Supplement: An exemplary computation of the quantities $\tau_d^{(i)}$ $d^{(l)}$, ξ_c , and α_c

Here, we consider the case where the distribution P is specified by: the random variable *X* is univariate and distributed according to some unknown distribution P_X , and the joint distribution of (Y, X) is given by the simple model $Y = \beta_0 + \beta_1 X + \varepsilon$, where $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ with β_0 and σ^2 unknown. The goal is to compute the quantities $\tau_d^{(i)}$, ξ_c , and α_c analytically.

Since $\beta_0 = \mathbb{E}(Y - \beta_1 X)$, one has $\widehat{\beta}_0 = g^{-1} \sum_{i=1}^g (Y_i - \beta_1 X_i)$ and Γ takes the form

$$
\Gamma(1,\ldots,g;g+1) = G((X_1,Y_1),\ldots,(X_g,Y_g);(X_{g+1},Y_{g+1}))
$$

= $(g^{-1}\sum_{i=1}^g (Y_i - \beta_1 X_i) + \beta_1 X_{g+1} - Y_{g+1})^2$,

using the mean squared error as the loss function. By a slight abuse of notation, let us write $Z_i := Y_i - \beta_1 X_i = \beta_0 + \varepsilon_i$. (Correctly, one would have to use yet another notation, say W_i instead of Z_i ; however, one would then obtain

$$
G(Z_1, \ldots, Z_g; Z_{g+1}) = G(W_1, \ldots, W_g; W_{g+1})
$$

as equality of random variables on the entire probability space which is why we use the notation Z_i in the first place.) Then, Z_i is *i.i.d.* from $Z \sim \mathcal{N}(\beta_0, \sigma^2)$ and Γ can be written in terms of these variables as

$$
\Gamma(1,\ldots,g;g+1) = G(Z_1,\ldots,Z_g;Z_{g+1}) = (g^{-1}\sum_{i=1}^g Z_i - Z_{g+1})^2 = (g^{-1}\sum_{i=1}^g \varepsilon_i - \varepsilon_{g+1})^2.
$$

Therefore, Γ is $\sigma^2(1/g+1)$ times a chi-square variable with one degree of freedom. Moreover, $\Theta = \mathbb{E} \Gamma = \mathbb{V}(g^{-1} \sum_{i=1}^{g} \varepsilon_i - \varepsilon_{g+1}) = \sigma^2 (1 + g^{-1})$. This formula is similar to [Zhang and Qian](#page-2-0) [\(2013,](#page-2-0) (9), (10)).

Recall that the covariance between two chi-square random variables can be computed as follows. Let (P, Q) be a bivariate normal distribution with covariance matrix $\begin{pmatrix} a & b \\ b & c \end{pmatrix}$ and mean $(0,0)^T$. Then, $Cov(P^2, Q^2) = 2b^2$. Hence, all $\tau_d^{(i)}$ $d_d^{(i)}$ are non-negative in this case.

Some care has to be taken: the degree of Θ is two rather than $g + 1$; thus, Assumption 1 is not valid in this case. However, in this chapter we will only make use of the non-degeneracy of the associated *U*-statistic which is a slightly weaker statement than the assumption; non-degeneracy still remains valid. On a related note, let *s* ² denote the usual unbiased variance estimator for σ^2 , which is a *U*-statistic of degree two. Then one can check that the symmetrized form Γ_0 of Γ coincides with $s^2(1+g^{-1})$, which also follows from the uniqueness of the *U*-statistic for a regular parameter.

Another possibility to resolve the issue would be to add a negligibly small term of degree $g+1$ to Γ ; in other words, the collection of choices of Γ such that the assumption is violated is a null set in some sense.

Let us abbreviate $A = \sum_{i=1}^{d} \varepsilon_i, C = \sum_{i=1}^{g}$ e_i^g
 $e_i, D = \sum_{i=g+2}^{2g-d+1}$ $\frac{2g-d+1}{g+2}$ ε_i . Then, $A \sim (d\sigma^2)^{1/2} \mathcal{N}(0,1),$ *C* ∼ ((*g*−*d*)σ²)^{1/2} ∕ ∕ (0,1),*D* ∼ ((*g*−*d*)σ²)^{1/2} ∕ ⁄ (0,1). Furthermore, E*A*⁴ = 3(*d*σ²)² due to the normal kurtosis, $\mathbb{E}A^3 = \mathbb{E}A = \mathbb{E}C = \mathbb{E}D = 0$, $\mathbb{E}A^2 = d\sigma^2$, $\mathbb{E}C^2 = \mathbb{E}D^2 =$ $(g-d)\sigma^2$.

Note that for type one, the overlap is only between the two learning sets, thus $d =$ *c*, and we only use the letter *d*. Making use of the mutual independences between $A, C, D, \varepsilon_{g+1}, \varepsilon_{2g+2-d}$, we obtain:

$$
\tau_c^{(1)} = Cov((g^{-1}(A+C) - \varepsilon_{g+1})^2, (g^{-1}(A+D) - \varepsilon_{2g+2-c})^2) =
$$

= 2(Cov(g^{-1}(A+C) - \varepsilon_{g+1}, g^{-1}(A+D) - \varepsilon_{2g+2-c}))^2 =
= c^2[2g^{-4}\sigma^4]

This is remarkable because there seem to be few places in the literature where the quantities σ_d of a *U*-statistic are explicitly calculated. In particular, no variance formulae for the leave-*p*-out error of linear regression are known, except in the "leave-one-out" case.

For type two, we have $d = c + 1$ and it is convenient to choose the following abbreviations: $A = \sum_{i=1}^{c} \varepsilon_i$, $C = \sum_{i=c+1}^{g} \varepsilon_i$, and $D = \sum_{i=g+1}^{2g-c}$ $\sum_{i=g+2}^{2g-c} \varepsilon_i$. Note that the symmetry between *C* and *D* is lost and we have $\mathbb{E}C^2 = (g - c)\sigma^2$ and $\mathbb{E}D^2 = (g - c - 1)\sigma^2$. We prefer to perform the index shift $c+1$ on the left hand-side of the equation in order to stress the analogy of the computation with type one above. We then have

$$
\tau_{c+1}^{(2)} = 2Cov[(g^{-1}(A+C) - \varepsilon_{g+1}), (g^{-1}(A+\varepsilon_{g+1}+D) - \varepsilon_{2g-c+1})]^2
$$

= $c^2[2g^{-4}\sigma^4] + c[-4g^{-3}\sigma^4] + 2g^{-2}\sigma^4.$ (1)

For type three, we have $d = c + 2$ and it is convenient to choose the following abbreviations: *A* and *D* as above, but $C = \sum_{c=1}^{g} \varepsilon_i$. We then have

$$
\tau_{c+2}^{(3)} = 2Cov[(g^{-1}(A + \varepsilon_{c+1} + C) - \varepsilon_{g+1}), (g^{-1}(A + \varepsilon_{g+1} + D) - \varepsilon_{c+1})]^2
$$

= $c^2[2g^{-4}\sigma^4] + c[-8g^{-3}\sigma^4] + 8g^{-2}\sigma^4.$ (2)

For type four, we abbreviate $A = \sum_{i=1}^{c} \varepsilon_i$, $C = \sum_{i=c+1}^{g} \varepsilon_i$, and $D = \sum_{i=g+2}^{2g-c+1}$ $\sum_{i=g+2}^{2g-c+1} \varepsilon_i$. Using that $\mathbb{E} \varepsilon_{g+1}^3 = 0$ because the third central moment of a normal random variate vanishes, we obtain:

$$
\tau_{c+1}^{(4)} = 2Cov[(g^{-1}(A+C) - \varepsilon_{g+1}), (g^{-1}(A+D) - \varepsilon_{g+1})]^2
$$

= $c^2[2g^{-4}\sigma^4] + c[4g^{-2}\sigma^4] + 2\sigma^4$.

By [\(3.5\)](#page-0-0), the expressions for the quantities τ as functions of *c* yield for ξ_c :

$$
\xi_c = 2\sigma^4 \bigg[c - 2g + n + \frac{c^2}{g^2} - \frac{2c}{g} + \frac{2c^2 n}{g^3} - \frac{4cn}{g^2} + \frac{2n}{g} + \frac{c^2 n^2}{g^4} \bigg].
$$

By (3.12) , we have

$$
\alpha_0 = 2\sigma^4 \left[-2g + n + 2ng^{-1} \right] \n\alpha_1 = 2\sigma^4 \left[-\frac{2}{g} - \frac{4n}{g^2} + \frac{1}{g^2} + \frac{2n}{g^3} + \frac{n^2}{g^4} + 1 \right] \n\alpha_2 = 4\sigma^4 \left[g^{-2} + 2ng^{-3} + n^2g^{-4} \right] \n\alpha_\gamma = 0, \quad \gamma \ge 3.
$$

References

Zhang Q., Qian P.Z.G., 2013. Designs for crossvalidating approximation models. *Biometrika*, 100(4), 997–1004.