S1 Text. Supplementary material for the manuscript "On the accuracy of genomic selection"

1. Proof of the main result

In what follows, the quantities X and Q are supposed to be known. In other words, all the results will be conditional on X and Q. Recall that θ is fixed, and also that $q_{n_{\text{TRN}+1}}$ and $x_{n_{\text{TRN}+1}}$ are considered random.

Using the causal model, we have

$$\operatorname{Cov}\left(\hat{Y}_{n_{\mathrm{TRN}}+1}, Y_{n_{\mathrm{TRN}}+1}\right) = \operatorname{Cov}\left(\boldsymbol{x}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{Y}, \boldsymbol{q}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{\theta} + \boldsymbol{e}_{n_{\mathrm{TRN}}+1}\right)$$
$$= \operatorname{Cov}\left(\boldsymbol{x}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{Q}\boldsymbol{\theta}, \boldsymbol{q}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{\theta}\right) .$$

Besides, since $x_{n_{\text{TRN}}+1}$ and $q_{n_{\text{TRN}}+1}$ are centered, we have

$$\operatorname{Cov}\left(\hat{Y}_{n_{\mathrm{TRN}}+1}, Y_{n_{\mathrm{TRN}}+1}\right) = \mathbb{E}\left(\boldsymbol{x}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{Q}\boldsymbol{\theta}\boldsymbol{q}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{\theta}\right) .$$
(1)

Let us now focus on the terms present at the denominator, that is to say $\operatorname{Var}(Y_{n_{\mathrm{TRN}}+1})$ and $\operatorname{Var}(\hat{Y}_{n_{\mathrm{TRN}}+1})$. By definition,

$$\operatorname{Var}\left(Y_{n_{\mathrm{TRN}}+1}\right) = \sigma_{G}^{2} + \sigma_{e}^{2} \quad \text{where} \quad \sigma_{G}^{2} = \boldsymbol{\theta}' \operatorname{Var}\left(\boldsymbol{q_{n_{\mathrm{TRN}}+1}}\right) \boldsymbol{\theta} \,. \tag{2}$$

Besides, we have the relationship

$$\begin{aligned} \operatorname{Var}\left(\hat{Y}_{n_{\mathrm{TRN}}+1}\right) &= \mathbb{E}\left(\operatorname{Var}\left(\hat{Y}_{n_{\mathrm{TRN}}+1} \mid \boldsymbol{x}_{\boldsymbol{n}_{\mathrm{TRN}}+1}\right)\right) + \operatorname{Var}\left(\mathbb{E}\left(\hat{Y}_{n_{\mathrm{TRN}}+1} \mid \boldsymbol{x}_{\boldsymbol{n}_{\mathrm{TRN}}+1}\right)\right) & (3) \end{aligned}$$
To begin with, let us compute the quantity $\mathbb{E}\left(\operatorname{Var}\left(\hat{Y}_{n_{\mathrm{TRN}}+1} \mid \boldsymbol{x}_{\boldsymbol{n}_{\mathrm{TRN}}+1}\right)\right)$. We have

$$\operatorname{Var}\left(\hat{Y}_{n_{\mathrm{TRN}}+1} \mid \boldsymbol{x}_{n_{\mathrm{TRN}}+1}\right) = \mathbb{E}\left(\hat{Y}_{n_{\mathrm{TRN}}+1}^{2} \mid \boldsymbol{x}_{n_{\mathrm{TRN}}+1}\right) - \left(\boldsymbol{x}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{Q}\boldsymbol{\theta}\right)^{2}$$

and

$$\mathbb{E}\left(\hat{Y}_{n_{\mathrm{TRN}}+1}^{2} \mid \boldsymbol{x}_{n_{\mathrm{TRN}}+1}\right) = \mathbb{E}\left(\left(\boldsymbol{x}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{Q}\boldsymbol{\theta} + \boldsymbol{x}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{e}\right)^{2} \mid \boldsymbol{x}_{n_{\mathrm{TRN}}+1}\right) \\ = \mathbb{E}\left(\left(\left(\boldsymbol{x}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{Q}\boldsymbol{\theta}\right)^{2} \mid \boldsymbol{x}_{n_{\mathrm{TRN}}+1}\right) + \mathbb{E}\left(\left(\left(\boldsymbol{x}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{e}\right)^{2} \mid \boldsymbol{x}_{n_{\mathrm{TRN}}+1}\right) \\ = \left(\boldsymbol{x}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{Q}\boldsymbol{\theta}\right)^{2} + \sigma_{e}^{2} \left\|\boldsymbol{x}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\right\|^{2}$$

where $\|.\|$ is the L^2 norm. As a result,

$$\mathbb{E}\left(\operatorname{Var}\left(\hat{Y}_{n_{\mathrm{TRN}}+1} \mid \boldsymbol{x}_{n_{\mathrm{TRN}}+1}\right)\right) = \sigma_{e}^{2} \mathbb{E}\left(\left\|\boldsymbol{x}_{n_{\mathrm{TRN}}+1}^{\prime} \boldsymbol{X}^{\prime} \boldsymbol{V}^{-1}\right\|^{2}\right) .$$

On the other hand, the second term in formula (3) is

$$\operatorname{Var}\left(\mathbb{E}\left(\hat{Y}_{n_{\mathrm{TRN}}+1} \mid \boldsymbol{x}_{\boldsymbol{n}_{\mathrm{TRN}}+1}\right)\right) = \operatorname{Var}\left(\boldsymbol{x}'_{\boldsymbol{n}_{\mathrm{TRN}}+1}\boldsymbol{X}'\boldsymbol{V}^{-1}\boldsymbol{Q}\boldsymbol{\theta}\right)$$
$$= \boldsymbol{\theta}'\boldsymbol{Q}'\boldsymbol{V}^{-1}\boldsymbol{X}\operatorname{Var}\left(\boldsymbol{x}_{\boldsymbol{n}_{\mathrm{TRN}}+1}\right)\boldsymbol{X}'\boldsymbol{V}^{-1}\boldsymbol{Q}\boldsymbol{\theta}$$

where $\operatorname{Var}(\boldsymbol{x_{n_{\text{TRN}}+1}})$ is the covariance matrix of size $p \times p$. Then,

$$\operatorname{Var}\left(\hat{Y}_{n_{\mathrm{TRN}}+1}\right) = \sigma_{e}^{2} \mathbb{E}\left(\left\|\boldsymbol{x}_{\boldsymbol{n}_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\right\|^{2}\right) + \boldsymbol{\theta}^{\prime}\boldsymbol{Q}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{X}\operatorname{Var}\left(\boldsymbol{x}_{\boldsymbol{n}_{\mathrm{TRN}}+1}\right)\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{Q}\boldsymbol{\theta}$$

$$(4)$$

To conclude, according to formulae (1), (2), (4), the accuracy $\rho_{\rm RR}$ satisfies the following expression

$$\rho_{\rm RR} = \frac{\mathbb{E}\left(\boldsymbol{x}_{\boldsymbol{n}_{\rm TRN}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{Q}\boldsymbol{\theta}\boldsymbol{q}_{\boldsymbol{n}_{\rm TRN}+1}^{\prime}\boldsymbol{\theta}\right)}{\left(\sigma_{e}^{2} \mathbb{E}\left(\left\|\boldsymbol{x}_{\boldsymbol{n}_{\rm TRN}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\right\|^{2}\right) + \boldsymbol{\theta}^{\prime}\boldsymbol{Q}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{X}\operatorname{Var}\left(\boldsymbol{x}_{\boldsymbol{n}_{\rm TRN}+1}\right)\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{Q}\boldsymbol{\theta}\right)^{1/2}\left(\sigma_{G}^{2} + \sigma_{e}^{2}\right)^{1/2}}$$
(5)

.

Note that the formula can be rewritten:

$$\rho_{\mathrm{RR}} = \frac{\theta' \mathbb{E} \left(q_{n_{\mathrm{TRN}}+1} x'_{n_{\mathrm{TRN}}+1} \right) X' V^{-1} Q \theta}{\left(\sigma_e^2 \mathbb{E} \left(\left\| x'_{n_{\mathrm{TRN}}+1} X' V^{-1} \right\|^2 \right) + \theta' Q' V^{-1} X \operatorname{Var} \left(x_{n_{\mathrm{TRN}}+1} \right) X' V^{-1} Q \theta \right)^{1/2} \left(\sigma_G^2 + \sigma_e^2 \right)^{1/2}}$$

2. A new proxy (QTLs in perfect LD with some markers)

Let us assume that we have the relationship

$$x'_{n_{\mathrm{TRN}}+1}X'V^{-1}Q heta=q'_{n_{\mathrm{TRN}}+1} heta$$

Let us consider the different terms present in the general formula (5). First, we have

$$\mathbb{E}\left(\boldsymbol{x}_{\boldsymbol{n}_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{Q}\boldsymbol{\theta}\boldsymbol{q}_{\boldsymbol{n}_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{\theta}\right) = \mathbb{E}\left(\boldsymbol{q}_{\boldsymbol{n}_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{\theta}\boldsymbol{q}_{\boldsymbol{n}_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{\theta}\right) = \sigma_{G}^{2}$$

Besides, since

$$\operatorname{Var}\left(\mathbb{E}\left(\hat{Y}_{n_{\mathrm{TRN}}+1} \mid \boldsymbol{x}_{\boldsymbol{n}_{\mathrm{TRN}}+1}\right)\right) = \operatorname{Var}\left(\boldsymbol{x}_{\boldsymbol{n}_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\boldsymbol{Q}\boldsymbol{\theta}\right) = \operatorname{Var}\left(\boldsymbol{q}_{\boldsymbol{n}_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{\theta}\right) = \sigma_{G}^{2},$$

.

we have

$$\operatorname{Var}\left(\hat{Y}_{n_{\mathrm{TRN}}+1}\right) = \sigma_{e}^{2} \mathbb{E}\left(\left\|\boldsymbol{x}_{n_{\mathrm{TRN}}+1}^{\prime}\boldsymbol{X}^{\prime}\boldsymbol{V}^{-1}\right\|^{2}\right) + \sigma_{G}^{2} .$$

Then, the accuracy becomes,

$$\rho_{\text{pLD}} = \frac{\sigma_G^2}{\left(\sigma_e^2 \mathbb{E}\left(\left\|\boldsymbol{x'_{n_{\text{TRN}}+1} X' V^{-1}}\right\|^2\right) + \sigma_G^2\right)^{1/2} \left(\sigma_G^2 + \sigma_e^2\right)^{1/2}}$$

To conclude, since $\frac{\sigma_G^2}{\sigma_e^2} = \frac{h^2}{1-h^2}$, we obtain the final result

$$\rho_{\text{pLD}} = h \sqrt{\frac{h^2/(1-h^2)}{\mathbb{E}\left(\left\|\boldsymbol{x'_{n_{\text{TRN}}+1} X' V^{-1}}\right\|^2\right) + \frac{h^2}{1-h^2}}}$$

3. Link with the previous work of Daetwyler et al. [2008]

Estimators computed from Ridge Regression are equal to OLS estimators if λ is set to zero (see for instance Fan and Lv [2008]). So, by setting $\lambda = 0$, we obtain the prediction

$$\hat{Y}_{n_{ ext{TRN}}+1} = q'_{n_{ ext{TRN}}+1} \left(Q'Q
ight)^{-1}Q'Y$$
 .

Having replaced the terms $X'V^{-1}$ by $(Q'Q)^{-1}Q'$ and $x_{n_{\text{TRN}}+1}$ by $q_{n_{\text{TRN}}+1}$ in our general formula (5), the accuracy becomes

1

$$\rho = \frac{\mathbb{E}\left(q'_{n_{\text{TRN}}+1}(Q'Q)^{-1}Q'Q\theta q'_{n_{\text{TRN}}+1}\theta\right)}{\left(\sigma_{e}^{2}\mathbb{E}\left(\left\|q'_{n_{\text{TRN}}+1}(Q'Q)^{-1}Q'\right\|^{2}\right) + \theta'Q'Q(Q'Q)^{-1}\operatorname{Var}\left(q_{n_{\text{TRN}}+1}\right)(Q'Q)^{-1}Q'Q\theta\right)^{1/2}(\sigma_{G}^{2} + \sigma_{e}^{2})^{1/2}} \\
= \frac{\mathbb{E}\left(q'_{n_{\text{TRN}}+1}\theta q'_{n_{\text{TRN}}+1}\theta\right)}{\left(\sigma_{e}^{2}\mathbb{E}\left(\left\|q'_{n_{\text{TRN}}+1}(Q'Q)^{-1}Q'\right\|^{2}\right) + \theta'\operatorname{Var}\left(q_{n_{\text{TRN}}+1}\right)\theta\right)^{1/2}(\sigma_{G}^{2} + \sigma_{e}^{2})^{1/2}} \\
= \frac{\sigma_{G}^{2}}{\left(\sigma_{e}^{2}\mathbb{E}\left(\left\|q'_{n_{\text{TRN}}+1}(Q'Q)^{-1}Q'\right\|^{2}\right) + \sigma_{G}^{2}\right)^{1/2}(\sigma_{G}^{2} + \sigma_{e}^{2})^{1/2}} \\
= \frac{h\sigma_{G}}{\left(\sigma_{e}^{2}\mathbb{E}\left(\left\|q'_{n_{\text{TRN}}+1}(Q'Q)^{-1}Q'\right\|^{2}\right) + \sigma_{G}^{2}\right)^{1/2}}.$$
To finish, we use that (proof given in port section)

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$$\mathbb{E}\left(\left\|\boldsymbol{q}_{\boldsymbol{n}_{\mathrm{TRN}}+1}^{\prime}(\boldsymbol{Q}^{\prime}\boldsymbol{Q})^{-1}\boldsymbol{Q}^{\prime}\right\|^{2}\right)\approx\frac{C}{n_{\mathrm{TRN}}},$$

so the phenotypic accuracy and the genotypic accuracy are the following

$$\rho = h \sqrt{\frac{h^2/(1-h^2)}{\frac{C}{n_{\rm TRN}} + \frac{h^2}{1-h^2}}} , \tilde{\rho} = \sqrt{\frac{h^2/(1-h^2)}{\frac{C}{n_{\rm TRN}} + \frac{h^2}{1-h^2}}} .$$

In Daetwyler et al. [2008], the authors consider the case $\sigma_G^2 + \sigma_e^2 = 1$. As a result,

$$\rho = \frac{h^2}{\sqrt{\sigma_e^2 \frac{C}{n_{\text{TRN}}} + h^2}} \quad , \quad \tilde{\rho} = \frac{h}{\sqrt{\sigma_e^2 \frac{C}{n_{\text{TRN}}} + h^2}} \quad . \tag{6}$$

Besides, they use the approximation $\sigma_e^2 \approx 1$. Using this approximation in (6) and simplifying by h, we obtain

$$\rho = \frac{h}{\sqrt{\frac{1}{\eta h^2} + 1}} \ , \ \tilde{\rho} = \sqrt{\frac{h^2 \eta}{1 + h^2 \eta}} \ \text{where} \ \eta = n_{\text{\tiny TRN}}/C \ .$$

We can notice that this expression of $\tilde{\rho}$ is the same as the one presented in formula (1) of Daetwyler et al. [2008]. In the same way, the expression for ρ is the same as the one given at the end of Appendix A of Visscher et al. (2010), except that the focus was on the quantity ρ^2 .

Later, in their paper, Daetwyler et al. [2008] relaxed the assumption $\sigma_e^2 \approx 1$, and studied another approximation: $\sigma_e^2 \approx (1-h^2) + h^2(1-\tilde{\rho}^2)$. Using this new approximation in formula (6), we obtain

$$\tilde{\rho}^2 = \frac{h^2\eta}{(1-h^2\tilde{\rho}^2) + h^2\eta}$$

which is the same quantity as presented in formula (1) of Appendix S1 of Daetwyler et al. [2008].

4. Proof of
$$\mathbb{E}\left(\left\|q_{n_{\mathrm{TRN}}+1}'(Q'Q)^{-1}Q'\right\|^2\right) \approx C/n_{\mathrm{TRN}}$$

Recall that Daetwyler et al. [2008] suppose that the matrix $({\pmb Q' Q})^{-1}$ is diagonal and then,

$$(\mathbf{Q'Q})_{j,j}^{-1} = \left(\sum_{i=1}^{n_{\text{TRN}}} Q_{i,j}^2\right)^{-1}$$

Let $d_1, ..., d_C$ denote the quantities such as

$$(Q'Q)_{j,j} = d_j \ (j = 1, \cdots, C)$$
.

Let $q_{n_{\rm TRN}+1,j}$ denote the genotype of the TST individual at the $j{\rm th}$ QTL. We have the relationship

$$\left\| \boldsymbol{q}_{n_{\text{TRN}}+1}^{\prime}(\boldsymbol{Q}^{\prime}\boldsymbol{Q})^{-1}\boldsymbol{Q}^{\prime} \right\|^{2} = \sum_{j=1}^{C} \frac{(q_{n_{\text{TRN}}+1,j})^{2}}{d_{j}} + 2\sum_{j=1}^{C-1} \sum_{j^{\prime}=j+1}^{C} \frac{q_{n_{\text{TRN}}+1,j} \ q_{n_{\text{TRN}}+1,j^{\prime}} \sum_{i=1}^{n_{\text{TRN}}} (Q_{i,j}Q_{i,j^{\prime}})}{d_{j} \ d_{j^{\prime}}}$$

Since the QTLs are assumed to be in linkage equilibrium, we have

$$\forall j \neq j', \mathbb{E}\left(q_{n_{\mathrm{TRN}}+1,j} \; q_{n_{\mathrm{TRN}}+1,j'}\right) = 0$$

Recall that computations are conditional on Q. As a consequence,

$$\mathbb{E}\left(2\sum_{j=1}^{C-1}\sum_{j'=j+1}^{C}\frac{q_{n_{\mathrm{TRN}}+1,j} q_{n_{\mathrm{TRN}}+1,j'} \sum_{i=1}^{n_{\mathrm{TRN}}} (Q_{i,j}Q_{i,j'})}{d_j d_{j'}}\right) = 0.$$

Then,

$$\mathbb{E}\left(\left\|\boldsymbol{q}_{\boldsymbol{n}_{\mathrm{TRN}+1}}^{\prime}(\boldsymbol{Q}^{\prime}\boldsymbol{Q})^{-1}\boldsymbol{Q}^{\prime}\right\|^{2}\right) = \sum_{j=1}^{C} \frac{\mathbb{E}\left(\left(q_{\boldsymbol{n}_{\mathrm{TRN}+1,j}}\right)^{2}\right)}{d_{j}}$$

Finally, the authors use the approximation, $d_j \approx n_{\text{TRN}} \mathbb{E}\left(\left(Q_{n_{\text{TRN}},j}\right)^2\right)$ suitable when n_{TRN} is large. Besides, they assume that the TST and TRN samples come from the same population. In this context, $Q_{1,j}, \ldots, Q_{n_{\text{TRN}},j}, q_{n_{\text{TRN}}+1,j}$ are i.i.d. variables, and we have the relationship

$$\mathbb{E}\left(\sum_{j=1}^{C} \frac{\left(q_{n_{\mathrm{TRN}}+1,j}\right)^2}{d_j}\right) \approx \sum_{j=1}^{C} \frac{\mathbb{E}\left(\left(q_{n_{\mathrm{TRN}}+1,j}\right)^2\right)}{n_{\mathrm{TRN}} \mathbb{E}\left(\left(Q_{n_{\mathrm{TRN}},j}\right)^2\right)}$$
$$\approx C/n_{\mathrm{TRN}} .$$

As a result,

$$\mathbb{E}\left(\left\|\boldsymbol{q_{n_{\mathrm{TRN}}+1}^{\prime}}(\boldsymbol{Q^{\prime}Q})^{-1}\boldsymbol{Q^{\prime}}\right\|^{2}\right)\approx C/n_{\mathrm{TRN}}\;.$$

It concludes the proof.

References

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