$

and predicting on the training data takes the form $\hat{f}_S(\boldsymbol{X}) = \boldsymbol{A}\boldsymbol{Y}$ for some $\boldsymbol{A} \in \mathbb{R}^{n\times n}$. Now consider the model $f_\lambda^{-i} := \hat{f}_{\mathcal{S}_{-i}}^\lambda$ obtained from training on $\mathcal{S}_{-i}$. W.L.O.G. assume that $i = n$. We want to understand the quantity $\hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n)$, i.e. the k-th component of the prediction on $\boldsymbol{x}_i$. To that

end, consider the dataset $\mathcal{Z} := \mathcal{S}_{-n} \cup \left\{ \left(\boldsymbol{x}_n, \hat{f}_\lambda^{-n}(\boldsymbol{x}_n) \right) \right\}$. Notice that for any $f \in \mathcal{F}$, it holds

$$\begin{aligned}
L_{\mathcal{Z}}^{\lambda}(\hat{f}_\lambda^{-n}) &= \sum_{k=1}^{K} \left\{ \sum_{i=1}^{n-1} \left(\hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_i) - Y_{ik} \right)^2 + \left(\hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) - \hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) \right)^2 \right\} + \lambda ||\hat{f}_\lambda^{-n}||_{\mathcal{H}}^2 \\
&= \sum_{k=1}^{K} \sum_{i=1}^{n-1} \left(\hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_i) - Y_{ik} \right)^2 + \lambda ||\hat{f}_\lambda^{-n}||_{\mathcal{H}}^2 \\
&= L_{\mathcal{S}_{-n}}^{\lambda} \left(\hat{f}_\lambda^{-n} \right) \\
&\leq L_{\mathcal{S}_{-n}}^{\lambda}(f) \\
&\leq L_{\mathcal{S}_{-n}}^{\lambda}(f) + \sum_{k=1}^{K} \left(f_k(\boldsymbol{x}_n) - \hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) \right)^2 \\
&= L_{\mathcal{Z}}^{\lambda}(f)
\end{aligned}$$

where the first inequality follows because $\hat{f}^{-n}$ minimizes $L_{\mathcal{S}_{-n}}^{\lambda}$ by definition. Thus $\hat{f}_\lambda^{-n}$ also minimizes $L_{\mathcal{Z}}^{\lambda}$ and hence also takes the form

$$\hat{f}_\lambda^{-n}(\boldsymbol{X}) = \boldsymbol{A}\tilde{\boldsymbol{Y}}$$

where $\tilde{\boldsymbol{Y}} \in \mathbb{R}^{n \times K}$ such that $\tilde{Y}_{ik} = \begin{cases} Y_{ik} & \text{if } i \neq n \\ \hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) & \text{else} \end{cases}$. Now we care about the n-th prediction which is

$$\begin{aligned}
\hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) &= \sum_{j=1}^{n} A_{nj} \tilde{Y}_{jk} = \sum_{j=1}^{n-1} A_{nj} Y_{jk} + A_{nn} \hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) \\
&= \sum_{j=1}^{n} A_{nj} Y_{jk} - A_{nn} Y_{nk} + A_{nn} \hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) \\
&= \hat{f}_{\mathcal{S},k}^{\lambda}(\boldsymbol{x}_n) - A_{nn} Y_{nk} + A_{nn} \hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n)
\end{aligned}$$

Solving for $\hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n)$ gives

$$\hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) = \frac{\hat{f}_{\mathcal{S},k}^{\lambda}(\boldsymbol{x}_n) - A_{nn} Y_{nk}}{1 - A_{nn}} \tag{3}$$

Then, subtracting Y_{nk} leads to

$$Y_{nk} - \hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) = Y_{nk} - \frac{\hat{f}_{\mathcal{S},k}^{\lambda}(\boldsymbol{x}_n) - A_{nn} Y_{nk}}{1 - A_{nn}} = \frac{Y_{nk} - Y_{nk} A_{nn} - \hat{f}_{\mathcal{S},k}^{\lambda}(\boldsymbol{x}_n) + A_{nn} Y_{nk}}{1 - A_{nn}} = \frac{Y_{nk} - \hat{f}_{\mathcal{S},k}^{\lambda}(\boldsymbol{x}_n)}{1 - A_{nn}}$$

Squaring and summing the expression over n and k results in the formula.

For the accuracy, we know that we correctly predict if the maximal coordinate of $\hat{f}_\lambda^{-n}(\boldsymbol{x}_n)$ agrees with the maximal coordinate of $\boldsymbol{y}_n$, i.e.

$$\operatorname{argmax}_k \hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) = \operatorname{argmax}_k Y_{nk}$$

From equation 3, we notice that

$$\begin{aligned}
\operatorname{argmax}_k \hat{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) &= \operatorname{argmax}_k \frac{\hat{f}_{\mathcal{S},k}^{\lambda}(\boldsymbol{x}_n) - A_{nn} Y_{nk}}{1 - A_{nn}} = \operatorname{argmax}_k \frac{\hat{f}_{\mathcal{S},k}^{\lambda}(\boldsymbol{x}_n) - Y_{nk} + Y_{nk} - A_{nn} Y_{nk}}{1 - A_{nn}} \\
&= \operatorname{argmax}_k -\Delta_{nk}^{\lambda} + Y_{nk} \\
&= (\boldsymbol{y}_n - \boldsymbol{\Delta}_{n\bullet})^*
\end{aligned}$$

We thus have to check the indicator $\mathbb{1}_{\{(\boldsymbol{y}_n - \Delta_{n\bullet})^* = \boldsymbol{y}_n^*\}}$ and sum it over n to obtain the result. $\square$

A.2 BINARY CLASSIFICATION

Here we state the corresponding results in the case of binary classification. The formulation for the accuracy changes slightly as now the sign of the classifier serves as the prediction.

Proposition A.1. *Consider a kernel* $\mathrm{K} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ *and the associated objective with regularization parameter* $\lambda > 0$ *under mean squared loss. Define* $\boldsymbol{A} = \boldsymbol{K}\left(\boldsymbol{K} + \lambda \mathbf{1}_n\right)^{-1}$. *Then it holds that*

$$L_{LOO}\left(\mathcal{Q}_\lambda^{ERM}\right) = \frac{1}{n}\sum_{i=1}^{n}\left(\Delta_i^\lambda\right)^2, \qquad A_{LOO}\left(\mathcal{Q}_\lambda^{ERM}\right) = \frac{1}{n}\sum_{i=1}^{n}\mathbb{1}_{\{y_i\Delta_i^\lambda<1\}}$$

where the residuals $\Delta_i^\lambda \in \mathbb{R}$ *for* $i = 1, \ldots, n$ *is given by* $\Delta_i^\lambda = \frac{y_i - \hat{f}^\lambda(\boldsymbol{x}_i)}{1 - A_{ii}}$.

Proof. Notice that the result for L_{LOO} is analogous to the proof for Theorem 3.2 by setting $K = 1$. For binary classification we use the sign of the classifier as a decision rule, i.e. the classifier predicts correctly if $y\hat{f}^\lambda(\boldsymbol{x}) > 0$. We can thus calculate that

$$\begin{aligned}
y_n \hat{f}_\lambda^{-n}(\boldsymbol{x}_n) &= \frac{y_n \hat{f}_{\mathcal{S}}^\lambda(\boldsymbol{x}_n) - A_{nn}y_n^2}{1 - A_{nn}} = \frac{y_n \hat{f}_{\mathcal{S}}^\lambda(\boldsymbol{x}_n) - y_n^2 + y_n^2 - y_n^2 A_{nn}}{1 - A_{nn}} \\
&= y_n^2 - y_n \frac{y_n - \hat{f}_{\mathcal{S}}^\lambda(\boldsymbol{x}_n)}{1 - A_{nn}} \\
&= 1 - y_n \frac{y_n - \hat{f}_{\mathcal{S}}^\lambda(\boldsymbol{x}_n)}{1 - A_{nn}} \\
&= 1 - y_n \Delta_n^\lambda
\end{aligned}$$

Thus, the n-th sample is correctly classified if and only if

$$1 - y_n\Delta_n^\lambda > 0 \iff y_n\Delta_n^\lambda < 1$$

We now just count the correct predictions for the accuracy, i.e.

$$A_{\text{LOO}}\left(\mathcal{Q}_\lambda^{\text{ERM}}\right) = \frac{1}{n}\sum_{i=1}^{n}\mathbb{1}_{\{y_i\Delta_i^\lambda<1\}}$$

□

A.3 PROOF OF COROLLARY 3.3

Corollary 3.3. *Consider the eigendecomposition* $\boldsymbol{K} = \boldsymbol{V}\,\mathrm{diag}(\boldsymbol{\omega})\boldsymbol{V}^T$ *for* $\boldsymbol{V} \in O(n)$ *and* $\boldsymbol{\omega} \in \mathbb{R}^n$. *Denote its rank by* $r = \mathrm{rank}(\boldsymbol{K})$. *Then it holds that the residuals* $\Delta_{ik}^\lambda \in \mathbb{R}$ *can be expressed as*

$$\Delta_{ik}^\lambda(r) = \sum_{l=1}^{n} Y_{lk} \frac{\sum_{k=r+1}^{n} V_{ik}V_{lk} + \sum_{k=1}^{r}\frac{\lambda}{\lambda+\omega_k}V_{ik}V_{lk}}{\sum_{k=r+1}^{n} V_{ik}^2 + \sum_{k=1}^{r}\frac{\lambda}{\lambda+\omega_k}V_{ik}^2}$$

Moreover for zero regularization, i.e. $\lambda \to 0$, *it holds that*

$$\Delta_{ik}^\lambda(r) \to \Delta_{ik}(r) = \begin{cases} \sum_{l=1}^{n} Y_{lk}\frac{\sum_{j=r+1}^{n} V_{ij}V_{lj}}{\sum_{j=r+1}^{n} V_{ij}^2} & \text{if } r < n \\ \sum_{l=1}^{n} Y_{lk}\frac{\sum_{j=1}^{n}\frac{1}{\omega_j}V_{ij}V_{lj}}{\sum_{j=1}^{n}\frac{1}{\omega_j}V_{ij}^2} & \text{if } r = n \end{cases}$$

Proof. Define $\boldsymbol{A} = \boldsymbol{K}\left(\boldsymbol{K} + \lambda\mathbf{1}_n\right)^{-1} \in \mathbb{R}^{n\times n}$. Recall that $\hat{f}_{\mathcal{S}}^\lambda(\boldsymbol{X}) = \boldsymbol{A}\boldsymbol{y}$ and thus $\hat{f}_k^\lambda(\boldsymbol{x}_i) = \sum_{j=1}^{n} A_{ij}Y_{jk}$. Let us first simplify $\boldsymbol{A}$:

$$\begin{aligned}
\boldsymbol{A} &= \boldsymbol{K}\left(\boldsymbol{K} + \lambda\mathbf{1}_n\right)^{-1} = \boldsymbol{V}\,\mathrm{diag}\left(\boldsymbol{\omega}\right)\boldsymbol{V}^T\left(\boldsymbol{V}\,\mathrm{diag}\left(\boldsymbol{\omega}\right)\boldsymbol{V}^T + \lambda\mathbf{1}_n\right)^{-1} \\
&= \boldsymbol{V}\,\mathrm{diag}\left(\frac{\boldsymbol{\omega}}{\boldsymbol{\omega}+\lambda}\right)\boldsymbol{V}^T
\end{aligned}$$

We can characterize the off-diagonal elements for $i \neq j$ as follows:

$$A_{ij} = \sum_{k=1}^{n} V_{ik} \frac{\omega_i}{\omega_i + \lambda} V_{jk} = \sum_{k=1}^{r} V_{ik} V_{jk} \frac{\omega_i}{\omega_i + \lambda} = \sum_{k=1}^{r} V_{ik} V_{jk} - \sum_{k=1}^{r} \frac{\lambda}{\omega_k + \lambda} V_{ik} V_{jk}$$
$$= - \sum_{k=r+1}^{n} V_{ik} V_{jk} - \sum_{k=1}^{r} \frac{\lambda}{\omega_k + \lambda} V_{ik} V_{jk}$$

where we made use of the fact that $\boldsymbol{V}_{i\bullet} \perp \boldsymbol{V}_{j\bullet}$. The diagonal elements $i = j$ on the other hand can be written as

$$A_{ii} = \sum_{k=1}^{n} V_{ik}^2 \frac{\omega_i}{\omega_i + \lambda} = \sum_{k=1}^{r} V_{ik}^2 \frac{\omega_k}{\omega_k + \lambda} = \sum_{k=1}^{r} V_{ik}^2 - \sum_{k=1}^{r} V_{ik}^2 \frac{\lambda}{\omega_k + \lambda}$$
$$= 1 - \sum_{k=r+1}^{n} V_{ik}^2 - \sum_{k=1}^{r} V_{ik}^2 \frac{\lambda}{\omega_k + \lambda}$$

where we have made use of the fact that $\boldsymbol{V}_{i\bullet}$ is a unit vector. Plugging-in the quantities into L_{LOO} results in

$$\Delta_{ik}^{\lambda} = \frac{Y_{ik} - \hat{f}_k^{\lambda}(\boldsymbol{x}_i)}{1 - A_{ii}} = \frac{Y_{ik} - \sum_{l=1}^{n} A_{il} Y_{lk}}{1 - A_{ii}} = \frac{Y_{ik} - A_{ii} y_i - \sum_{l \neq i}^{n} A_{il} Y_{lk}}{1 - A_{ii}}$$
$$= \frac{Y_{ik} \left(\sum_{j=r+1}^{n} V_{ij}^2 + \sum_{k=1}^{r} V_{ij}^2 \frac{\lambda}{\omega_j + \lambda} \right) + \sum_{l \neq i}^{n} Y_{lk} \left(\sum_{j=r+1}^{n} V_{ij} V_{lj} + \sum_{j=1}^{r} \frac{\lambda}{\omega_j + \lambda} V_{ij} V_{lj} \right)}{\sum_{j=r+1}^{n} V_{ij}^2 + \sum_{j=1}^{r} V_{ij}^2 \frac{\lambda}{\omega_l + \lambda}}$$
$$= \frac{\sum_{l=1}^{n} Y_{lk} \left(\sum_{j=r+1}^{n} V_{ij} V_{lj} + \sum_{j=1}^{r} \frac{\lambda}{\omega_j + \lambda} V_{ij} V_{lj} \right)}{\sum_{j=r+1}^{n} V_{ij}^2 + \sum_{j=1}^{r} V_{ij}^2 \frac{\lambda}{\omega_k + \lambda}}$$

Now crucially, in the full rank case $r = n$, we have empty sums, i.e. $\sum_{l=r+1}^{n} = \sum_{l=n+1}^{n} = 0$ and we obtain

$$\Delta_{ik}^{\lambda} = \frac{\sum_{l=1}^{n} Y_{lk} \sum_{j=1}^{r} \frac{\lambda}{\omega_j + \lambda} V_{ij} V_{lj}}{\sum_{j=1}^{r} V_{ij}^2 \frac{\lambda}{\omega_j + \lambda}} = \frac{\sum_{l=1}^{n} Y_{lk} \sum_{j=1}^{r} \frac{1}{\omega_j + \lambda} V_{ij} V_{lj}}{\sum_{j=1}^{r} V_{ij}^2 \frac{1}{\omega_j + \lambda}}$$
$$\xrightarrow{\lambda \to 0} \sum_{l=1}^{n} Y_{lk} \frac{\sum_{j=1}^{r} \frac{1}{\omega_j} V_{ij} V_{lj}}{\sum_{j=1}^{r} \frac{1}{\omega_j} V_{ij}^2}$$

On the other hand, in the rank deficient case $r < n$ we can cancel the regularization term:

$$\Delta_{ik}^{\lambda} \xrightarrow{\lambda \to 0} \sum_{l=1}^{n} Y_{lk} \frac{\sum_{j=r+1}^{n} V_{ij} V_{lj}}{\sum_{j=r+1}^{n} V_{ij}^2}$$

Plugging this into the formulas for L_{LOO}^{λ} and A_{LOO}^{λ} concludes the proof. □

A.4 Proof of Proposition 4.1

Proposition 4.1. *Consider a kernel with spectral decomposition $\boldsymbol{K} = \boldsymbol{V} \operatorname{diag}(\boldsymbol{\omega}) \boldsymbol{V}^T$ for $\boldsymbol{V} \in \mathbb{R}^{n \times n}$ orthogonal and $\boldsymbol{\omega} \in \mathbb{R}^n$. Assume that $\operatorname{rank}(\boldsymbol{K}) = n$. Then it holds that the leave-one-out error $L_{LOO}(\tilde{\boldsymbol{Y}}; \boldsymbol{Y})$ for a model trained on $\tilde{\mathcal{S}} = \{(\boldsymbol{x}_i, \tilde{\boldsymbol{y}}_i)\}_{i=1}^n$ but evaluated on $\mathcal{S} = \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^n$ is given by*

$$L_{LOO}(\tilde{\boldsymbol{Y}}; \boldsymbol{Y}) = \frac{1}{n} \sum_{i=1}^{n} \sum_{k=1}^{K} \left(\tilde{\Delta}_{ik} + Y_{ik} - \tilde{Y}_{ik} \right)^2, \qquad A_{LOO}(\tilde{\boldsymbol{Y}}; \boldsymbol{Y}) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\left\{ (\tilde{\boldsymbol{y}}_i - \tilde{\boldsymbol{\Delta}}_{i\bullet})^* = \boldsymbol{y}_i^* \right\}}$$

where $\tilde{\Delta}_{ik} = \Delta_{ik}(\tilde{\boldsymbol{Y}}) \in \mathbb{R}$ is defined as in Corollary 3.3.

Proof. Denote by $\tilde{\mathcal{S}}_{-i}$ the dataset $\{(\boldsymbol{x}_j, \tilde{y}_j)\}_{j\neq i}^n$. Denote by $\tilde{f}_\lambda^{-i}$ the model trained on $\tilde{\mathcal{S}}_{-i}$. Recall from the proof of Theorem 3.2 that

$$\tilde{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) = \frac{\tilde{f}_k^\lambda(\boldsymbol{x}_n) - A_{nn}\tilde{Y}_{nk}}{1 - A_{nn}}$$

Instead of subtracting the same label $\tilde{Y}_{nk}$, we now subtract the evaluation label Y_{nk}:

$$\begin{aligned} Y_{nk} - \tilde{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) &= \frac{Y_{nk} - A_{nn}Y_{nk} - \tilde{f}_k^\lambda(\boldsymbol{x}_n) + A_{nn}\tilde{Y}_{nk}}{1 - A_{nn}} = \frac{(1 - A_{nn})(Y_{nk} - \tilde{Y}_{nk}) + \tilde{Y}_{nk} - \tilde{f}_k^\lambda(\boldsymbol{x}_n)}{1 - A_{nn}} \\ &= (Y_{nk} - \tilde{Y}_{nk}) + \frac{\tilde{Y}_{nk} - \tilde{f}_k^\lambda(\boldsymbol{x}_n)}{1 - A_{nn}} \\ &= (Y_{nk} - \tilde{Y}_{nk}) + \tilde{\Delta}_{ik}^\lambda \end{aligned}$$

The second term $\tilde{\Delta}_{ik}^\lambda$ is now the summand of the standard leave-one-out error where we evaluate on $\tilde{\boldsymbol{Y}}$. We can hence re-use Theorem 3.3 to decompose it. Squaring and summing over n concludes the LOO loss result. For the accuracy, we notice that a similar derivation as for Theorem 3.2 applies:

$$\begin{aligned} \operatorname{argmax}_k \tilde{f}_{\lambda,k}^{-n}(\boldsymbol{x}_n) &= \operatorname{argmax}_k \frac{\tilde{f}_k^\lambda(\boldsymbol{x}_n) - A_{nn}\tilde{Y}_{nk}}{1 - A_{nn}} = \operatorname{argmax}_k \frac{\hat{f}_k^\lambda(\boldsymbol{x}_n) - \tilde{Y}_{nk} + \tilde{Y}_{nk} - A_{nn}\tilde{Y}_{nk}}{1 - A_{nn}} \\ &= \operatorname{argmax}_k -\tilde{\Delta}_{nk}^\lambda + \tilde{Y}_{nk} \\ &= \left(\tilde{\boldsymbol{y}}_n - \tilde{\boldsymbol{\Delta}}_{n\bullet}\right)^* \end{aligned}$$

We thus have to check the indicator against the true label $\boldsymbol{y}_n$, i.e. $\mathbb{1}_{\{(\tilde{\boldsymbol{y}}_n - \tilde{\Delta}_{n\bullet})^* = \boldsymbol{y}_n^*\}}$ and sum it over n to obtain the result. □

A.5 Proof of Theorem 4.3

Theorem 4.3. *For large enough $n \in \mathbb{N}$, we can estimate as*

$$L_{LOO}^n(m^*) \gtrapprox 2nA$$

where $A \sim \Gamma(\frac{1}{2}, 1)$ is independent of n. $L_{LOO}^n(m^*)$ hence diverges a.s. with $n \to \infty$.

Proof. First we notice that for $m = m^*$, by definition it holds that $r = n - 1$, which simplifies the LOO expression to

$$L_{\text{LOO}}^n(m^*) \xrightarrow{\lambda \to 0} \frac{1}{n}\left(\sum_{i=1}^n \frac{1}{V_{in}^2}\right)\left(\sum_{i=1}^n y_i V_{in}\right)^2$$

For notational convenience, we will introduce $\boldsymbol{v} \in \mathbb{R}^n$ such that $v_i := V_{in}$. We will now bound the both factors one-by-one. The first part is a simple application of Proposition B.1 and Proposition B.5:

$$L_{LOO}^n(m^*) = \frac{1}{n}\left(\sum_{i=1}^n v_i\right)^2 \sum_{i=1}^n \frac{1}{v_i^2} \geq n^2 \frac{1}{n}\left(\sum_{i=1}^n v_i\right)^2 \overset{(d)}{=} n^2 B$$

Now for large enough n, we can use Lemma B.6 to make the following approximation in distribution:

$$nB \approx 2\frac{n-1}{2} B \xrightarrow{(d)} 2A$$

where $A \sim \Gamma(\frac{1}{2}, 1)$. Thus for large enough n, it holds that

$$L_{LOO}^n(m^*) \gtrapprox 2nA$$

As the approximation becomes exact for larger and larger n, we conclude that

$$L_{LOO}^n(m^*) \xrightarrow{n \to \infty} \infty \quad \text{a.s.}$$

□

B ADDITIONAL LEMMAS

In this section we present the additional technical Lemmas needed for the proofs of the main claims in A.

Lemma B.1. *Consider a unit vector $\boldsymbol{v} \in \mathbb{S}^{n-1}$. Then it holds that*

$$\sum_{i=1}^{n} \frac{1}{v_i^2} \geq n^2$$

Proof. Let's parametrize each v_i as

$$v_i = \frac{z_i}{\sqrt{\sum_{i=1}^{n} z_i^2}}$$

for $i = 1, \ldots, n$ and $\boldsymbol{z} \in \mathbb{R}^n$. One can easily check that $||\boldsymbol{v}||_2 = 1$ and hence $\boldsymbol{v} \in \mathbb{S}^{n-1}$. Plugging this in, we arrive at

$$\sum_{i=1}^{n} \frac{1}{v_i^2} = \sum_{i=1}^{n} \frac{\sum_{j=1}^{n} z_j^2}{z_i^2} = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{z_j^2}{z_i^2} = n + \sum_{i=1}^{n} \sum_{j \neq i}^{n} \frac{z_j^2}{z_i^2}$$

We can re-arrange the sum into pairs

$$\frac{z_j^2}{z_i^2} + \frac{z_i^2}{z_j^2} = a^2 + \frac{1}{a^2} \geq 2$$

for $a^2 = \frac{z_j^2}{z_i^2} > 0$ and using the fact that $x + \frac{1}{x} \geq 2$ for $x \geq 0$. We can find $\frac{n(n-1)}{2}$ such summands, and thus

$$\sum_{i=1}^{n} \frac{1}{v_i^2} \geq n + 2\frac{n(n-1)}{2} = n^2$$

□

Lemma B.2. *Consider $\boldsymbol{v} \sim \mathcal{U}\left(\mathbb{S}^{n-1}\right)$ and any fixed orthogonal matrix $\boldsymbol{U} \in O(n)$. Then it holds that*

$$\boldsymbol{U}\boldsymbol{v} \overset{(d)}{=} \boldsymbol{v}$$

Proof. This is a standard result and can for instance be found in Vershynin (2018). □

Lemma B.3. *Consider $\boldsymbol{w} \sim \mathcal{N}(\boldsymbol{0}, \mathbb{1}_n)$. Then it holds that*

$$\boldsymbol{v} = \frac{\boldsymbol{w}}{||\boldsymbol{w}||_2} \sim \mathcal{U}\left(\mathbb{S}^{n-1}\right)$$

Proof. This is a standard result and can for instance be found in Vershynin (2018). □

Lemma B.4. *Consider two independent Gamma variables $X \sim \text{Gamma}(\alpha, \nu)$ and $Y \sim \text{Gamma}(\beta, \nu)$. Then it holds that*

$$\frac{X}{X+Y} \sim \text{Beta}\left(\alpha, \beta\right)$$

Proof. This is a standard result and can for instance be found in Bowman et al. (1998). □

Lemma B.5. *Consider $\boldsymbol{v} \sim \mathcal{U}\left(\mathbb{S}^{n-1}\right)$. Then it holds that*

$$\frac{1}{n}\left(\sum_{i=1}^{n} y_i v_i\right)^2 \sim \text{Beta}\left(\frac{1}{2}, \frac{n-1}{2}\right)$$

Proof. First realize that we can write

$$\frac{1}{\sqrt{n}}\sum_{i=1}^{n} y_i v_i = \tilde{\mathbf{1}}_n^T (\boldsymbol{v} \odot \boldsymbol{y}) \overset{(d)}{=} \tilde{\mathbf{1}}_n^T \boldsymbol{v}$$

where $\tilde{\mathbf{1}}_n = \left(\frac{1}{\sqrt{n}}, \dots, \frac{1}{\sqrt{n}}\right)$ with $||\tilde{\mathbf{1}}_n||_2 = 1$ and the fact that $\boldsymbol{v} \odot \boldsymbol{y} \overset{(d)}{=} \boldsymbol{v}$ for fixed $\boldsymbol{y} \in \{-1, 1\}^n$. The idea is now to choose $\boldsymbol{U} \in O(n)$ such that $\boldsymbol{U}^T \tilde{\mathbf{1}}_n = \boldsymbol{e}_1 = (1, 0, \dots, 0)$. Then by using Lemma B.2, it holds

$$\tilde{\mathbf{1}}_n^T \boldsymbol{v} \overset{(d)}{=} \tilde{\mathbf{1}}_n^T \boldsymbol{U} \boldsymbol{v} \overset{(d)}{=} \left(\boldsymbol{U}\tilde{\mathbf{1}}_n\right)^T \boldsymbol{v} \overset{(d)}{=} \boldsymbol{e}_1^T \boldsymbol{v} \overset{(d)}{=} v_1$$

Thus, surprisingly, it suffices to understand the distribution of v_1. By Lemma B.3, we know that

$$v_1 \overset{(d)}{=} \frac{z_1}{\sqrt{z_1^2 + \dots + z_n^2}}$$

where $\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \mathbb{1}_n)$. We are interested in the square of this expression,

$$\frac{1}{n}\left(\sum_{i=1}^{n} v_i\right)^2 \overset{(d)}{=} v_1^2 \overset{(d)}{=} \frac{z_1^2}{z_1^2 + \dots + z_n^2} \overset{(d)}{=} \frac{z_1^2}{z_1^2 + w}$$

where we define $w = \sum_{i=2}^{n} z_i^2$, clearly independent of z_1^2. Moreover, it holds that $z_1^2 \sim \text{Gamma}\left(\frac{1}{2}, \frac{1}{2}\right)$ and $w \sim \text{Gamma}\left(\frac{n-1}{2}, \frac{1}{2}\right)$. Thus, by Lemma B.4 we can conclude that

$$\frac{1}{n}\left(\sum_{i=1}^{n} v_i\right)^2 \sim \text{Beta}\left(\frac{1}{2}, \frac{n-1}{2}\right)$$

□

Lemma B.6. *Consider the sequence of Beta distributions* $X_n \sim \text{Beta}(k, n)$. *Then it holds that*

$$nX_n \xrightarrow{(d)} \text{Gamma}(k, 1)$$

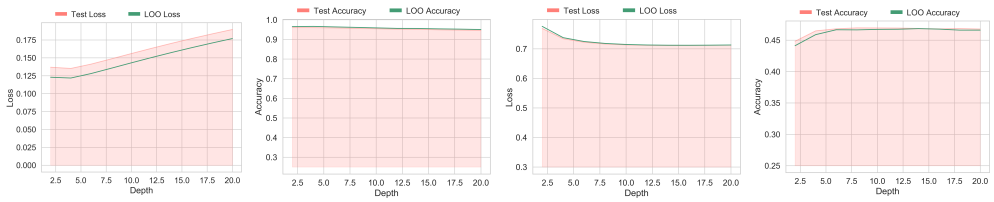
Proof. This is a standard result and can for instance be found in Walck (1996). □

C Further Experiments

In this section we present additional experimental results on the leave-one-out error.

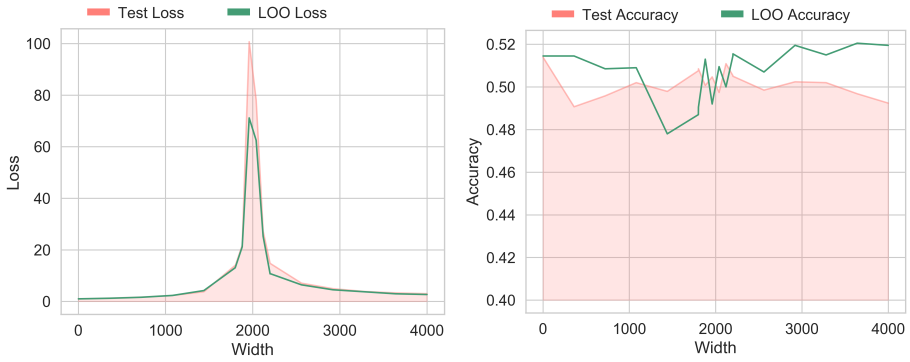
C.1 LOO as function of depth L

We study how the depth L of the NTK kernel $\Theta^{(L)}$ affects the performance of LOO loss and accuracy. We use the datasets *MNIST* and *CIFAR10* with $n = 5000$ and evaluate NTK models with depth ranging from 3 to 20. We present our findings in Figure 4. Again we see a very close match between LOO and the corresponding test quantity for *CIFAR10*. Interestingly the performance is slightly worse for very shallow models. For *MNIST* we see a gap between LOO loss and test loss, which is due to the very zoomed-in nature of the plot (the gap is actually only 0.015) as the loss values are very small in general. Indeed we observe an excellent match between the test and LOO accuracy.



(a) Loss (b) Accuracy (c) L_{LOO}, *CIFAR10* (d) A_{LOO}, *CIFAR10*

Figure 4: Test and LOO losses (a, c) and accuracies (b, d) as a function of depth L. We use fully-connected NTK model on *MNIST* and *CIFAR10*.



(a) Loss (b) Accuracy

Figure 5: Test and LOO losses (a) and accuracies (b) as a function of sample width m. We use a random feature model on binary *MNIST* with random labels.

C.2 Double Descent with Random Labels

Here we demonstrate how the spike in double descent is a very universal phenomenon as demonstrated by Theorem 4.3. We consider a random feature model of varying width m on binary *MNIST* with $n = 2000$, where the labels are fully randomized ($p = 1$), destroying thus any relationship between the inputs and targets. Of course, there will be no double descent behaviour in the test accuracy as the network has to perform random guessing at any width. We display this in Figure 5. We observe that indeed the model is randomly guessing throughout all the regimes of overparametrization. Both the test and LOO loss however, exhibit a strong spike around the interpolation threshold. This underlines the universal nature of the phenomenon, connecting with the fact that Theorem 4.3 does not need any assumptions on the targets.