Supplement: An exemplary computation of the quantities $\tau_d^{(i)}, \xi_c$, 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 $\tau_d^{(i)}, \xi_c$, 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

$$\begin{split} \Gamma(1,\ldots,g;g+1) &= G((X_1,Y_1),\ldots,(X_g,Y_g);(X_{g+1},Y_{g+1})) \\ &= \left(g^{-1}\sum_{i=1}^g (Y_i-\beta_1X_i) + \beta_1X_{g+1} - Y_{g+1}\right)^2, \end{split}$$

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 (2013, (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 $\tau_d^{(i)}$ 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 $A = \sum_{i=1}^{d} \varepsilon_i, C = \sum_{i=d+1}^{g} \varepsilon_i, D = \sum_{i=g+2}^{2g-d+1} \varepsilon_i$. Then, $A \sim (d\sigma^2)^{1/2} \mathcal{N}(0,1)$, $C \sim ((g-d)\sigma^2)^{1/2} \mathcal{N}(0,1), D \sim ((g-d)\sigma^2)^{1/2} \mathcal{N}(0,1)$. Furthermore, $\mathbb{E}A^4 = 3(d\sigma^2)^2$ 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:

$$\begin{aligned} \tau_c^{(1)} &= Cov((g^{-1}(A+C) - \varepsilon_{g+1})^2, (g^{-1}(A+D) - \varepsilon_{2g+2-c})^2) = \\ &= 2(Cov(g^{-1}(A+C) - \varepsilon_{g+1}, g^{-1}(A+D) - \varepsilon_{2g+2-c}))^2 = \\ &= c^2 [2g^{-4}\sigma^4] \end{aligned}$$

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 $D = \sum_{i=g+2}^{2g-c} \varepsilon_i$. 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

$$\begin{aligned} \tau_{c+1}^{(2)} &= 2Cov \big[(g^{-1}(A+C) - \varepsilon_{g+1}), (g^{-1}(A+\varepsilon_{g+1}+D) - \varepsilon_{2g-c+1}) \big]^2 \\ &= c^2 [2g^{-4}\sigma^4] + c [-4g^{-3}\sigma^4] + 2g^{-2}\sigma^4. \end{aligned}$$
(1)

For type three, we have d = c + 2 and it is convenient to choose the following abbreviations: *A* and *D* as above, but $C = \sum_{c+2}^{g} \varepsilon_i$. 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 $D = \sum_{i=g+2}^{2g-c+1} \varepsilon_i$. Using that $\mathbb{E} \varepsilon_{g+1}^3 = 0$ because the third central moment of a normal random variate vanishes, we obtain:

$$\begin{split} \tau_{c+1}^{(4)} &= 2Cov \big[(g^{-1}(A+C) - \varepsilon_{g+1}), (g^{-1}(A+D) - \varepsilon_{g+1}) \big]^2 \\ &= c^2 [2g^{-4}\sigma^4] + c [4g^{-2}\sigma^4] + 2\sigma^4. \end{split}$$

By (3.5), the expressions for the quantities τ as functions of *c* yield for ξ_c :

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

By (3.12), we have

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

References

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