

## I. SUPPLEMENTARY INFORMATION

In this section we introduce the necessary notation to understand the formulae of the variance analyses from the previous sections. We focus on a simple example of a quantity  $y$  that depends on the variable  $x$ . In Figure 1 we show several measurements (full black circles) of the quantity  $y$  with the corresponding fitted curve. For a certain value  $x$  we perform several different measurements of the quantity  $y$ , thus, every point in the graph can be labeled with an index  $ij$  where the index  $i$  corresponds to the  $x$  value (also called level) and the index  $j$  corresponds to different measurements of the same level  $x$ , say  $y_{ij}$ . We define the mean value of the measurements at a certain  $x$  (or index  $i$ ) as  $\bar{y}_i$ . Moreover, we define the mean value of all the quantities  $y_{ij}$  as  $\bar{y}$ , and the value of the fitted curve at  $x$  as  $\hat{y}_i$ . Now, if we perform  $n_i$  measurements for each level  $i$  we obtain that the total number of observations are  $n = \sum n_i$ . Finally, defining as  $m$  the number of different levels for  $x$  and as  $p$  the number of parameters of our least square fitted model, we can build the formulae for the variance analysis of Table I. The differences in the expressions of the sum of squares of Table I are depicted in Figure 1. The difference  $(\hat{y}_i - \bar{y}_i)^2$  is a measure of the deviation of the mean value of a level with the value of the fitted model at the same level. These differences can be small depending on the fitted model employed and they are called adjust error differences. The difference  $(y_{ij} - \bar{y}_i)^2$  is a measure of the deviation of the measurement on a level with respect to its level mean value. In this case, these differences do not depend on the model and they are called pure error differences. The sum of the adjust error differences with the pure error differences is called the residual. For the  $F$ -distribution and  $F$ -criterion employed in the this article, as well as for more detailed information about variance analysis, see [1].

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[1] D.C. Montgomery, Design and Analysis of Experiments, 8 edition, Wiley.

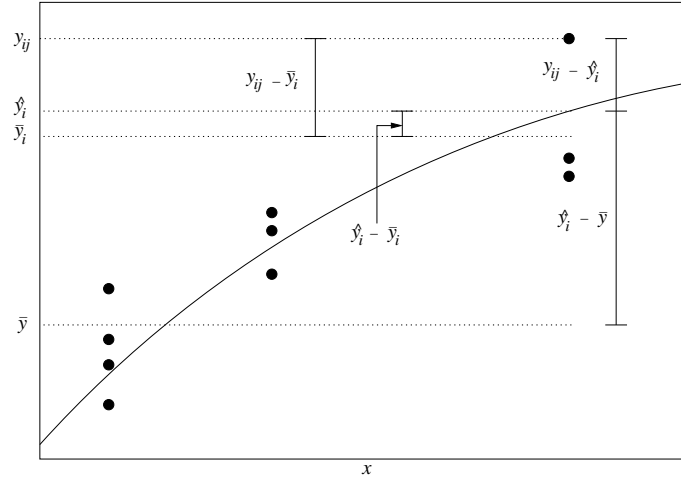


FIG. 1. Figure showing the elements present in the variance formulae of Table I.

TABLE I. Formulae for the variance analysis

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square
Regression	$SS_{\text{REG}} = \sum_i^m \sum_j^{n_i} (\hat{y}_i - \bar{y})^2$	$p - 1$	$MS_{\text{REG}} = \frac{SS_{\text{REG}}}{p - 1}$
Residual	$SS_{\text{RES}} = \sum_i^m \sum_j^{n_i} (y_{ij} - \hat{y}_i)^2$	$n - p$	$MS_{\text{RES}} = \frac{SS_{\text{RES}}}{n - p}$
Adjust Error	$SS_{\text{ADJ}} = \sum_i^m \sum_j^{n_i} (\hat{y}_i - \bar{y}_i)^2$	$m - p$	$MS_{\text{ADJ}} = \frac{SS_{\text{ADJ}}}{m - p}$
Pure Error	$SS_{\text{PURE}} = \sum_i^m \sum_j^{n_i} (y_{ij} - \bar{y}_i)^2$	$n - m$	$MS_{\text{PURE}} = \frac{SS_{\text{PURE}}}{n - m}$
Total	$SS_{\text{TOT}} = \sum_i^m \sum_j^{n_i} (y_{ij} - \bar{y})^2$	$n - 1$	
	% of the explained variation: $\frac{SS_{\text{REG}}}{SS_{\text{RES}}}$		
	% of the maximum explained variation: $\frac{SS_{\text{TOT}} - SS_{\text{PURE}}}{SS_{\text{TOT}}}$		