The contributions of distinct sets of explanatory variables to the model are typically captured by breaking up the overall regression (or model) sum of squares into distinct components.

This is useful quite generally in linear models, but especially in ANOVA models where the response is modeled in terms of one or more class variables or factors. In such cases, the model sum of squares is decomposed into sums of squares for each of the distinct sets of dummy, or indicator, variables necessary to capture each of the factors in the model.

For example, the following model is appropriate for a randomized complete block design (RCBD)

$$y_{ij} = \mu + \beta_j + \alpha_i + e_{ij}$$

where y_{ij} is the response from the ith treatment in the jth block, and β_j and α_i are block and treatment effects, respectively. This model can also be written as

$$\mathbf{y} = \mu\mathbf{j}_n + \beta_1\mathbf{b}_1 + \cdots + \beta_b\mathbf{b}_b + \alpha_1\mathbf{t}_1 + \cdots + \alpha_a\mathbf{t}_a + \mathbf{e} \qquad (*)$$

In this context, the notation $SS(\alpha|\beta,\mu)$ denotes *the extra regression sum of squares due to fitting the* α_i*s after fitting* μ *and the* β_j*s* and is given by

$$SS(\alpha|\beta,\mu) = \mathbf{y}^T(\mathbf{P}_{C(\mathbf{X})} - \mathbf{P}_{C(\mathbf{X}_1)})\mathbf{y}$$

where $\mathbf{X}_1 = (\mathbf{j}_n, \mathbf{b}_1, \ldots, \mathbf{b}_b)$ and $\mathbf{X} = (\mathbf{X}_1, \mathbf{t}_1, \ldots, \mathbf{t}_a)$.

- Sums of squares like this one that can be computed by fitting successively more complex models and taking the difference in regression/model sum of squares at each step are called *sequential sums of squares.*

- They represent the contribution of each successive group of explanatory variables above and beyond those explanatory variables already in the model.

Any model that can be written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \mathbf{X}_3\boldsymbol{\beta}_3 + \cdots + \mathbf{e}$$

has a sequential sum of squares decomposition. That is, the regression or model sum of squares $SS_{\text{Model}} = \mathbf{y}^T\mathbf{P}_{C(\mathbf{X})}\mathbf{y} = \|\mathbf{P}_{C(\mathbf{X})}\mathbf{y}\|^2$ can always be decomposed as follows:

$$\begin{aligned} SS_{\text{Model}} &= \|\mathbf{P}_{C(\mathbf{X})}\mathbf{y}\|^2 \\ &= \|\mathbf{P}_{C(\mathbf{X}_1)}\mathbf{y}\|^2 + \|(\mathbf{P}_{C(\mathbf{X}_1,\mathbf{X}_2)} - \mathbf{P}_{C(\mathbf{X}_1)})\mathbf{y}\|^2 \\ &\qquad + \|(\mathbf{P}_{C(\mathbf{X}_1,\mathbf{X}_2,\mathbf{X}_3)} - \mathbf{P}_{C(\mathbf{X}_1,\mathbf{X}_2)})\mathbf{y}\|^2 + \cdots \\ \text{or} \quad SS_{\text{Model}} &= SS(\boldsymbol{\beta}_1) + SS(\boldsymbol{\beta}_2|\boldsymbol{\beta}_1) + SS(\boldsymbol{\beta}_3|\boldsymbol{\beta}_1,\boldsymbol{\beta}_2) + \cdots \end{aligned}$$

- Note that by construction, the projections and squared lengths of projections in such a decomposition are independent because the spaces onto which we are projecting are mutually orthogonal.
- Such a decomposition can be extended to any number of terms.

Consider the RCBD model (*). This model can be written as

$$\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \mathbf{X}_3\boldsymbol{\beta}_3 + \mathbf{e}$$

where

$$\mathbf{X}_1 = \mathbf{j}_N, \quad \mathbf{X}_2 = (\mathbf{b}_1, \ldots, \mathbf{b}_b), \quad \mathbf{X}_3 = (\mathbf{t}_1, \ldots, \mathbf{t}_a)$$

and $\boldsymbol{\beta}_1 = \mu$, $\boldsymbol{\beta}_2 = (\beta_1, \ldots, \beta_b)^T$, and $\boldsymbol{\beta}_3 = (\alpha_1, \ldots, \alpha_a)^T$.

The sequential break-down of the model sum of squares here is

$$SS_{\text{Model}} = SS(\mu) + SS(\beta|\mu) + SS(\alpha|\beta, \mu) \qquad (**)$$

Consider the null hypothesis $H_0 : \alpha_1 = \cdots = \alpha_a = 0$. The null model corresponding to this hypothesis is $y_{ij} = \mu + \beta_j + e_{ij}$.

Fitting just the null model we have

$$SS_{\text{Model0}} = SS(\mu) + SS(\beta|\mu).$$

Note that SSE $= SS_T - SS_{\text{Model}}$, where $SS_T = \|\mathbf{y}\|^2$ is the total (uncorrected) sum of squares. Therefore, the difference in error sums of squares between the null model and the maintained model is

$$\begin{aligned}\text{SSE}_0 - \text{SSE} &= (SS_T - SS_{\text{Model0}}) - (SS_T - SS_{\text{Model}}) \\ &= SS_{\text{Model}} - SS_{\text{Model0}} = SS(\alpha|\beta, \mu).\end{aligned}$$

- That is, $SS(\alpha|\beta, \mu)$ is an appropriate sum of squares for the numerator of the $F-$ test for testing $y_{ij} = \mu + \beta_j + e_{ij}$ versus $y_{ij} = \mu + \beta_j + \alpha_i + e_{ij}$.
- Similarly, we can test $y_{ij} = \mu + e_{ij}$ versus $y_{ij} = \mu + \beta_j + e_{ij}$ using $SS(\beta|\mu)$ as the numerator sum of squares.
- Finally, we can test $y_{ij} = \mu + e_{ij}$ versus $y_{ij} = \mu + \beta_j + \alpha_i + e_{ij}$ using $SS(\alpha, \beta|\mu) \equiv SS(\alpha|\beta, \mu) + SS(\beta|\mu)$.

This last test is a test for significance of the entire model (other than the constant term), or the overall regression test we have already encountered.

The sequential sums of squares used in decomposition (**) are known as **Type I sums of squares.** This terminology is from SAS, but it has taken hold more generally.

Notice that with Type I (sequential) sums of squares we can decompose SS_{Model} either as

$$SS_{\text{Model}} = SS(\mu) + SS(\beta|\mu) + SS(\alpha|\beta,\mu)$$

or as

$$SS_{\text{Model}} = SS(\mu) + SS(\alpha|\mu) + SS(\beta|\alpha,\mu)$$

- That is, if we happen to add the block effects to the model first, then the appropriate test statistic is based on $SS(\alpha|\beta,\mu)$. If we happen to add the treatment effects first then the test is based on $SS(\alpha|\mu)$.
- In addition, although $SS(\alpha|\beta,\mu) = SS(\alpha|\mu)$ for <u>some</u> models (e.g., balanced ANOVA models), such a result is not true, in general.
  - Clearly, there's something dissatisfying about obtaining different tests based on the order of the terms in the model.
  - There's an asymmetry in the way that the α's and β's are treated in the Type I SSs.
- In contrast we might choose to always test the α's based on $SS(\alpha|\beta,\mu)$ and to test the β's based on $SS(\beta|\alpha,\mu)$.
- Sums of squares like $SS(\alpha|\beta,\mu)$ and $SS(\beta|\alpha,\mu)$ are called **Type II sums of squares** in SAS.

- Type II SS's correct the order-dependence of Type I SS's. In the RCBD mode, for example, Type II SS's treat main effects for blocks ($SS(\beta|\alpha,\mu)$) and treatments ($SS(\alpha|\beta,\mu)$) in a symmetric way.

- For a full definition of Type II SS's we need to understand what a hierarchical model is.

Hierarchical models: Hierarchical models are models in which the inclusion of any interaction effect necessarily implies the inclusion of all lower-level interactions and main effects involving the factors of the original interaction.

- E.g., in the context of a two-way layout, the usual model has main effects α_i and β_j for the levels of each of the two factors A and B, and interaction effects $(\alpha\beta)_{ij}$ corresponding to $A * B$. However, there is nothing to prevent us from considering simpler models.

- The model
$$y_{ijk} = \mu + \alpha_i + (\alpha\beta)_{ij} + e_{ijk}$$
is not a hierachical model, because we have included an $A * B$ interaction, but no main effect for factor B. In a hierarchical model, the inclusion of $(\alpha\beta)_{ij}$ requires the inclusion of both α_i and β_j.

- Similarly, suppose we have a three-way layout. The full hierarchical model is
$$y_{ijkl} = \mu + \alpha_i + \beta_j + \gamma_k + (\alpha\beta)_{ij} + (\alpha\gamma)_{ik} + (\beta\gamma)_{jk} + (\alpha\beta\gamma)_{ijk} + e_{ijkl}$$
Here, γ_k is an effect for the k^{th} level of factor C, $(\alpha\gamma)_{ik}$ and $(\beta\gamma)_{jk}$ are two way interactions for $A * C$ and $B * C$, and $(\alpha\beta\gamma)_{ijk}$ is the three-way interaction $A * B * C$. Two examples of non-hierarchical three-factor models are
$$y_{ijkl} = \mu + \alpha_i + \beta_j + \gamma_k + (\alpha\beta)_{ij} + (\beta\gamma)_{jk} + (\alpha\beta\gamma)_{ijk} + e_{ijkl}$$
$$\text{and} \quad y_{ijkl} = \mu + \alpha_i + \gamma_k + (\alpha\beta)_{ij} + (\alpha\gamma)_{ik} + (\alpha\beta\gamma)_{ijk} + e_{ijkl}$$

- I believe (and most statisticians would agree) that, in general, it is best to restrict attention to hierarchical models unless there is a compelling reason that in a particular application the omission of a lower-order term makes sense (e.g., is suggested by some theory or known fact from the context of the problem).

  - This principle is similar to the notion that in a polynomial regression model: $y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_q x_i^q + e_i$ one should not consider any model in which a term $\beta_k x_i^k$ is included, but where any of the terms $\beta_0, \beta_1 x_i, \ldots, \beta_{k-1} x_i^{k-1}$ are excluded.

Type II SS's computes the SS for a factor U, say, as the reduction in SS's obtained by adding a term for factor U to the model that is the largest hierarchical model that does not contain U.

- E.g., in the two-way layout, the Type II SS's are

$$SS_A = SS(\alpha|\beta,\mu), \quad SS_B = SS(\beta|\alpha,\mu), \quad SS_{AB} = SS((\alpha\beta)|\alpha,\beta,\mu)$$

  - Notice that there is no longer an order effect. Factor B is adjusted for A and factor A is adjusted for B.

- Another example: in the three-way layout, the Type II SS's are

$$SS_A = SS(\alpha|\mu,\beta,\gamma,(\beta\gamma)), \quad SS_B = SS(\beta|\mu,\alpha,\gamma,(\alpha\gamma)), \quad SS_C = SS(\gamma|\mu,\alpha,\beta,(\alpha\beta))$$
$$SS_{AB} = SS((\alpha\beta)|\mu,\alpha,\beta,\gamma,(\alpha\gamma),(\beta\gamma)) \quad SS_{AC} = SS((\alpha\gamma)|\mu,\alpha,\beta,\gamma,(\alpha\beta),(\beta\gamma))$$
$$SS_{BC} = SS((\beta\gamma)|\mu,\alpha,\beta,\gamma,(\alpha\beta),(\alpha\gamma)) \quad SS_{ABC} = SS((\alpha\beta\gamma)|\mu,\alpha,\beta,\gamma,(\alpha\beta),(\alpha\gamma),(\beta\gamma))$$

Type III SS's:

When using ANOVA models for the analysis of experimental data, the scientific focus is often on comparing mean responses across different levels of the treatment factors (e.g., low, medium high doses of a drug; presence vs. abscence of fertilizer,; etc.).

In an expperiment with only one treatment factor, the levels of that factor are the treatments, and means across these treatments are typically of interest. However, in a factorial design, the treatments are the experimental conditions corresponding to combinations of the levels of two or more factors.

- E.g., in a two-way layout with two factors, A and B, with a and b levels, respectively, we may be interested in comparing means across the treatments, where the treatment means correspond to the cells of the following table

Levels of Factor A	Levels of Factor B 1	2	$\cdots$	b	
1	μ_{11}	μ_{12}	$\cdots$	μ_{1b}	$\bar{\mu}_{1\cdot}$
2	μ_{21}	μ_{22}	$\cdots$	μ_{2b}	$\bar{\mu}_{2\cdot}$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
a	μ_{a1}	μ_{a2}	$\cdots$	μ_{ab}	$\bar{\mu}_{a\cdot}$
	$\bar{\mu}_{\cdot 1}$	$\bar{\mu}_{\cdot 2}$	$\cdots$	$\bar{\mu}_{\cdot b}$	

Here, μ_{ij} is the population mean for the i,jth treatment, or the treatment corresponding to the ith level of factor A combinaed with the jth level of factor B. These μ_{ij} are the parameters of the full-rank cell means model:

$$y_{ijk} = \mu_{ij} + e_{ijk}, \quad i = 1, \ldots, a, j = 1, \ldots, b, k = 1, \ldots, n_{ij}$$

or, in terms of the overparameterized effects model,

$$y_{ijk} = \underbrace{\mu + \alpha_i + \beta_j + (\alpha\beta)_{ij}}_{=\mu_{ij}} + e_{ijk}$$

While it is often of interest to compare treatment means (e.g., to test $H_0 : \mu_{ij} = \mu_{i'j'}$), it also often of interest to compare the mean response across levels of factor A *marginally*; that is, after averaging across factor B (or vice versa).

We define the marginal mean at the ith level of factor A to be $\bar{\mu}_{i\cdot} = \frac{1}{b}\sum_{j=1}^{b} \mu_{ij}$ or, in terms of the effects model,

$$\bar{\mu}_{i\cdot} = \frac{1}{b}\sum_{j=1}^{b}(\mu + \alpha_i + \beta_j + (\alpha\beta)_{ij}) = \mu + \alpha_i + \bar{\beta}_{\cdot} + (\bar{\alpha\beta})_{i\cdot}.$$

- Marginal means for each of the level of factor B are defined similarly.

If we are interested in making comparisons among the marginal means, it would be nice if our sum of squares for factor A, and for factor B led to an F test, $F = \frac{SS_A/\mathrm{df}_A}{MSE}$, which tested a simple hypothesis of interest like $H_0 : \bar{\mu}_{1\cdot} = \bar{\mu}_{2\cdot} = \cdots = \bar{\mu}_{a\cdot}$.

- It turns out that both the Type I and Type II approach to calculating SS_A do not test such a hypothesis. Type III SS's, also know as **marginal sums of squares**, do.

It can be shown that, in terms of the marginal means, the hypotheses tested by Type I and Type II SS's are difficult to interpret, and not at all the sorts of hypotheses that one would typically be interested in if the focus of the analysis was to compare treatment means (which it usually is).

- For example, in the two-way layout, the hypotheses tested by $F_A = \frac{SS_A/\text{df}_A}{MS_E}$ for Type I and II versions of SS_A are:

$$\text{Type I:} \qquad H_0 : \sum_{j=1}^{b} \frac{n_{1j}\mu_{1j}}{n_{1\cdot}} = \cdots = \sum_{j=1}^{b} \frac{n_{aj}\mu_{aj}}{n_{a\cdot}}$$

$$\text{Type II:} \qquad H_0 : \sum_{j=1}^{b} n_{1j}\mu_{1j} = \sum_{i=1}^{a}\sum_{j=1}^{b} \frac{n_{1j}n_{ij}\mu_{ij}}{n_{\cdot j}}, \ldots, \sum_{j=1}^{b} n_{aj}\mu_{aj} = \sum_{i=1}^{a}\sum_{j=1}^{b} \frac{n_{aj}n_{ij}\mu_{ij}}{n_{\cdot j}}$$

- These hypotheses (especially those from Type II) are strange. They correspond to testing whether certain weighted marginal averages of the treatment means are equal. Testing such hypotheses is seldom of interest. If one is interested in comparing means across the levels of factor A, these SS's are definitely not what one would want to use.

Type III SS's are designed to always test simple hypotheses on (unweighted) marginal population means. In particular, for the Type III version of SS_A, F_A tests the hypothesis

$$\text{Type III:} \qquad H_0 : \bar{\mu}_{1\cdot} = \cdots = \bar{\mu}_{a\cdot}$$

Similarly, the Type III version of SS_B leads to a test of

$$\text{Type III:} \qquad H_0 : \bar{\mu}_{\cdot 1} = \cdots = \bar{\mu}_{\cdot b}$$

- All three types of SS's lead to the same (reasonable and appropriate) hypothesis for $F_{AB} = MS_{AB}/MS_E$. Namely,

$$H_0 : (\mu_{ij} - \mu_{ij'}) - (\mu_{i'j} - \mu_{i'j'}) = 0, \quad \text{for all } i, i', j, j'$$

Type III SS's also have an interpretation in terms of reduction in SS's. For the two way layout model **with sum-to-zero restrictions on the parameters** the Type III SS's are:

$$SS_A = SS(\alpha|\mu, \beta, (\alpha\beta)), \quad SS_B = SS(\beta|\mu, \alpha, (\alpha\beta)), \quad SS_{AB} = SS((\alpha\beta)|\mu, \alpha, \beta).$$

- Note that this interpretation only applies to the sum-to-zero restricted version of the two-way layout model. For other restrictions, the interpretation would be different. A much better way to understand Type III SS's is in terms of the hypotheses tested on the marginal means, as described above.

Type IV SS's:

The fourth type of SS's is useful when there are certain treatment combinations for which $n_{ij} = 0$.

- My recommendation is to avoid the use of Type IV SSs. If factorial designs are encountered with missing treatments, I suggest instead the use of a one-way anova model, treating the treatments with data as levels of a single treatment factor. Interactions and main effects can be investigated by testing hypotheses on the treatment means.

- If you're really interested, you can refer to Milliken & Johnson (1992) or Littell, Freund, & Spector (*SAS System for Linear Models, Third Edition, 1991*) for information on Type IV SS's.

Relationships Among the Types and Recommendations:

In certain situations, the following equalities among the types of SS's hold:

$$
\begin{aligned}
I = II = III = IV &\qquad \text{for balanced data} \\
II = III = IV &\qquad \text{for no-interaction models} \\
III = IV &\qquad \text{for all-cells-filled data}
\end{aligned}
$$

If one is interested in model-building (finding a parsimonious well-fitting model for the data) then

i. use Type I for choosing between models of sequentially increasing complexity; and

ii. use Type II for choosing between hierarchical models.

If one is interested in testing hypotheses that compare means across the levels of experimentally controlled factors

iii. use Type III.

- Note that Type I SS's are the only type of sum of squares that, in general, lead decompose the total sum of squares. E.g., in the two-way anova model, they are the only type of SS that guarantee that $SS_T = SS_A + SS_B + SS_{AB} + SS_E$ holds, in general.
- However, all four types yield sums of squares that are independent of SS_E and all lead to valid F tests (just of different hypotheses).
- Independence of these SSs from the SSE is guaranteed because all four types of SSs are squared lengths of projections onto some subspace of $C(\mathbf{X})$, whereas SSE is the squared length of a projection onto $C(\mathbf{X})^{\perp}$.