# Supplementary material. Optimal response surface designs for detection and minimization of model contamination

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## A Trace-based Criteria

### A.1 Lack-of-fit criterion

Together with the Lack-of-fit DP-criterion derived in Section 3.1, we formulate a criterion to estimate the lack-of-fit by minimizing the average squared lengths of posterior confidence intervals for linear functions of $\boldsymbol{\beta}_q$ defined by matrix $\boldsymbol{P}$. We define the "Lack-of-fit LP-criterion" using the mean of the squared lengths of the $100(1-\alpha_{LoF})\%$ posterior confidence intervals for these linear functions, i.e. we minimize

$$\frac{1}{q}\text{trace}\left[\boldsymbol{P}\boldsymbol{P}^T\left(\boldsymbol{L}+\frac{\boldsymbol{I}_q}{\tau^2}\right)^{-1}\right]F_{1,d;1-\alpha_{LoF}}. \tag{1}$$

This trace-based criterion is linked to the lack-of-fit part of Generalized $L$-optimality (**?**), and the pure error estimation approach retains the corresponding upper point of the F-distribution. Henceforth we mainly consider the case when $\boldsymbol{P}\boldsymbol{P}^T$ is diagonal, and the criterion above is reduced to weighted-$AP$-optimality. In other words, the "Lack-of-fit AP-criterion" stands for minimization of the weighted average of the $q$-dimensional vector of the posterior confidence intervals' squared lengths for the potential parameters.

Maximizing the (weighted) trace of the dispersion matrix $\boldsymbol{L}$ translates into maximizing the (weighted) mean distance of potential terms from the linear subspace spanned by the primary terms. Aiming towards the primary and potential subspaces being as near to orthogonal to each other as possible also works towards maximizing the power of the lack-of-fit test.

### A.2 MSE-based criterion

To derive the trace-based form of the MSE criterion, we calculate the expectation of the trace function of the MSE matrix (**??**), under the prior for the potential terms $\boldsymbol{\beta}_q \sim$

$\mathcal{N}(\mathbf{0}, \tau^2\sigma^2\boldsymbol{I}_q)$:

$$\begin{aligned}
\mathtt{E}_{\boldsymbol{\beta}_q}\text{trace}[\text{MSE}(\hat{\boldsymbol{\beta}}_p|\boldsymbol{\beta}_q)] &= \text{trace}[\mathtt{E}_{\boldsymbol{\beta}_q}\text{MSE}(\hat{\boldsymbol{\beta}}_p|\boldsymbol{\beta}_q)] \\
&= \text{trace}[\sigma^2(\boldsymbol{X}_p^T\boldsymbol{X}_p)^{-1} + \mathtt{E}_{\boldsymbol{\beta}_q}(\boldsymbol{A}\boldsymbol{\beta}_q\boldsymbol{\beta}_q^T\boldsymbol{A}^T)] \\
&= \text{trace}[\sigma^2(\boldsymbol{X}_p^T\boldsymbol{X}_p)^{-1} + \sigma^2\tau^2\boldsymbol{A}\boldsymbol{A}^T] \\
&= \sigma^2\text{trace}[(\boldsymbol{X}_p^T\boldsymbol{X}_p)^{-1} + \tau^2\boldsymbol{A}\boldsymbol{A}^T] \\
&= \sigma^2[\text{trace}\{(\boldsymbol{X}_p^T\boldsymbol{X}_p)^{-1}\} + \tau^2\text{trace}\boldsymbol{A}\boldsymbol{A}^T].
\end{aligned}$$

The operations of calculating trace and expectation are commutative, hence there is no necessity of any additional numerical evaluations, and in the case of the trace-based criterion using the point prior for $\boldsymbol{\beta}_q$ at $\boldsymbol{\beta}_q = \pm\sigma\tau\mathbf{1}_q$ would lead to the same resulting function. By minimizing the whole function above, we simultaneously minimize both the average variance of the primary terms and the expected squared norm of the bias vector in the direction of the potential terms, scaled by $\tau^2$ which regulates the magnitude of the potential terms relative to the error variance. We formally define the "MSE(L)-criterion" to minimize

$$\frac{1}{p}\text{trace}\{(\boldsymbol{X}_p^T\boldsymbol{X}_p)^{-1} + \tau^2\boldsymbol{A}\boldsymbol{A}^T\}. \tag{2}$$

## A.3 Compound criterion

Similarly, we obtain the trace-based "compound MSE-LP$_S$-criterion" by joining the LP$_S$ criterion with trace-based lack-of-fit (1) and MSE components to minimize

$$\begin{aligned}
&\left[\frac{1}{p-1}\text{trace}(\boldsymbol{W}\boldsymbol{X}_{p-1}^T\boldsymbol{Q}_0\boldsymbol{X}_{p-1})^{-1}F_{1,d;1-\alpha_{LP}}\right]^{\kappa_{LP}} \times \\
&\left[\frac{1}{q}\text{trace}\left(\boldsymbol{L} + \frac{\boldsymbol{I}_q}{\tau^2}\right)^{-1}F_{1,d;1-\alpha_{LoF}}\right]^{\kappa_{LoF}} \times \\
&\left[\frac{1}{p-1}\text{trace}[\boldsymbol{M}^{-1} + \tau^2\boldsymbol{A}\boldsymbol{A}^T]_{[p-1,p-1]}\right]^{\kappa_{MSE}}.
\end{aligned} \tag{3}$$

Here $[\boldsymbol{M}^{-1} + \tau^2\boldsymbol{A}\boldsymbol{A}^T]_{[p-1,p-1]}$ stands for the submatrix corresponding to the parameters of interest, that is with the first row and first column removed. Confidence levels $\alpha_{LP}$ and $\alpha_{LoF}$ play similar roles here, although they do not have to be the same as in the determinant-based criterion. Moreover, it would be sensible to take into account the multiple testing corrections, as we are dealing with minimizing the lengths of multiple confidence intervals rather than with the volume of a single region.

## A.4 Example

Figures 1 and 2 below provide a summary of MSE-LP$_S$-optimal designs (optimality criterion as in (3)) for the example considered in Section 3.4. The values of weights $\kappa_i$ and $\tau^2$ are the same as for the MSE-DP$_S$-optimal designs. Matrix $\boldsymbol{W}$ is diagonal, so that the $LP_S$-optimality is reduced to weighted AP-optimality; weights sum to 1, and are all equal except for the ones on the quadratic terms which are 1/4 of each of the rest of them; this weighting allows us to even out the contributions to the total variance.

Each point on the simplex plots corresponds to a design that has been obtained as optimal in terms of the 3 individual criteria (vertex points) and 7 more weight combinations; similar plots displaying pure error and lack-of-fit degrees of freedom across these designs are presented in Figure 3.

In general, the designs tend to be quite $DP$- and $LP$-efficient. $DP$-efficient designs (Figures **??**, **??**) are not bad in terms of $LP$-efficiency and vice versa, but the same cannot be observed for the lack-of-fit components and seems not to be true at all for the $MSE$ components, especially, for the $MSE(L)$-optimal design when $\tau^2 = 1$.

$MSE - LP_S$-optimal designs tend to have larger $LP$- and $MSE(L)$-efficiencies in the case of smaller $\tau^2$, which makes sense – smaller potential contamination leads to a more easily achievable compromise between the contradicting components of the criteria (the same is observed for the trace-based efficiencies of the $MSE - DP_S$-optimal designs).

The $MSE(L)$-component seems to be much more sensitive to the weight allocations than the $MSE(D)$ component: in the case of $\tau^2 = 1$ reasonable efficiencies are achieved only when most of the weight is on the 'potential terms' criterion components, i.e. designs in the lower right part of the simplex plot.

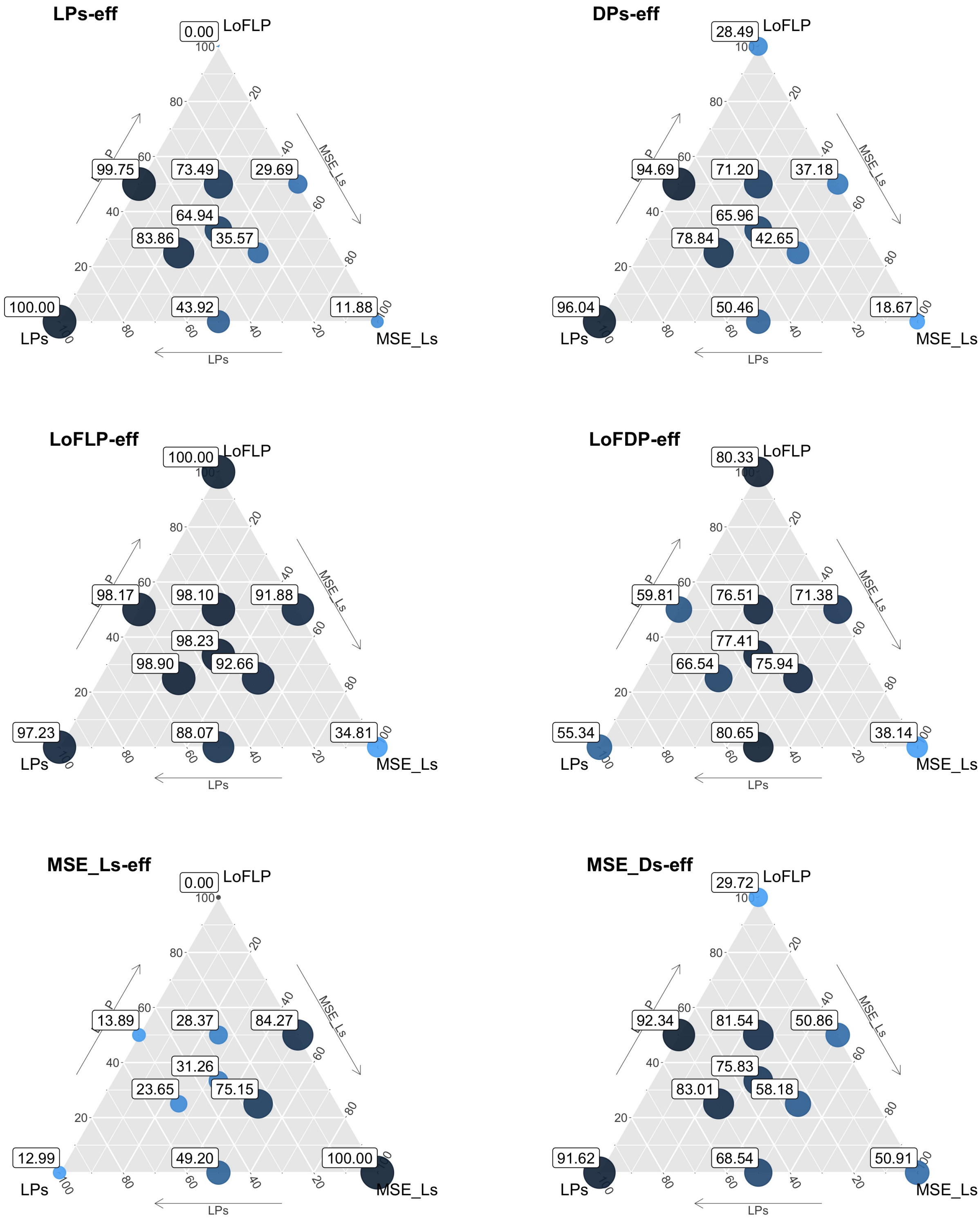


Figure 1: Efficiency values of $MSE - LP_S$-optimal designs, $\tau^2 = 1$.

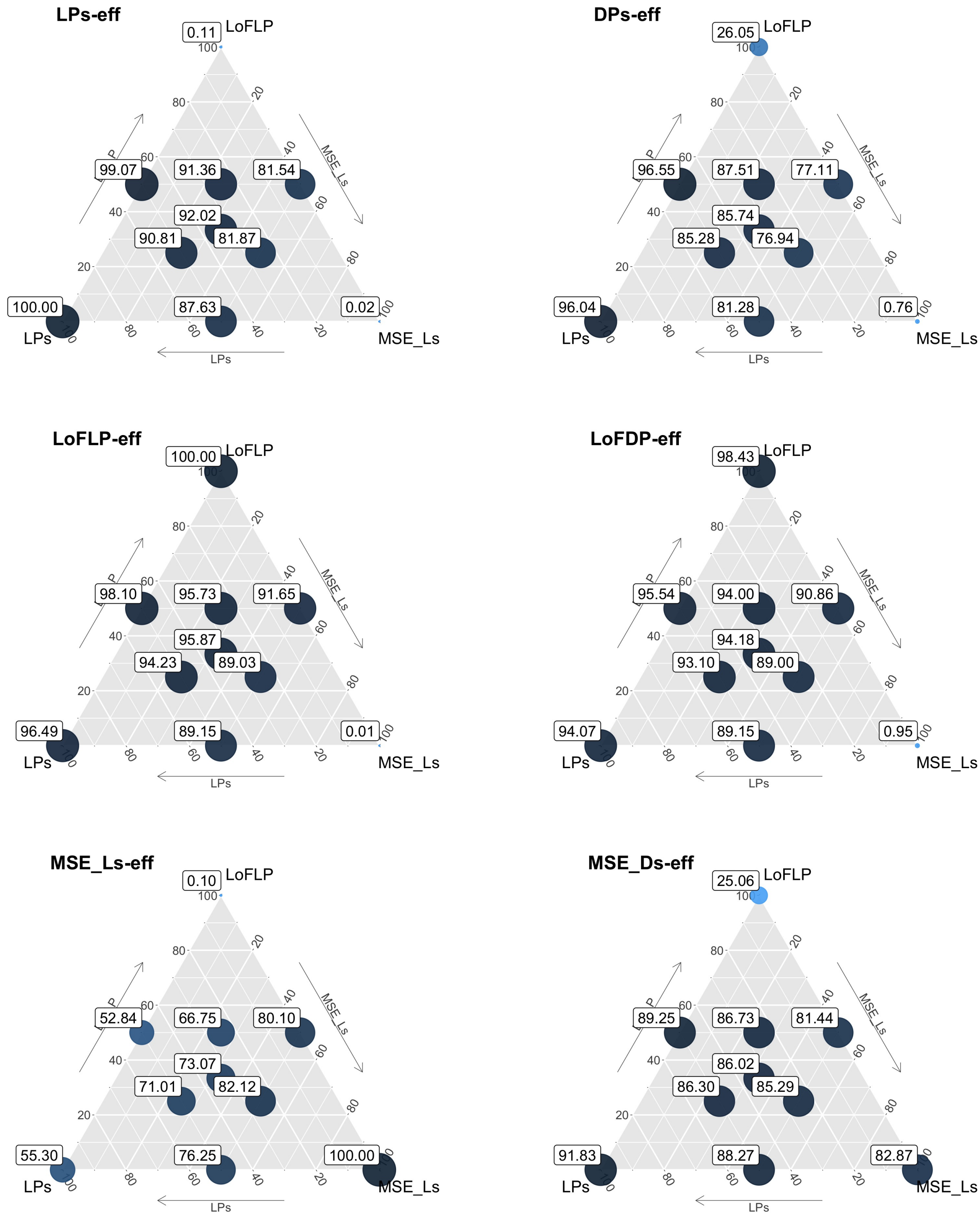


Figure 2: Efficiency values of $MSE - LP_S$-optimal designs, $\tau^2 = 1/q$.

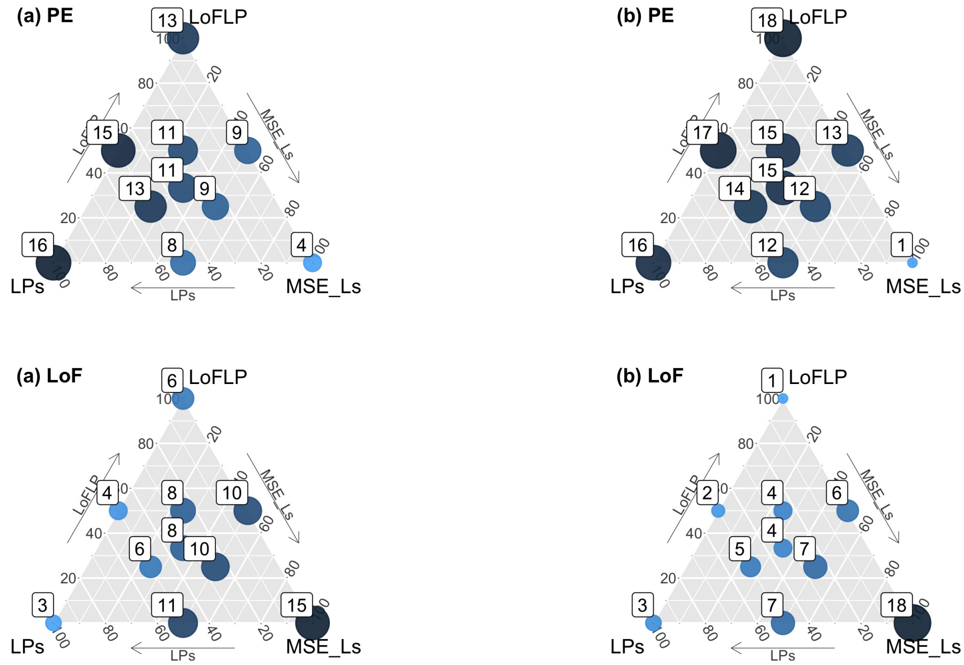


Figure 3: Pure error and lack-of-fit degrees of freedom of $MSE-LP_S$-optimal designs: (a) $\tau^2 = 1$ and (b) $\tau^2 = 1/q$.

# B MSE-DP$_S$ - optimal designs

## B.1 DP$_S$-optimal completely randomized design

The $DP_S$-optimal design from the example in Section **??** is shown in Table 1, and is also optimal: (i) for the uniform weight allocation across the three components; (ii) for the weight equally distributed between the DP$_S$- and LoF(DP)-components; and (iii) in terms of the criterion with half weight on the DP-component and a quarter on the LoF(DP) and MSE(D$_S$) components (all for $\tau^2 = 1/q$). The design has 18 pure error degrees of freedom which arise from pairs of replicated points – the only unreplicated points are #11, #16, #19 and #20. Fourteen of these pairs come from replicates of the $2^{5-1}$ fractional factorial, and the 4 remaining replicated points have 2 or 3 factors set to 0.

Table 1: MSE-DP$_S$-optimal design

| | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -1 | -1 | -1 | 0 | 0 | 11 | -1 | 0 | 1 | 1 | 0 | 21 | 0 | 0 | 1 | 0 | 1 | 31 | 1 | -1 | 1 | 1 | -1 |
| 2 | -1 | -1 | -1 | 0 | 0 | 12 | -1 | 1 | -1 | -1 | -1 | 22 | 0 | 0 | 1 | 0 | 1 | 32 | 1 | -1 | 1 | 1 | -1 |
| 3 | -1 | -1 | -1 | 1 | -1 | 13 | -1 | 1 | -1 | -1 | -1 | 23 | 0 | 1 | 0 | -1 | 0 | 33 | 1 | 1 | -1 | -1 | 1 |
| 4 | -1 | -1 | -1 | 1 | -1 | 14 | -1 | 1 | -1 | 1 | 1 | 24 | 0 | 1 | 0 | -1 | 0 | 34 | 1 | 1 | -1 | -1 | 1 |
| 5 | -1 | -1 | 1 | -1 | -1 | 15 | -1 | 1 | -1 | 1 | 1 | 25 | 1 | -1 | -1 | -1 | -1 | 35 | 1 | 1 | -1 | 1 | -1 |
| 6 | -1 | -1 | 1 | -1 | -1 | 16 | -1 | 1 | 0 | 0 | -1 | 26 | 1 | -1 | -1 | -1 | -1 | 36 | 1 | 1 | -1 | 1 | -1 |
| 7 | -1 | -1 | 1 | 1 | 1 | 17 | -1 | 1 | 1 | -1 | 1 | 27 | 1 | -1 | -1 | 1 | 1 | 37 | 1 | 1 | 1 | -1 | -1 |
| 8 | -1 | -1 | 1 | 1 | 1 | 18 | -1 | 1 | 1 | -1 | 1 | 28 | 1 | -1 | -1 | 1 | 1 | 38 | 1 | 1 | 1 | -1 | -1 |
| 9 | -1 | 0 | 0 | -1 | 1 | 19 | -1 | 1 | 1 | 1 | -1 | 29 | 1 | -1 | 1 | -1 | 1 | 39 | 1 | 1 | 1 | 1 | 1 |
| 10 | -1 | 0 | 0 | -1 | 1 | 20 | 0 | -1 | -1 | -1 | 1 | 30 | 1 | -1 | 1 | -1 | 1 | 40 | 1 | 1 | 1 | 1 | 1 |

## B.2 Sensitivity of $MSE - DP_S$-optimal design to $\tau^2$.

The sensitivity of the $MSE - DP_S$-optimal designs to $\tau^2$ is shown in Figure 4. Designs which include all three criterion components seem to be fairly insensitive to the prior value of $\tau$ chosen.

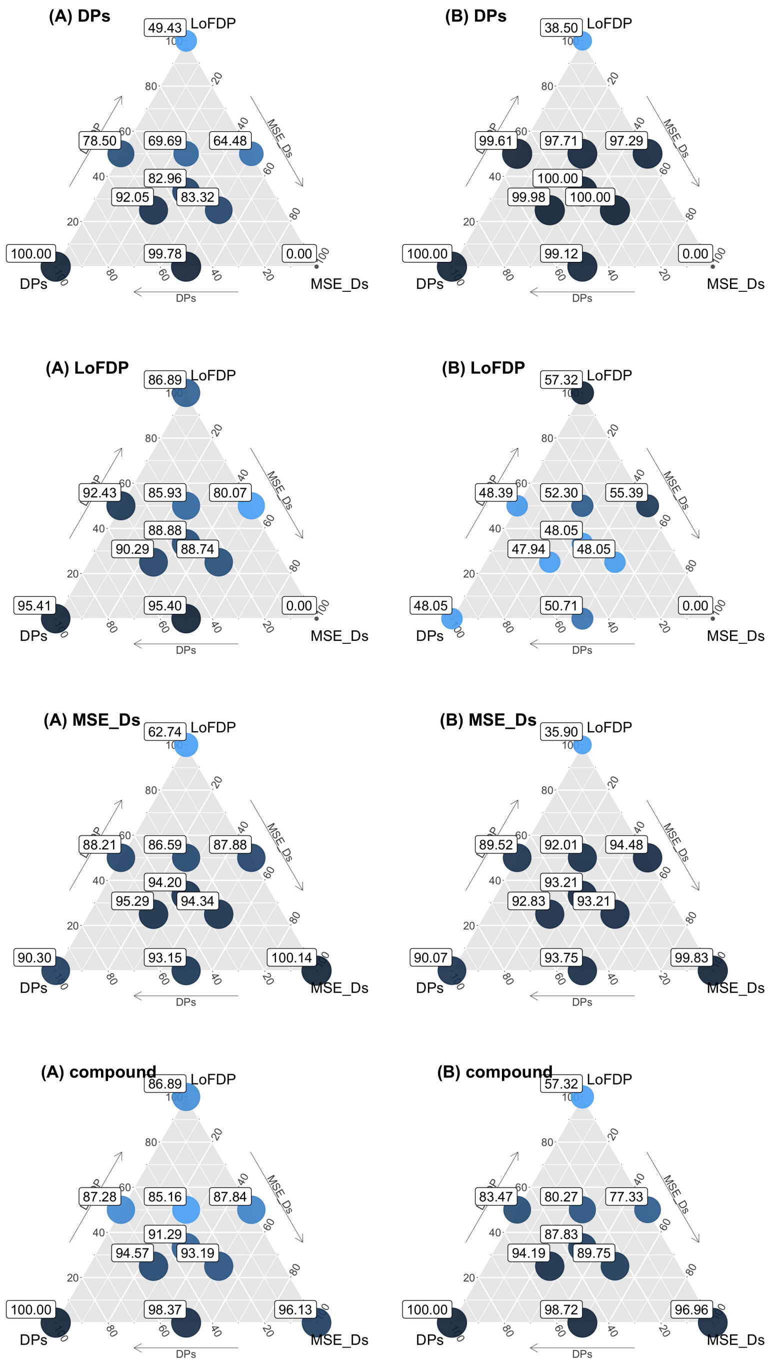


Figure 4: Sensitivity of $MSE - DP_S$-optimal design to $\tau^2$ values: individual and compound efficiency values. (A) ($\tau^2 = 1/q$)- efficiency values for ($\tau^2 = 1$)-optimal designs (*left*), (B) ($\tau^2 = 1$)- efficiency values for ($\tau^2 = 1/q$)-optimal designs (*right*).

## C Performance overview of the Pareto frontier designs, for MSE(DP)-optimality criteria

For 3000 random starts (which took $10-20$ hours), the resulting sets contain 769 ($\tau^2 = 1$) and 304 ($\tau^2 = 1/q$) designs optimized with respect to the $\mathrm{DP}_S$, LoF(DP) and $\mathrm{MSE(D}_S)$ criteria. There are two immediate observations: firstly, the $\mathrm{DP}_S$-optimal design(s) have not been found, and the best one is only $\sim 78\%$ $\mathrm{DP}_S$-efficient (88% and 98% for the other two criteria). This might occur due to the number of (conflicting) objectives, and the large number of candidate designs; increasing the number of random starts might improve that, but it is hard to tell how many would be sufficient for a specific example – we initially had 1000 starts, and no substantial improvement was noticeable. So, a search for designs optimal with respect to individual criteria would be recommended for reliable performance evaluation of the results.

Secondly, the large number of designs obtained results in the need to select the "best" one (and to define what "best" means). There are a few options here, e.g. choosing the ones closest to the utopia point, but in order to get a general overview of the designs obtained, we take the weighted product of the efficiency values and see which designs perform best in terms of various weight allocations; top performing designs for nine weight sets are presented in Tables 2 and3 for $\tau^2 = 1$, and $\tau^2 = 1/q$ respectively.

The designs have between 7 and 11 pure error degrees of freedom. Designs optimal with respect to the equal weight allocation, particularly #171 and #185 (highlighted), also perform well for other weight allocations, except when no weight was put on the DP-component, or when the majority of weight was on the MSE(D) criterion – the designs with such performance tendencies might be considered as good candidates if we are to choose from the Pareto frontier. Similar patterns are observed in case of the criteria with smaller $\tau^2$ (Table 3 below). As in the case of compound optimality, better performing designs across the board seem to be more similar: having $10-11$ pure error degrees of freedom, and seemingly with a compromise across the components being easier to find, compared to the case of larger $\tau^2$.

Table 2: Efficiency values (%) of some Pareto frontier designs, ordered with respect to various weight combinations. LoF(DP) and MSE($D_S$) criteria with $\tau^2 = 1$.

| **(1/3, 1/3, 1/3)** | **$DP_S$** | **LoF(DP)** | **MSE($D_S$)** | **(0, 1/2, 1/2)** | **$DP_S$** | **LoF(DP)** | **MSE($D_S$)** | **(1/3, 0, 2/3)** | **$DP_S$** | **LoF(DP)** | **MSE($D_S$)** |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 225 | 72.01 | 85.00 | 89.60 | 10 | 62.37 | 84.82 | 91.43 | 555 | 72.58 | 82.64 | 90.44 |
| *171* | *74.51* | *83.17* | *87.60* | 17 | 62.23 | 84.92 | 91.21 | 530 | 72.55 | 82.65 | 90.41 |
| 555 | 72.58 | 82.64 | 90.44 | 60 | 62.15 | 85.01 | 91.12 | 557 | 72.38 | 82.79 | 90.06 |
| *185* | *74.54* | *83.15* | *87.49* | 19 | 62.26 | 84.91 | 91.20 | 559 | 72.39 | 82.77 | 90.05 |
| 530 | 72.55 | 82.65 | 90.41 | 9 | 62.20 | 84.98 | 91.08 | 533 | 72.35 | 82.80 | 90.00 |
| 180 | 74.41 | 83.25 | 87.42 | 4 | 62.21 | 84.94 | 91.12 | 545 | 72.30 | 82.84 | 90.03 |
| 187 | 74.40 | 83.26 | 87.34 | 8 | 62.17 | 85.00 | 91.04 | 531 | 72.33 | 82.82 | 90.00 |
| 179 | 74.33 | 83.30 | 87.34 | 6 | 62.18 | 84.99 | 91.04 | 552 | 72.23 | 82.86 | 90.04 |
| 182 | 74.37 | 83.27 | 87.29 | 68 | 62.00 | 85.12 | 90.89 | 551 | 72.27 | 82.86 | 90.01 |
| 184 | 74.34 | 83.31 | 87.24 | 11 | 62.13 | 85.04 | 90.98 | 757 | 69.18 | 81.95 | 91.99 |
| **(1/2, 1/2, 0)** | $DP_S$ | LoF(DP) | MSE($D_S$) | **(1/2, 1/4, 1/4)** | $DP_S$ | LoF(DP) | MSE($D_S$) | **(1/4, 1/4, 1/2)** | $DP_S$ | LoF(DP) | MSE($D_S$) |
| 185 | 74.54 | 83.15 | 87.49 | 171 | 74.51 | 83.17 | 87.60 | 225 | 72.01 | 85.00 | 89.60 |
| 171 | 74.51 | 83.17 | 87.60 | 185 | 74.54 | 83.15 | 87.49 | 555 | 72.58 | 82.64 | 90.44 |
| 180 | 74.41 | 83.25 | 87.42 | 180 | 74.41 | 83.25 | 87.42 | 530 | 72.55 | 82.65 | 90.41 |
| 187 | 74.40 | 83.26 | 87.34 | 187 | 74.40 | 83.26 | 87.34 | 557 | 72.38 | 82.79 | 90.06 |
| 182 | 74.37 | 83.27 | 87.29 | 182 | 74.37 | 83.27 | 87.29 | 559 | 72.39 | 82.77 | 90.05 |
| 184 | 74.34 | 83.31 | 87.24 | 179 | 74.33 | 83.30 | 87.34 | 545 | 72.30 | 82.84 | 90.03 |
| 181 | 74.31 | 83.33 | 87.22 | 184 | 74.34 | 83.31 | 87.24 | 531 | 72.33 | 82.82 | 90.00 |
| 179 | 74.33 | 83.30 | 87.34 | 181 | 74.31 | 83.33 | 87.22 | 533 | 72.35 | 82.80 | 90.00 |
| 186 | 74.29 | 83.34 | 87.19 | 186 | 74.29 | 83.34 | 87.19 | 551 | 72.27 | 82.86 | 90.01 |
| 135 | 74.14 | 83.50 | 86.98 | 172 | 74.27 | 83.36 | 87.17 | 552 | 72.23 | 82.86 | 90.04 |
| **(1/2, 0, 1/2)** | $DP_S$ | LoF(DP) | MSE($D_S$) | **(1/4, 1/2, 1/4)** | $DP_S$ | LoF(DP) | MSE($D_S$) | **(1/3, 2/3, 0)** | $DP_S$ | LoF(DP) | MSE($D_S$) |
| 555 | 72.58 | 82.64 | 90.44 | 225 | 72.01 | 85.00 | 89.60 | 700 | 69.92 | 86.59 | 87.27 |
| 530 | 72.55 | 82.65 | 90.41 | 700 | 69.92 | 86.59 | 87.27 | 92 | 69.73 | 86.60 | 86.66 |
| 171 | 74.51 | 83.17 | 87.60 | 223 | 70.79 | 85.56 | 88.18 | 485 | 67.71 | 87.87 | 84.18 |
| 185 | 74.54 | 83.15 | 87.49 | 104 | 70.30 | 86.16 | 87.48 | 93 | 69.94 | 86.45 | 86.91 |
| 559 | 72.39 | 82.77 | 90.05 | 113 | 70.40 | 86.02 | 87.61 | 497 | 67.73 | 87.84 | 84.20 |
| 557 | 72.38 | 82.79 | 90.06 | 95 | 70.24 | 86.19 | 87.44 | 506 | 67.81 | 87.79 | 84.34 |
| 533 | 72.35 | 82.80 | 90.00 | 111 | 70.36 | 86.05 | 87.57 | 96 | 69.98 | 86.42 | 86.94 |
| 531 | 72.33 | 82.82 | 90.00 | 107 | 70.23 | 86.21 | 87.33 | 496 | 67.81 | 87.78 | 84.29 |
| 545 | 72.30 | 82.84 | 90.03 | 106 | 70.31 | 86.16 | 87.32 | 504 | 67.72 | 87.84 | 84.20 |
| 551 | 72.27 | 82.86 | 90.01 | 102 | 70.13 | 86.28 | 87.29 | 488 | 67.73 | 87.83 | 84.28 |

Table 3: Efficiency values (%) of some Pareto frontier designs ordered by various weight combinations. LoF(DP) and MSE($D_S$) criteria with $\tau^2 = 1/q$.

| **(1/3, 1/3, 1/3)** | $DP_S$ | LoF(DP) | MSE($D_S$) | **(0,1/2, 1/2)** | $DP_S$ | LoF(DP) | MSE($D_S$) | **(1/3, 0, 2/3)** | $DP_S$ | LoF(DP) | MSE($D_S$) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 186 | 76.73 | 90.59 | 85.61 | 186 | 76.73 | 90.59 | 85.61 | 120 | 76.95 | 84.94 | 90.04 |
| 185 | 76.71 | 90.64 | 85.51 | 185 | 76.71 | 90.64 | 85.51 | 117 | 76.96 | 84.96 | 89.91 |
| 184 | 76.52 | 90.73 | 85.31 | 184 | 76.52 | 90.73 | 85.31 | 119 | 76.87 | 84.94 | 89.94 |
| 181 | 76.84 | 89.81 | 85.62 | 187 | 76.30 | 90.78 | 85.09 | 165 | 76.88 | 84.98 | 89.91 |
| 189 | 76.75 | 89.91 | 85.53 | 81 | 75.80 | 87.08 | 88.63 | 163 | 76.82 | 84.95 | 89.94 |
| 180 | 76.80 | 89.85 | 85.52 | 188 | 76.09 | 90.88 | 84.87 | 122 | 76.87 | 85.00 | 89.90 |
| 187 | 76.30 | 90.78 | 85.09 | 183 | 76.03 | 90.93 | 84.82 | 118 | 76.81 | 84.97 | 89.92 |
| 120 | 76.95 | 84.94 | 90.04 | 78 | 75.67 | 87.11 | 88.52 | 162 | 76.75 | 85.01 | 89.69 |
| 117 | 76.96 | 84.96 | 89.91 | 166 | 76.08 | 90.79 | 84.92 | 116 | 76.73 | 85.03 | 89.67 |
| 165 | 76.88 | 84.98 | 89.91 | 85 | 75.70 | 87.13 | 88.47 | 164 | 76.67 | 85.04 | 89.68 |
| **(1/2, 1/2, 0)** | $DP_S$ | LoF(DP) | MSE($D_S$) | **(1/2, 1/4, 1/4)** | $DP_S$ | LoF(DP) | MSE($D_S$) | **(1/4, 1/4, 1/2)** | $DP_S$ | LoF(DP) | MSE($D_S$) |
| 185 | 76.71 | 90.64 | 85.51 | 186 | 76.73 | 90.59 | 85.61 | 120 | 76.95 | 84.94 | 90.04 |
| 186 | 76.73 | 90.59 | 85.61 | 185 | 76.71 | 90.64 | 85.51 | 117 | 76.96 | 84.96 | 89.91 |
| 184 | 76.52 | 90.73 | 85.31 | 181 | 76.84 | 89.81 | 85.62 | 119 | 76.87 | 84.94 | 89.94 |
| 187 | 76.30 | 90.78 | 85.09 | 184 | 76.52 | 90.73 | 85.31 | 165 | 76.88 | 84.98 | 89.91 |
| 188 | 76.09 | 90.88 | 84.87 | 180 | 76.80 | 89.85 | 85.52 | 122 | 76.87 | 85.00 | 89.90 |
| 183 | 76.03 | 90.93 | 84.82 | 189 | 76.75 | 89.91 | 85.53 | 163 | 76.82 | 84.95 | 89.94 |
| 166 | 76.08 | 90.79 | 84.92 | 120 | 76.95 | 84.94 | 90.04 | 118 | 76.81 | 84.97 | 89.92 |
| 181 | 76.84 | 89.81 | 85.62 | 117 | 76.96 | 84.96 | 89.91 | 133 | 76.52 | 85.68 | 89.47 |
| 189 | 76.75 | 89.91 | 85.53 | 165 | 76.88 | 84.98 | 89.91 | 162 | 76.75 | 85.01 | 89.69 |
| 180 | 76.80 | 89.85 | 85.52 | 122 | 76.87 | 85.00 | 89.90 | 116 | 76.73 | 85.03 | 89.67 |
| **(1/2, 0, 1/2)** | $DP_S$ | LoF(DP) | MSE($D_S$) | **(1/4, 1/2, 1/4)** | $DP_S$ | LoF(DP) | MSE($D_S$) | **(1/3, 2/3, 0)** | $DP_S$ | LoF(DP) | MSE($D_S$) |
| 120 | 76.95 | 84.94 | 90.04 | 186 | 76.73 | 90.59 | 85.61 | 185 | 76.71 | 90.64 | 85.51 |
| 117 | 76.96 | 84.96 | 89.91 | 185 | 76.71 | 90.64 | 85.51 | 184 | 76.52 | 90.73 | 85.31 |
| 119 | 76.87 | 84.94 | 89.94 | 184 | 76.52 | 90.73 | 85.31 | 186 | 76.73 | 90.59 | 85.61 |
| 165 | 76.88 | 84.98 | 89.91 | 187 | 76.30 | 90.78 | 85.09 | 187 | 76.30 | 90.78 | 85.09 |
| 122 | 76.87 | 85.00 | 89.90 | 188 | 76.09 | 90.88 | 84.87 | 183 | 76.03 | 90.93 | 84.82 |
| 163 | 76.82 | 84.95 | 89.94 | 183 | 76.03 | 90.93 | 84.82 | 188 | 76.09 | 90.88 | 84.87 |
| 118 | 76.81 | 84.97 | 89.92 | 166 | 76.08 | 90.79 | 84.92 | 166 | 76.08 | 90.79 | 84.92 |
| 162 | 76.75 | 85.01 | 89.69 | 181 | 76.84 | 89.81 | 85.62 | 176 | 75.34 | 91.09 | 83.97 |
| 116 | 76.73 | 85.03 | 89.67 | 189 | 76.75 | 89.91 | 85.53 | 171 | 75.16 | 91.20 | 83.69 |
| 164 | 76.67 | 85.04 | 89.68 | 180 | 76.80 | 89.85 | 85.52 | 172 | 75.35 | 91.08 | 83.96 |

# D Derivation of MSE(DP)- and MSE(LP)-criteria for blocked experiments

## D.1 Lack-of-fit criterion

The information matrix for the extended model

$$\boldsymbol{Y} = \boldsymbol{Z}\boldsymbol{\beta}_B + \boldsymbol{X}_p\boldsymbol{\beta}_p + \boldsymbol{X}_q\boldsymbol{\beta}_q + \boldsymbol{\varepsilon},$$

up to a multiple of $1/\sigma^2$, is

$$\boldsymbol{M_B} = \begin{pmatrix} \boldsymbol{Z}^T\boldsymbol{Z} & \boldsymbol{Z}^T\boldsymbol{X}_p & \boldsymbol{Z}^T\boldsymbol{X}_q \\ \boldsymbol{X}_p^T\boldsymbol{Z} & \boldsymbol{X}_p^T\boldsymbol{X}_p & \boldsymbol{X}_p^T\boldsymbol{X}_q \\ \boldsymbol{X}_q^T\boldsymbol{Z} & \boldsymbol{X}_q^T\boldsymbol{X}_p & \boldsymbol{X}_q^T\boldsymbol{X}_q + \boldsymbol{I}_q/\tau^2 \end{pmatrix} = \begin{pmatrix} \tilde{\boldsymbol{X}}_p^T\tilde{\boldsymbol{X}}_p & \tilde{\boldsymbol{X}}_p^T\boldsymbol{X}_q \\ \boldsymbol{X}_q^T\tilde{\boldsymbol{X}}_p & \boldsymbol{X}_q^T\boldsymbol{X}_q + \boldsymbol{I}_q/\tau^2 \end{pmatrix}.$$

Adopting the same prior on $\boldsymbol{\beta}_q \sim \mathcal{N}(\boldsymbol{0}, \tau^2\sigma^2\boldsymbol{I}_q)$ as for completely randomized designs, we construct the variance-covariance matrix corresponding to the potential terms – that is the lower right submatrix of the inverse of $\boldsymbol{M_B}$: $\tilde{\boldsymbol{\Sigma}}_{qq} = \sigma^2[\boldsymbol{M}_B^{-1}]_{22}$, i.e.

$$\begin{aligned}
\tilde{\boldsymbol{\Sigma}}_{qq} &= \sigma^2([\boldsymbol{M_B}]_{22} - [\boldsymbol{M_B}]_{21}([\boldsymbol{M_B}]_{11})^{-1}[\boldsymbol{M_B}]_{12})^{-1} \\
&= \sigma^2(\boldsymbol{X}_q^T\boldsymbol{X}_q + \boldsymbol{I}_q/\tau^2 - \boldsymbol{X}_q^T\tilde{\boldsymbol{X}}_p(\tilde{\boldsymbol{X}}_p^T\tilde{\boldsymbol{X}}_p)^{-1}\tilde{\boldsymbol{X}}_p^T\boldsymbol{X}_q)^{-1} \\
&= \sigma^2\left(\tilde{\boldsymbol{L}} + \frac{\boldsymbol{I}_q}{\tau^2}\right), \text{ where } \tilde{\boldsymbol{L}} = \boldsymbol{X}_q^T\boldsymbol{X}_q - \boldsymbol{X}_q^T\tilde{\boldsymbol{X}}_p(\tilde{\boldsymbol{X}}_p^T\tilde{\boldsymbol{X}}_p)^{-1}\tilde{\boldsymbol{X}}_p^T\boldsymbol{X}_q.
\end{aligned}$$

Therefore, the lack-of-fit criteria for the completely randomized case are adjusted for blocked experiments by replacing the primary terms matrix $\boldsymbol{X}_p$ by the extended matrix $\tilde{\boldsymbol{X}}_p$ and the dispersion matrix $\boldsymbol{L}$ by $\tilde{\boldsymbol{L}}$ as obtained above.

## D.2 MSE-based criterion

As for the MSE-based measure of the shift in the primary terms estimates, we first consider the overall mean square error matrix

$$\text{MSE}(\hat{\tilde{\boldsymbol{\beta}}}_p|\tilde{\boldsymbol{\beta}}) = \mathtt{E}_{\boldsymbol{Y}|\boldsymbol{\beta}}[(\hat{\tilde{\boldsymbol{\beta}}}_p - \tilde{\boldsymbol{\beta}}_p)(\hat{\tilde{\boldsymbol{\beta}}}_p - \tilde{\boldsymbol{\beta}}_p)^T] = \sigma^2(\tilde{\boldsymbol{X}}_p^T\tilde{\boldsymbol{X}}_p)^{-1} + \tilde{\boldsymbol{A}}\boldsymbol{\beta}_q\boldsymbol{\beta}_q^T\tilde{\boldsymbol{A}}^T, \quad (4)$$

with $\tilde{\boldsymbol{A}} = (\tilde{\boldsymbol{X}}_p^T\tilde{\boldsymbol{X}}_p)^{-1}\tilde{\boldsymbol{X}}_p'^T\boldsymbol{X}_q$ being the alias matrix, and then its partition with respect to block and primary effects, to get

$$\begin{aligned}
&\mathtt{E}_{\boldsymbol{Y}|\boldsymbol{\beta}}[(\hat{\tilde{\boldsymbol{\beta}}}_p - \tilde{\boldsymbol{\beta}}_p)(\hat{\tilde{\boldsymbol{\beta}}}_p - \tilde{\boldsymbol{\beta}}_p)^T] \\
&= \mathtt{E}_{\boldsymbol{Y}|\boldsymbol{\beta}}\{[\hat{\tilde{\beta}}_{p1} - \tilde{\beta}_{p1}, \ldots, \hat{\tilde{\beta}}_{pb} - \tilde{\beta}_{pb}, \hat{\tilde{\beta}}_{pb+1} - \tilde{\beta}_{pb+1}, \ldots, \hat{\tilde{\beta}}_{pb+p} - \tilde{\beta}_{pb+p}]\times \\
&[\hat{\tilde{\beta}}_{p1} - \tilde{\beta}_{p1}, \ldots, \hat{\tilde{\beta}}_{pb} - \tilde{\beta}_{pb}, \hat{\tilde{\beta}}_{pb+1} - \tilde{\beta}_{pb+1}, \ldots, \hat{\tilde{\beta}}_{pb+p} - \tilde{\beta}_{pb+p}]^T\} \\
&= \mathtt{E}_{\boldsymbol{Y}|\boldsymbol{\beta}}\{[\hat{\boldsymbol{\beta}}_B - \boldsymbol{\beta}_B, \hat{\boldsymbol{\beta}}_p - \boldsymbol{\beta}_p][\hat{\boldsymbol{\beta}}_B - \boldsymbol{\beta}_B, \hat{\boldsymbol{\beta}}_p - \boldsymbol{\beta}_p]^T\} \\
&= \begin{bmatrix} \mathtt{E}_{\boldsymbol{Y}|\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}_B - \boldsymbol{\beta}_B)(\hat{\boldsymbol{\beta}}_B - \boldsymbol{\beta}_B)^T & \mathtt{E}_{\boldsymbol{Y}|\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}_B - \boldsymbol{\beta}_B)(\hat{\boldsymbol{\beta}}_p - \boldsymbol{\beta}_p)^T \\ \mathtt{E}_{\boldsymbol{Y}|\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}_p - \boldsymbol{\beta}_p)(\hat{\boldsymbol{\beta}}_B - \boldsymbol{\beta}_B)^T & \mathtt{E}_{\boldsymbol{Y}|\boldsymbol{\beta}}(\hat{\boldsymbol{\beta}}_p - \boldsymbol{\beta}_p)(\hat{\boldsymbol{\beta}}_p - \boldsymbol{\beta}_p)^T \end{bmatrix}.
\end{aligned}$$

The bottom right $p \times p$ submatrix corresponds to the bias of the primary terms $\boldsymbol{\beta}_p$, and we can extract it from the MSE expression in (4). The respective submatrix of the first summand is

$$[\sigma^2(\tilde{\boldsymbol{X}}_p^T\tilde{\boldsymbol{X}}_p)^{-1}]_{22} = \sigma^2(\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_p)^{-1}, \text{ where } \boldsymbol{Q} = \boldsymbol{I} - \boldsymbol{Z}(\boldsymbol{Z}^T\boldsymbol{Z})^{-1}\boldsymbol{Z}.^T$$

Using the matrix inversion rule for block matrices (Harville 2006), we now consider

$$\begin{aligned}
\tilde{\boldsymbol{A}} &= \left(\begin{bmatrix}\boldsymbol{Z}^T\\ \boldsymbol{X}_p^T\end{bmatrix}\begin{bmatrix}\boldsymbol{Z} & \boldsymbol{X}_p\end{bmatrix}\right)^{-1}\begin{bmatrix}\boldsymbol{Z}^T\\ \boldsymbol{X}_p^T\end{bmatrix}\boldsymbol{X}_q = \begin{pmatrix}\boldsymbol{Z}^T\boldsymbol{Z} & \boldsymbol{Z}^T\boldsymbol{X}_p\\ \boldsymbol{X}_p^T\boldsymbol{Z} & \boldsymbol{X}_p^T\boldsymbol{X}_p\end{pmatrix}^{-1}\begin{bmatrix}\boldsymbol{Z}^T\\ \boldsymbol{X}_p^T\end{bmatrix}\boldsymbol{X}_q\\
&= \begin{bmatrix}(\boldsymbol{Z}^T\boldsymbol{P}\boldsymbol{Z})^{-1} & -(\boldsymbol{Z}^T\boldsymbol{P}\boldsymbol{Z})^{-1}\boldsymbol{Z}^T\boldsymbol{X}_p(\boldsymbol{X}_p^T\boldsymbol{X}_p)^{-1}\\ -(\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_p)^{-1}\boldsymbol{X}_p^T\boldsymbol{Z}(\boldsymbol{Z}^T\boldsymbol{Z})^{-1} & (\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_p)^{-1}\end{bmatrix}\begin{bmatrix}\boldsymbol{Z}^T\\ \boldsymbol{X}_p^T\end{bmatrix}\boldsymbol{X}_q\\
&= \begin{bmatrix}(\boldsymbol{Z}^T\boldsymbol{P}\boldsymbol{Z})^{-1}\boldsymbol{Z}^T\boldsymbol{P}\boldsymbol{X}_q\\ (\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_p)^{-1}\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_q\end{bmatrix},
\end{aligned}$$

where $\boldsymbol{P} = \boldsymbol{I} - \boldsymbol{X}_p(\boldsymbol{X}_p^T\boldsymbol{X}_p)^{-1}\boldsymbol{X}_p^T$, $\boldsymbol{Z}\boldsymbol{Z}^T$, $\boldsymbol{X}_p^T\boldsymbol{X}_p$ and $\boldsymbol{Z}^T\boldsymbol{P}\boldsymbol{Z}$ are all invertible and, therefore, the operations are legitimate. Now denote $\boldsymbol{R}_{\boldsymbol{P}} = (\boldsymbol{Z}^T\boldsymbol{P}\boldsymbol{Z})^{-1}\boldsymbol{Z}^T\boldsymbol{P}\boldsymbol{X}_q$ and $\boldsymbol{R}_{\boldsymbol{Q}} = (\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_p)^{-1}\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_q$, and consider the second summand in (4),

$$\tilde{\boldsymbol{A}}\boldsymbol{\beta}_q\boldsymbol{\beta}_q^T\tilde{\boldsymbol{A}}^T = \begin{bmatrix}\boldsymbol{R}_{\boldsymbol{P}}\boldsymbol{\beta}_q\\ \boldsymbol{R}_{\boldsymbol{Q}}\boldsymbol{\beta}_q\end{bmatrix}\begin{bmatrix}\boldsymbol{\beta}_q^T\boldsymbol{R}_{\boldsymbol{P}}^T & \boldsymbol{\beta}_q^T\boldsymbol{R}_{\boldsymbol{Q}}^T\end{bmatrix} = \begin{bmatrix}\boldsymbol{R}_{\boldsymbol{P}}\boldsymbol{\beta}_q\boldsymbol{\beta}_q^T\boldsymbol{R}_{\boldsymbol{P}}^T & \boldsymbol{R}_{\boldsymbol{P}}\boldsymbol{\beta}_q\boldsymbol{\beta}_q^T\boldsymbol{R}_{\boldsymbol{Q}}^T\\ \boldsymbol{R}_{\boldsymbol{Q}}\boldsymbol{\beta}_q\boldsymbol{\beta}_q^T\boldsymbol{R}_{\boldsymbol{P}}^T & \boldsymbol{R}_{\boldsymbol{Q}}\boldsymbol{\beta}_q\boldsymbol{\beta}_q^T\boldsymbol{R}_{\boldsymbol{Q}}^T\end{bmatrix}.$$

Then the submatrix of (4) corresponding to the primary terms is

$$\begin{aligned}
\text{MSE}(\hat{\tilde{\boldsymbol{\beta}}}_p|\tilde{\boldsymbol{\beta}})_{pp} =&\sigma^2(\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_p)^{-1} + \boldsymbol{R}_{\boldsymbol{Q}}\boldsymbol{\beta}_q\boldsymbol{\beta}_q^T\boldsymbol{R}_{\boldsymbol{Q}}^T\\
=&\sigma^2\tilde{\boldsymbol{M}}^{-1} + \tilde{\boldsymbol{M}}^{-1}\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_q\boldsymbol{\beta}_q\boldsymbol{\beta}_q^T\boldsymbol{X}_q^T\boldsymbol{Q}\boldsymbol{X}_p\tilde{\boldsymbol{M}},^{-1}
\end{aligned} \tag{5}$$

where $\tilde{\boldsymbol{M}} = \boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_p$.

As in the unblocked case, we first look at the determinant of the submatrix (5):

$$\begin{aligned}
\det[\text{MSE}(\hat{\tilde{\boldsymbol{\beta}}}_p|\tilde{\boldsymbol{\beta}})_{pp}] =& \det[\sigma^2\tilde{\boldsymbol{M}}^{-1} + \tilde{\boldsymbol{M}}^{-1}\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_q\boldsymbol{\beta}_q\boldsymbol{\beta}_q^T\boldsymbol{X}_q^T\boldsymbol{Q}\boldsymbol{X}_p\tilde{\boldsymbol{M}}^{-1}]\\
=&\sigma^{2p}\det[\tilde{\boldsymbol{M}}^{-1} + \tilde{\boldsymbol{M}}^{-1}\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_q\tilde{\boldsymbol{\beta}}_q\tilde{\boldsymbol{\beta}}_q^T\boldsymbol{X}_q^T\boldsymbol{Q}\boldsymbol{X}_p\tilde{\boldsymbol{M}}^{-1}]\\
=&\sigma^{2p}\det[\tilde{\boldsymbol{M}}^{-1}](1 + \tilde{\boldsymbol{\beta}}_q^T\boldsymbol{X}_q^T\boldsymbol{Q}\boldsymbol{X}_p^T\tilde{\boldsymbol{M}}^{-1}\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_q\tilde{\boldsymbol{\beta}}_q).
\end{aligned} \tag{6}$$

The $q$-dimensional random vector $\tilde{\boldsymbol{\beta}}_q$, as before, follows $\mathcal{N}(\boldsymbol{0}, \tau^2\boldsymbol{I}_q)$, so that this prior does not depend on the error variance $\sigma.^2$ Next, taking the expectation of the logarithm of (6) over the prior distribution is identical to the derivations in Section 3.2. The MSE(D)-component in the blocked case then becomes

$$\log(\det[\tilde{\boldsymbol{M}}^{-1}]) + \mathtt{E}_{\tilde{\boldsymbol{\beta}}_q}\{\log(1 + \tilde{\boldsymbol{\beta}}_q^T\boldsymbol{X}_q^T\boldsymbol{Q}\boldsymbol{X}_p\tilde{\boldsymbol{M}}^{-1}\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_q\tilde{\boldsymbol{\beta}}_q)\}, \tag{7}$$

and the determinant-based compound criterion for a blocked experiment is minimizing

$$\begin{aligned}
&\left[\left|(\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_p)^{-1}\right|^{1/p} F_{p,d_B;1-\alpha_{DP}}\right]^{\kappa_{DP}} \times\\
&\left[\left|\tilde{\boldsymbol{L}} + \frac{\boldsymbol{I}_q}{\tau^2}\right|^{-1/q} F_{q,d_B;1-\alpha_{LoF}}\right]^{\kappa_{LoF}} \times\\
&\left[|\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_p|^{-1}\exp\left(\frac{1}{N}\sum_{i=1}^{N}\log(1 + \tilde{\boldsymbol{\beta}}'_{qi}\boldsymbol{X}_q^T\boldsymbol{Q}\boldsymbol{X}_p\tilde{\boldsymbol{M}}^{-1}\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_q\tilde{\boldsymbol{\beta}}_{qi})\right)\right]^{\kappa_{MSE}/p}.
\end{aligned} \tag{8}$$

The probability levels $\alpha_i$ and weights $\kappa_j$ have the same meanings as in the unblocked case and, as was noted earlier, the number of pure error degrees of freedom $d_B$ accounts for the comparisons between blocks.

## D.3 Trace-based criteria for blocked experiments

Following the derivations for determinant-based criteria in the previous sections, we take the expectation of the trace of (5) to obtain the trace-based MSE-criterion:

$$\begin{aligned}
\mathtt{E}_{\beta_q}\text{trace}[\text{MSE}(\hat{\tilde{\boldsymbol{\beta}}}_p|\tilde{\boldsymbol{\beta}})_{pp}] &= \text{trace}[\mathtt{E}_{\beta_q}\text{MSE}(\hat{\tilde{\boldsymbol{\beta}}}_p|\tilde{\boldsymbol{\beta}})_{pp}] \\
&= \text{trace}[\sigma^2\tilde{\boldsymbol{M}}_{pp}^{-1} + \mathtt{E}_{\beta_q}(\tilde{\boldsymbol{A}}\boldsymbol{\beta}_q\boldsymbol{\beta}_q^T\tilde{\boldsymbol{A}})_{pp}] \\
&= \sigma^2\text{trace}[\tilde{\boldsymbol{M}}_{pp}^{-1} + \tau^2\{\tilde{\boldsymbol{A}}\tilde{\boldsymbol{A}}^T\}_{pp}] \\
&= \sigma^2[\text{trace}(\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_p)^{-1} + \tau^2\text{trace}\{\tilde{\boldsymbol{A}}\tilde{\boldsymbol{A}}^T\}_{pp}]. \qquad (9)
\end{aligned}$$

The MSE-LP compound criterion for a blocked experiment is then to minimize

$$\begin{aligned}
&\left[\frac{1}{p}\text{trace}(\boldsymbol{W}\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_p)^{-1}F_{1,d_B;1-\alpha_{LP}}\right]^{\kappa_{LP}} \times \\
&\left[\frac{1}{q}\text{trace}\left(\tilde{\boldsymbol{L}} + \boldsymbol{I}_q/\tau^2\right)^{-1}F_{1,d_B;1-\alpha_{LoF}}\right]^{\kappa_{LoF}} \times \\
&\left[\frac{1}{p}\text{trace}\{(\boldsymbol{X}_p^T\boldsymbol{Q}\boldsymbol{X}_p)^{-1} + \tau^2[\tilde{\boldsymbol{A}}\tilde{\boldsymbol{A}}^T]_{pp}\}\right]^{\kappa_{MSE}}. \qquad (10)
\end{aligned}$$

# E Case-study, blocked experiment

The MSE-DP-optimal blocked design that was used to run the experiment described in Section 4.1. The design itself is shown in Table 4 and Figure 5.

Table 4: Case-study: $MSE-DP$-optimal design with two center points, $\tau^2 = 1$

| Block I | | | | | | | | Block II | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | X1 | X2 | X3 | | X1 | X2 | X3 | | X1 | X2 | X3 | | X1 | X2 | X3 |
| 1 | -1 | -1 | -1 | 10 | 0 | 0 | 0 | 1 | -1 | -1 | -1 | 10 | 0 | 0 | 0 |
| 2 | -1 | -1 | 0 | 11 | 0 | 1 | -1 | 2 | -1 | -1 | 0 | 11 | 0 | 1 | 1 |
| 3 | -1 | -1 | 1 | 12 | 1 | -1 | -1 | 3 | -1 | -1 | 1 | 12 | 1 | -1 | -1 |
| 4 | -1 | 0 | -1 | 13 | 1 | -1 | 0 | 4 | -1 | 0 | 1 | 13 | 1 | -1 | 0 |
| 5 | -1 | 1 | -1 | 14 | 1 | -1 | 1 | 5 | -1 | 1 | -1 | 14 | 1 | -1 | 1 |
| 6 | -1 | 1 | 1 | 15 | 1 | 0 | 1 | 6 | -1 | 1 | 0 | 15 | 1 | 0 | -1 |
| 7 | -1 | 1 | 1 | 16 | 1 | 1 | -1 | 7 | 0 | -1 | -1 | 16 | 1 | 0 | 1 |
| 8 | 0 | -1 | 1 | 17 | 1 | 1 | 0 | 8 | 0 | -1 | 1 | 17 | 1 | 1 | -1 |
| 9 | 0 | 0 | 0 | 18 | 1 | 1 | 1 | 9 | 0 | 0 | 0 | 18 | 1 | 1 | 1 |

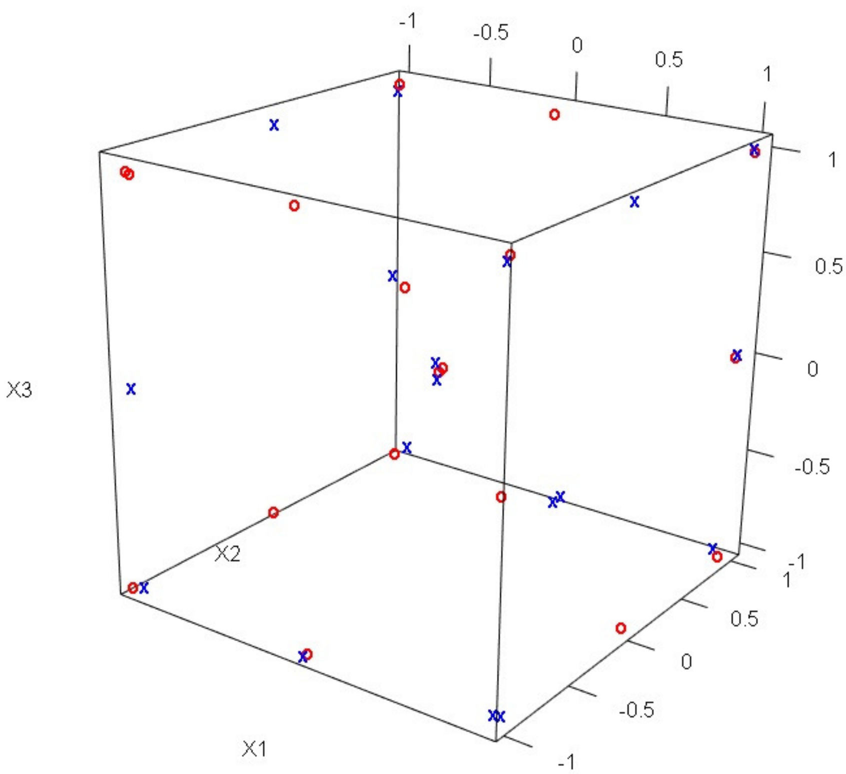


Figure 5: $MSE-DP$-optimal design: colours (blue and red) and symbols (‘x’ and ‘o’) serve as block indicators.

# References

Harville, D. A. (2006), *Matrix Algebra From a Statistician's Perspective*, Springer New York.