

[SUPPLEMENTARY MATERIALS]

Stochastic Variance Inflation Factor with Collective Information Content Pre-analysis for Detecting Linkage Disequilibrium in Indonesian Rice SNPs

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Definition 1. By deriving from Eq. (2) and minimizing the residual sum of squares (RSS) or the cost function $\sum_{i=1}^N (y_i - \hat{y}_i)^2$, the normal Ordinary Least Squares (OLS) can be formulated as

$$\frac{1}{N} \sum_{i=1}^N (y_i - \beta_0 - \beta_1 x_i)^2 = 0$$

where β_0 and β_1 are the coefficients, act as the regression parameters.

Proof 1. The sum of all residuals is equal to zero, $\sum_{i=1}^N \varepsilon_i = 0$.

1. Estimate value of β_0 that minimizes the OLS:

$$\begin{aligned} \frac{\partial}{\partial \beta_0} \sum_{i=1}^N (y_i - \beta_0 - \beta_1 x_i)^2 &= 0 \\ -2 \sum_{i=1}^N (y_i - \beta_0 - \beta_1 x_i) &= 0 \end{aligned}$$

Ignore the constant for a while. Since $\varepsilon_i = y_i - \hat{y}_i = y_i - (\beta_0 + \beta_1 x_i)$, it is proved that $\sum_{i=1}^N \varepsilon_i = 0$. Remember, since a partial derivative has been done w.r.t. β_0 , this property applies when $\beta_0 = 0$.

2. Estimate value of β_1 that minimizes the OLS:

$$\begin{aligned} \frac{\partial}{\partial \beta_1} \sum_{i=1}^N (y_i - \beta_0 - \beta_1 x_i)^2 &= 0 \\ -2 \sum_{i=1}^N x_i (y_i - \beta_0 - \beta_1 x_i) &= 0 \end{aligned}$$

Omit the constant and thus it is proved that $\sum_{i=1}^N x_i \varepsilon_i = 0$. Remember, since a partial derivative has been done w.r.t. β_1 , this property applies when $\beta_{1,\dots,N} = 0$.

Proof 2. Residual and the predicted value are uncorrelated, $\text{corr}(\hat{y}, \varepsilon) = 0$.

$$\begin{aligned}
\text{Corr}(\hat{y}, \varepsilon) &= \frac{\text{Cov}(\hat{y}, \varepsilon)}{\sqrt{\sigma_{\hat{y}}^2 \sigma_{\varepsilon}^2}} \\
&= \frac{N^{-1} \sum_{i=1}^N (\hat{y} - \mu_{\hat{y}})(\varepsilon - \mu_{\varepsilon})}{\sqrt{\sigma_{\hat{y}}^2 \sigma_{\varepsilon}^2}} \\
&= \frac{N^{-1} \sum_{i=1}^N \varepsilon (\hat{y} - \mu_{\hat{y}})}{\sqrt{\sigma_{\hat{y}}^2 \sigma_{\varepsilon}^2}} \quad \dots \mu_{\varepsilon} = 0 \\
&= \frac{N^{-1} (\sum_{i=1}^N \hat{y} \varepsilon - \mu_{\hat{y}} \sum_{i=1}^N \varepsilon)}{\sqrt{\sigma_{\hat{y}}^2 \sigma_{\varepsilon}^2}} \quad \dots \sum_{i=1}^N \varepsilon = 0 \\
&\quad \text{and } \sum_{i=1}^N \hat{y} \varepsilon = 0, \text{ has been proved in } \textbf{Proof 1}. \\
&= 0
\end{aligned}$$

Hence, it is proved that $\text{Corr}(\hat{y}, \varepsilon) = 0$, as well as $\text{Cov}(\hat{y}, \varepsilon) = 0$.

Proof 3. The coefficient of determination is equivalent to the squared Pearson correlation coefficient, $R^2(y, \hat{y}) \equiv r_{y\hat{y}}^2$.

$$\begin{aligned}
r^2(y, \hat{y}) &= \left(\frac{\text{Cov}(y, \hat{y})}{\sqrt{\sigma_y^2 \sigma_{\hat{y}}^2}} \right)^2 \\
&= \frac{\text{Cov}(y, \hat{y}) \text{Cov}(y, \hat{y})}{\sigma_y^2 \sigma_{\hat{y}}^2}
\end{aligned}$$

Recall that residual, $\varepsilon = y - \hat{y} \Leftrightarrow y = \hat{y} + \varepsilon$.

$$= \frac{\text{Cov}(\hat{y} + \varepsilon, \hat{y}) \text{Cov}(\hat{y} + \varepsilon, \hat{y})}{\sigma_y^2 \sigma_{\hat{y}}^2}$$

This equation can be expanded since $\text{Cov}(a, (b + c)) = \text{Cov}(a, b) + \text{Cov}(a, c)$, and then can be further simplified since $\text{Cov}(a, a) = \sigma_a^2$. The cancellation of $\text{Cov}(\hat{y}, \varepsilon)$ is due to the second property of residuals, as proved in *Proof 2*.

$$= \frac{(\text{Cov}(\hat{y}, \hat{y}) + \text{Cov}(\hat{y}, \varepsilon))(\text{Cov}(\hat{y}, \hat{y}) + \text{Cov}(\hat{y}, \varepsilon))}{\sigma_y^2 \sigma_{\hat{y}}^2}$$

$$\begin{aligned}
&= \frac{\text{Cov}(\hat{y}, \hat{y}) \text{Cov}(\hat{y}, \hat{y})}{\sigma_y^2 \sigma_{\hat{y}}^2} \\
&= \frac{\sigma_{\hat{y}}^2 \sigma_{\hat{y}}^2}{\sigma_y^2 \sigma_{\hat{y}}^2} \\
r^2(y, \hat{y}) &= \frac{N^{-1} \sum_{i=1}^N (\hat{y}_i - \mu_{\hat{y}_i})^2}{N^{-1} \sum_{i=1}^N (y_i - \mu_{y_i})^2}
\end{aligned}$$

where explained sum of squares, $ESS = N^{-1} \sum_{i=1}^N (\hat{y}_i - \mu_{\hat{y}_i})^2$, total sum of squares, $TSS = N^{-1} \sum_{i=1}^N (y_i - \mu_{y_i})^2$, and hence $R_{y\hat{y}}^2 = \frac{ESS}{TSS} = r^2(y, \hat{y})$.