EFFICIENT DESIGNS FOR THE ESTIMATION OF MIXED AND SELF CARRYOVER EFFECTS

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Supplementary Material

S1 Proof of Proposition 1

For given $\lambda_2 \geq \lambda_3 > 0$, we have that $\lambda_1 \leq L - \lambda_2 - \lambda_3$. Hence,

$$\varphi_A(d) = \frac{1}{\frac{1}{\lambda_1} + \frac{1}{\lambda_2} + \frac{1}{\lambda_3}} \leq \frac{1}{\frac{1}{L-\lambda_2-\lambda_3} + \frac{1}{\lambda_2} + \frac{1}{\lambda_3}}.$$

Holding λ_3 fixed, this bound is maximal if $\lambda_2 = L - \lambda_2 - \lambda_3$, i.e. if $\lambda_2 = (L - \lambda_3)/2$. This implies that

$$\varphi_A(d) \leq \frac{1}{\frac{2}{L-\lambda_3} + \frac{2}{L-\lambda_3} + \frac{1}{\lambda_3}}.$$

This bound, however, gets maximal if λ_3 gets as near to $(L - \lambda_3)/2$ as possible, which means that $\lambda_3 = q$. This gives

$$\varphi_A(d) \leq \frac{1}{\frac{2}{L-q} + \frac{2}{L-q} + \frac{1}{q}}.$$

If $\lambda_3 = 0$ we get $\varphi_A(d) = 0$, which completes the proof.

S2 Proof of Proposition 2

In our notation, the equation at the bottom of page 75 of Pukelsheim (1993) becomes

$$\begin{bmatrix} \mathbf{C}_{d11} & \mathbf{C}_{d12} \\ \mathbf{C}_{d12}^T & \mathbf{C}_{d22} \end{bmatrix} = \begin{bmatrix} \mathbf{I}_2 & \mathbf{C}_{d12}\mathbf{C}_{d22}^+ \\ \mathbf{0} & \mathbf{I}_4 \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{C}}_d & \mathbf{0} \\ \mathbf{0} & \mathbf{C}_{d22} \end{bmatrix} \begin{bmatrix} \mathbf{I}_2 & \mathbf{0} \\ \mathbf{C}_{d22}^+\mathbf{C}_{d12}^T & \mathbf{I}_4 \end{bmatrix}.$$

Multiplying this by $\begin{bmatrix} \mathbf{I}_2 & -\mathbf{X}^T \end{bmatrix}$ from the left and by $\begin{bmatrix} \mathbf{I}_2 \\ -\mathbf{X} \end{bmatrix}$ from the right, we get

$$\begin{aligned} & \mathbf{C}_{d11} - \mathbf{C}_{d12}\mathbf{X} - \mathbf{X}^T\mathbf{C}_{d12}^T + \mathbf{X}^T\mathbf{C}_{d22}\mathbf{X} \\ = & \begin{bmatrix} \mathbf{I}_2 & \mathbf{C}_{d12}\mathbf{C}_{d22}^+ - \mathbf{X}^T \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{C}}_d & \mathbf{0} \\ \mathbf{0} & \mathbf{C}_{d22} \end{bmatrix} \begin{bmatrix} \mathbf{I}_2 & \mathbf{C}_{d22}^+\mathbf{C}_{d12}^T - \mathbf{X} \end{bmatrix} \\ = & \tilde{\mathbf{C}}_d + \left(\mathbf{C}_{d12}\mathbf{C}_{d22}^+ - \mathbf{X}^T\right)\mathbf{C}_{d22}\left(\mathbf{C}_{d22}^+\mathbf{C}_{d12}^T - \mathbf{X}\right). \end{aligned}$$

This is almost the same as (5.2) in Kushner (1997), except that $\mathbf{X}$ is not square. Since $\left(\mathbf{C}_{d12}\mathbf{C}_{d22}^+ - \mathbf{X}^T\right)\mathbf{C}_{d22}\left(\mathbf{C}_{d22}^+\mathbf{C}_{d12}^T - \mathbf{X}\right) \geq 0$, it follows that

$$\mathbf{C}_{d11} - \mathbf{C}_{d12}\mathbf{X} - \mathbf{X}^T\mathbf{C}_{d12}^T + \mathbf{X}^T\mathbf{C}_{d22}\mathbf{X} \geq \tilde{\mathbf{C}}_d,$$

with equality for $\mathbf{X} = \mathbf{C}_{d22}^+\mathbf{C}_{d12}^T$.

S3 Proof of Proposition 3

Define $Q(x) = \mathbf{k}^T\mathbf{C}_{d11}\mathbf{k} - 2\mathbf{k}^T\mathbf{C}_{d12}\mathbf{b}_2x + \mathbf{b}_2^T\mathbf{C}_{d22}\mathbf{b}_2x^2$.

Case 1: $\mathbf{k}^T\mathbf{C}_{d12}\mathbf{b}_2 \neq 0$.

Consider the matrix

$$\mathbf{X} = \mathbf{C}_{d12}^T\frac{x}{\mathbf{k}^T\mathbf{C}_{d12}^T\mathbf{b}_2} \in \mathbb{R}^{2\times 4}.$$

Then $\mathbf{k}^T\mathbf{X}^T\mathbf{b}_2 = x$.

It follows from Proposition 2 that

$$\mathbf{k}^T\tilde{C}_d\mathbf{k} \leq \mathbf{k}^T\mathbf{C}_{d11}\mathbf{k} - \mathbf{k}^T\mathbf{C}_{d12}\mathbf{X}\mathbf{k} - \mathbf{k}^T\mathbf{X}^T\mathbf{C}_{d12}^T\mathbf{k} + \mathbf{k}^T\mathbf{X}^T\mathbf{C}_{d22}\mathbf{X}\mathbf{k}.$$

Since $\mathbf{C}_{d12}$ has row-sums 0, we have $\mathbf{C}_{d12}\mathbf{b}_2\mathbf{b}_2^T = \mathbf{C}_{d12}$. Since $\mathbf{C}_{d22}$ has both row- and column-sums 0, we even have $\mathbf{b}_2\mathbf{b}_2^T\mathbf{C}_{d22}\mathbf{b}_2\mathbf{b}_2^T = \mathbf{C}_{d22}$. Hence

$$\begin{aligned}
\mathbf{k}^T\tilde{C}_d\mathbf{k} &\leq \mathbf{k}^T\mathbf{C}_{d11}\mathbf{k} - \mathbf{k}^T\mathbf{C}_{d12}\mathbf{b}_2\mathbf{b}_2^T\mathbf{X}\mathbf{k} \\
&\quad -\mathbf{k}^T\mathbf{X}^T\mathbf{b}_2\mathbf{b}_2^T\mathbf{C}_{d12}^T\mathbf{k} + \mathbf{k}^T\mathbf{X}^T\mathbf{b}_2\mathbf{b}_2^T\mathbf{C}_{d22}\mathbf{b}_2\mathbf{b}_2^T\mathbf{X}\mathbf{k} \\
&= \mathbf{k}^T\mathbf{C}_{d11}\mathbf{k} - \mathbf{k}^T\mathbf{C}_{d12}\mathbf{b}_2x - x\mathbf{b}_2^T\mathbf{C}_{d12}^T\mathbf{k} + x\mathbf{b}_2^T\mathbf{C}_{d22}\mathbf{b}_2x \\
&= Q(x).
\end{aligned}$$

Because of Proposition 2, we get equality for $\mathbf{X} = \mathbf{X}_d = \mathbf{C}_{d22}^+\mathbf{C}_{d12}^T$, i.e., for

$$x = \mathbf{b}_2^T\mathbf{C}_{d22}^+\mathbf{C}_{d12}^T\mathbf{k} = x_d.$$

Case 2: $\mathbf{k}^T\mathbf{C}_{d12}\mathbf{b}_2 = 0$.

Then $Q(x) = \mathbf{k}^T \mathbf{C}_{d11} \mathbf{k} + \mathbf{b}_2^T \mathbf{C}_{d22} \mathbf{b}_2 x^2 \geq \mathbf{k}^T \mathbf{C}_{d11} \mathbf{k}$ with equality for $x = 0$.

On the other hand, it follows from $\mathbf{k}^T \mathbf{C}_{d12} \mathbf{b}_2 = 0$ that $\mathbf{k}^T \mathbf{C}_{d12} \mathbf{b}_2 \mathbf{b}_2^T = 0$, and, therefore, that $\mathbf{k}^T \mathbf{C}_{d12} = \mathbf{0}$. Hence, $\mathbf{k}^T \mathbf{C}_{d11} \mathbf{k} = \mathbf{k}^T \tilde{\mathbf{C}}_d \mathbf{k}$. Furthermore, $x_d = \mathbf{k}^T \mathbf{C}_{d12} \mathbf{C}_{d22}^+ \mathbf{b}_2 = \mathbf{k}^T \mathbf{C}_{d12} \mathbf{b}_2 \mathbf{b}_2^T \mathbf{C}_{d22}^+ \mathbf{b}_2 = 0$. This completes the proof.

S4 Proof of Proposition 4

It follows from Proposition 3 and Equation (3.6) that

$$\begin{aligned} \frac{1}{n} \mathbf{k}^T \tilde{\mathbf{C}}_d \mathbf{k} &\leq \sum_{z \in Z_p} \pi_d(z) \{ \mathbf{k}^T \mathbf{C}_{11}(z) \mathbf{k} - 2\mathbf{k}^T \mathbf{C}_{12}(z) \mathbf{b}_2 x + \mathbf{b}_2^T \mathbf{C}_{22}(z) \mathbf{b}_2 x^2 \} \\ &\leq \max_{z \in Z_p} \{ \mathbf{k}^T \mathbf{C}_{11}(z) \mathbf{k} - 2\mathbf{k}^T \mathbf{C}_{12}(z) \mathbf{b}_2 x + \mathbf{b}_2^T \mathbf{C}_{22}(z) \mathbf{b}_2 x^2 \}. \end{aligned}$$

From the Courant-Fischer Theorem it follows that

$$\lambda_3(\tilde{\mathbf{C}}_d) = \min_{\mathbf{h}: \mathbf{h}^T \mathbf{1}_4 = 0} \frac{1}{\mathbf{h}^T \mathbf{h}} \mathbf{h}^T \tilde{\mathbf{C}}_d \mathbf{h}$$

and since

$$\lambda_3(\mathbf{C}_d) \leq \lambda_3(\tilde{\mathbf{C}}_d),$$

the desired inequality follows.

S5 Proof of Proposition 5

Since $tr(\tilde{\mathbf{C}}_d) \geq tr(\mathbf{C}_d)$, it follows directly from Proposition 2 and Equation (3.6) that

$$\begin{aligned} & tr(\mathbf{C}_d)/n \\ \leq \; & tr\left(\sum_{z\in Z_p} \pi_d(z)\big(\mathbf{C}_{11}(z) - \mathbf{C}_{12}(z)\mathbf{X} - \mathbf{X}^T\mathbf{C}_{12}^T(z) + \mathbf{X}^T\mathbf{C}_{22}(z)\mathbf{X}\big)\right) \\ \leq \; & \max_{z\in Z_p}\Big(tr(\mathbf{C}_{11}(z)) - 2tr(\mathbf{C}_{12}(z)\mathbf{X}) + tr(\mathbf{X}^T\mathbf{C}_{22}(z)\mathbf{X})\Big). \end{aligned}$$

This completes the proof.

S6 Proof of Proposition 6

Choosing $\mathbf{X} = \mathbf{X}_f$, it follows from (3.7) for any design $d \in \Delta_{2,n,p}$ that $tr(\mathbf{C}_d) \leq \max_{z\in Z_p} L_z(\mathbf{X}_f)$. The conditions of Proposition 6 imply that $\max_{z\in Z_p} L_z(\mathbf{X}_f) \leq tr(\mathbf{C}_f)$ and, hence, that $tr(\mathbf{C}_d) \leq tr(\mathbf{C}_f)$.

S7 Proof of Proposition 7

The design d has weights $\pi_d(z)$, $z \in Z_p$. Consider the dual design $\bar{d} \in \Delta_{2,n,p}$ with weights $\pi_{\bar{d}}(z)$, $z \in Z_p$, where for each $z \in Z_p$ the dual design $\bar{d}$ allots the weight that d has allotted to the dual sequence $\bar{z}$, i.e. $\pi_{\bar{d}}(z) = \pi_d(\bar{z})$. If we define

$$\mathbf{H}_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

then $\mathbf{S}_{\bar{d}} = \mathbf{S}_d\mathbf{H}_2$, $\mathbf{M}_{\bar{d}} = \mathbf{M}_d\mathbf{H}_2$ and $\mathbf{T}_{\bar{d}} = \mathbf{T}_d\mathbf{H}_2$. Therefore,

$$\mathbf{C}_{\bar{d}11} = \begin{bmatrix} \mathbf{H}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_2 \end{bmatrix} \mathbf{C}_{d11} \begin{bmatrix} \mathbf{H}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_2 \end{bmatrix}, \ \mathbf{C}_{\bar{d}12} = \begin{bmatrix} \mathbf{H}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_2 \end{bmatrix} \mathbf{C}_{d12}\mathbf{H}_2$$

and

$$\mathbf{C}_{\bar{d}22} = \mathbf{H}_2\mathbf{C}_{d22}\mathbf{H}_2.$$

This implies that

$$\begin{aligned} \tilde{\mathbf{C}}_{\bar{d}} &= \begin{bmatrix} \mathbf{H}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_2 \end{bmatrix} \mathbf{C}_{d11} \begin{bmatrix} \mathbf{H}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_2 \end{bmatrix} \\ &\quad - \begin{bmatrix} \mathbf{H}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_2 \end{bmatrix} \mathbf{C}_{d12}\mathbf{H}_2(\mathbf{H}_2\mathbf{C}_{d22}^{+}\mathbf{H}_2)\mathbf{H}_2\mathbf{C}_{d12}^{T} \begin{bmatrix} \mathbf{H}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_2 \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{H}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_2 \end{bmatrix} \tilde{\mathbf{C}}_d \begin{bmatrix} \mathbf{H}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_2 \end{bmatrix}. \end{aligned}$$

It follows that $\tilde{C}_{\bar{d}}$ has the same eigenvalues as $\tilde{C}_d$ and, consequently, that $\tilde{\varphi}_A(\bar{d}) = \tilde{\varphi}_A(d)$.

Now consider the dual balanced design f which allots to each sequence z the weight $\pi_f(z) = \frac{1}{2}\pi_d(z) + \frac{1}{2}\pi_{\bar{d}}(z)$. It then follows from Proposition 1 of Kunert and Martin (2000) that

$$\tilde{\mathbf{C}}_f \geq \frac{1}{2}\tilde{\mathbf{C}}_d + \frac{1}{2}\tilde{\mathbf{C}}_{\bar{d}},$$

which implies that

$$\tilde{\varphi}_A(f) \geq \frac{1}{2}\tilde{\varphi}_A(d) + \frac{1}{2}\tilde{\varphi}_A(\bar{d}) = \tilde{\varphi}_A(d),$$

since the A-criterion is concave and increasing.

S8 Proof of Proposition 8

The first row of both $\mathbf{S}_z$ and $\mathbf{M}_z$ is $[0,0]$. The first row of $\mathbf{T}_z$ is either $[1,0]$ or $[0,1]$, depending on whether the sequence z starts with R or T. Therefore, the first element of $\mathbf{S}_z\mathbf{b}_2 - \mathbf{M}_z\mathbf{b}_2 - \mathbf{T}_z\mathbf{b}_2$ is eitherl 1 or -1.

Now consider the i-th element, for $i \geq 2$.

Case 1: The preceding treatment was R, the current treatment is R. Then the i-th row of $\mathbf{S}_z$ is $[1,0]$, the i-th row of $\mathbf{M}_z$ is $[0,0]$, and the i-th row of $\mathbf{T}_z$ is $[1,0]$. Hence, the i-th element of $\mathbf{S}_z\mathbf{b}_2 - \mathbf{M}_z\mathbf{b}_2 - \mathbf{T}_z\mathbf{b}_2$ equals 0.

Case 2: The preceding treatment was R, the current treatment is T. Then the i-th row of $\mathbf{S}_z$ is $[0,0]$, the i-th row of $\mathbf{M}_z$ is $[1,0]$, and the i-th row of $\mathbf{T}_z$ is $[0,1]$. Hence, the i-th element of $\mathbf{S}_z\mathbf{b}_2 - \mathbf{M}_z\mathbf{b}_2 - \mathbf{T}_z\mathbf{b}_2$ equals 0.

Case 3: The preceding treatment was T, the current treatment is R. Then the i-th row of $\mathbf{S}_z$ is $[0,0]$, the i-th row of $\mathbf{M}_z$ is $[0,1]$, and the i-th row of

$\mathbf{T}_z$ is $[0,1]$. Again, the i-th element of $\mathbf{S}_z\mathbf{b}_2 - \mathbf{M}_z\mathbf{b}_2 - \mathbf{T}_z\mathbf{b}_2$ equals 0.

Case 4: The preceding treatment was T, the current treatment is T. Then the i-th row of $\mathbf{S}_z$ is $[0,1]$, the i-th row of $\mathbf{M}_z$ is $[0,0]$, and the i-th row of $\mathbf{T}_z$ is $[0,1]$. So also in this case, the i-th element of $\mathbf{S}_z\mathbf{b}_2 - \mathbf{M}_z\mathbf{b}_2 - \mathbf{T}_z\mathbf{b}_2$ equals 0.

This completes the proof.

S9 Proof of Proposition 9

Observing that

$$\mathbf{k} = \frac{1}{\sqrt{2}} \begin{bmatrix} \mathbf{b}_2 \\ -\mathbf{b}_2 \end{bmatrix}$$

we get

$$\begin{aligned} J_z(\frac{1}{\sqrt{2}}) &= \frac{1}{2}\left[\mathbf{b}_2^T, -\mathbf{b}_2^T\right]\mathbf{C}_{11}(z)\begin{bmatrix} \mathbf{b}_2 \\ -\mathbf{b}_2 \end{bmatrix} - \frac{1}{2}\left[\mathbf{b}_2^T, -\mathbf{b}_2^T\right]\mathbf{C}_{12}(z)\mathbf{b}_2 \\ &\quad -\frac{1}{2}\mathbf{b}_2^T\mathbf{C}_{12}^T(z)\begin{bmatrix} \mathbf{b}_2 \\ -\mathbf{b}_2 \end{bmatrix} + \mathbf{b}_2^T\mathbf{C}_{22}(z)\mathbf{b}_2 \\ &= \frac{1}{2}\left[\mathbf{b}_2^T, -\mathbf{b}_2^T, -\mathbf{b}_2^T\right]\begin{bmatrix} \mathbf{C}_{11}(z) & \mathbf{C}_{12}(z) \\ \mathbf{C}_{12}^T(z) & \mathbf{C}_{22}(z) \end{bmatrix}\begin{bmatrix} \mathbf{b}_2 \\ -\mathbf{b}_2 \\ -\mathbf{b}_2 \end{bmatrix}. \end{aligned}$$

Using (3.3)-(3.5) and the fact that

$$\mathbf{B}_4 \begin{bmatrix} \mathbf{b}_2 \\ -\mathbf{b}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{b}_2 \\ -\mathbf{b}_2 \end{bmatrix},$$

we get

$$J_z(\frac{1}{\sqrt{2}}) = \frac{1}{2} \left[\mathbf{b}_2^T, -\mathbf{b}_2^T, -\mathbf{b}_2^T\right] \begin{bmatrix} \mathbf{S}_z^T \\ \mathbf{M}_z^T \\ \mathbf{T}_z^T \end{bmatrix} \mathbf{B}_p \left[\mathbf{S}_z, \mathbf{M}_z, \mathbf{T}_z\right] \begin{bmatrix} \mathbf{b}_2 \\ -\mathbf{b}_2 \\ -\mathbf{b}_2 \end{bmatrix}.$$

In Proposition 8 we have seen that

$$\left[\mathbf{S}_z, \mathbf{M}_z, \mathbf{T}_z\right] \begin{bmatrix} \mathbf{b}_2 \\ -\mathbf{b}_2 \\ -\mathbf{b}_2 \end{bmatrix} = \begin{bmatrix} a \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

where a is either 1 or -1. It follows that

$$J_z(\frac{1}{\sqrt{2}}) = [1, 0, \ldots, 0]\, \mathbf{B}_p \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \frac{p-1}{2p}$$

which completes the proof.

S10 Proof of Proposition 10

For $\mathbf{X}^* = c\,[\mathbf{B}_2, -\mathbf{B}_2]$, as in the statement of Proposition 10, define

$$G_z = L_z(\mathbf{X}^*)/n = tr(\mathbf{C}_{11}(z)) - 2tr(\mathbf{C}_{12}(z)\mathbf{X}^*) + tr(\mathbf{X}^{*T}\mathbf{C}_{22}(z)\mathbf{X}^*).$$

We get from (3.3)-(3.5)

$$\begin{aligned} G_z &= tr\left(\mathbf{B}_4 \begin{bmatrix} \mathbf{S}_z^T \\ \mathbf{M}_z^T \end{bmatrix} \mathbf{B}_p\,[\mathbf{S}_z, \mathbf{M}_z]\,\mathbf{B}_4\right) \\ &\quad -2c\,tr\left(\mathbf{B}_4 \begin{bmatrix} \mathbf{S}_z^T \\ \mathbf{M}_z^T \end{bmatrix} \mathbf{B}_p\mathbf{T}_z\,[\mathbf{B}_2, -\mathbf{B}_2]\right) \\ &\quad +c^2 tr\left(\begin{bmatrix} \mathbf{B}_2 \\ -\mathbf{B}_2 \end{bmatrix} \mathbf{T}_z^T\mathbf{B}_p\mathbf{T}_z\,[\mathbf{B}_2, -\mathbf{B}_2]\right) \\ &= tr\Big(\mathbf{B}_4 \begin{bmatrix} (\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2)^T \\ (\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2)^T \end{bmatrix} \mathbf{B}_p\big[\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2, \mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2\big]\mathbf{B}_4\Big), \end{aligned}$$

where we have used that $[\mathbf{B}_2, -\mathbf{B}_2]\,\mathbf{B}_4 = [\mathbf{B}_2, -\mathbf{B}_2]$ and, for any $\mathbf{A}_1, \mathbf{A}_2$, that $tr(\mathbf{A}_1\mathbf{A}_2) = tr(\mathbf{A}_2\mathbf{A}_1)$.

We split G_z up into several parts. Define

$$G_z^{(1)} = tr\left(\begin{bmatrix} (\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2)^T \\ (\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2)^T \end{bmatrix} \Big[\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2, \mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2\Big]\right),$$

$$G_z^{(2)} = tr\left(\begin{bmatrix}(\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2)^T \\ (\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2)^T\end{bmatrix}\frac{1}{p}\mathbf{1}_p\mathbf{1}_p^T\Big[\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2, \mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2\Big]\right),$$

and

$$G_z^{(3)} = \frac{1}{4}\mathbf{1}_4^T\begin{bmatrix}(\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2)^T \\ (\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2)^T\end{bmatrix}\mathbf{B}_p\Big[\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2, \mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2\Big]\mathbf{1}_4.$$

Then $G_z = G_z^{(1)} - G_z^{(2)} - G_z^{(3)}$, because $tr\,(\mathbf{B}_4\mathbf{A}\mathbf{B}_4) = tr(\mathbf{A}) - \frac{1}{4}\mathbf{1}_4^T\mathbf{A}\mathbf{1}_4$.

If z starts with R, the first row of $\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2$ equals $\big[-c/2, c/2\big]$. Otherwise it is $\big[c/2, -c/2\big]$.

For $i \geq 2$, the i-th row of $\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2$ equals

$$\begin{aligned}
&[1 - c/2,\ c/2]\,, \text{ if } z(i-1) = R,\ z(i) = R,\\
&[c/2,\ -c/2]\,, \quad \text{if } z(i-1) = R,\ z(i) = T,\\
&[-c/2,\ c/2]\,, \quad \text{if } z(i-1) = T,\ z(i) = R,\\
&[c/2,\ 1 - c/2]\,, \text{ if } z(i-1) = T,\ z(i) = T.
\end{aligned}$$

On the other hand, the first row of $\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2$ is $\big[c/2, -c/2\big]$ if z starts with R, and $\big[-c/2, c/2\big]$ if it starts with T. For $i \geq 2$, the i-th row of $\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2$ equals

$$\begin{aligned}
&[c/2,\ -c/2]\,, \quad \text{if } z(i-1) = R,\ z(i) = R,\\
&[1 - c/2,\ c/2]\,, \text{ if } z(i-1) = R,\ z(i) = T,
\end{aligned}$$

$$[c/2,\, 1-c/2]\,, \text{ if } z(i-1)=T,\, z(i)=R,$$

$$[-c/2,\, c/2]\,, \quad \text{ if } z(i-1)=T,\, z(i)=T.$$

We therefore have that

$$(\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2)^T(\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2) =$$
$$\begin{bmatrix} \frac{c^2}{4} & -\frac{c^2}{4} \\ -\frac{c^2}{4} & \frac{c^2}{4} \end{bmatrix} + s_{RR} \begin{bmatrix} (1-\frac{c}{2})^2 & \frac{c}{2}(1-\frac{c}{2}) \\ \frac{c}{2}(1-\frac{c}{2}) & \frac{c^2}{4} \end{bmatrix}$$
$$+m_{RT} \begin{bmatrix} \frac{c^2}{4} & -\frac{c^2}{4} \\ -\frac{c^2}{4} & \frac{c^2}{4} \end{bmatrix} + m_{TR} \begin{bmatrix} \frac{c^2}{4} & -\frac{c^2}{4} \\ -\frac{c^2}{4} & \frac{c^2}{4} \end{bmatrix} + s_{TT} \begin{bmatrix} \frac{c^2}{4} & \frac{c}{2}(1-\frac{c}{2}) \\ \frac{c}{2}(1-\frac{c}{2}) & (1-\frac{c}{2})^2 \end{bmatrix}$$

and

$$tr\big((\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2)^T(\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2)\big) =$$
$$(1+m_{RT}+m_{TR})\frac{c^2}{2} + \big(s_{RR}+s_{TT}\big)(\frac{c^2}{4} + (1-\frac{c}{2})^2).$$

Similarly,

$$\begin{aligned} & tr\big((\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2)^T(\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2)\big) \\ = \; & (1+s_{RR}+s_{TT})\frac{c^2}{2} + \big(m_{RT}+m_{TR}\big)(\frac{c^2}{4} + (1-\frac{c}{2})^2). \end{aligned}$$

Noting that $s_{RR}+s_{TT}+m_{RT}+m_{TR}=p-1$, we get

$$\begin{aligned} G_z^{(1)} &= tr\big((\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2)^T(\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2)\big) \\ &\quad + tr\big((\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2)^T(\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2)\big) \end{aligned}$$

$$
\begin{aligned}
&= (p+1)\frac{c^2}{2} + (p-1)(\frac{c^2}{4} + (1-\frac{c}{2})^2) \\
&= \frac{3p^3+4p^2-2p-4}{4(p+1)^2}.
\end{aligned}
$$

We also get from our analysis of the rows of $\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2$ and of $\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2$ that

$$
\mathbf{1}_4^T \begin{bmatrix} (\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2)^T \\ (\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2)^T \end{bmatrix} = \begin{bmatrix} 0, \, 1, \ldots, \, 1 \end{bmatrix}
$$

for any sequence z. Therefore,

$$
G_z^{(3)} = \frac{1}{4}\begin{bmatrix}0, 1, \ldots, 1\end{bmatrix}\mathbf{B}_p\begin{bmatrix}0, 1, \ldots, 1\end{bmatrix}^T = \frac{p-1}{4p}.
$$

To determine $G_z^{(2)}$, we calculate

$$
\begin{aligned}
\begin{bmatrix} (\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2)^T \\ (\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2)^T \end{bmatrix} \mathbf{1}_p = &\begin{bmatrix} -\frac{c}{2} \\ \frac{c}{2} \\ \frac{c}{2} \\ -\frac{c}{2} \end{bmatrix} + s_{RR} \begin{bmatrix} 1-\frac{c}{2} \\ \frac{c}{2} \\ \frac{c}{2} \\ -\frac{c}{2} \end{bmatrix} \\
+m_{RT} \begin{bmatrix} \frac{c}{2} \\ -\frac{c}{2} \\ 1-\frac{c}{2} \\ \frac{c}{2} \end{bmatrix} + m_{TR} &\begin{bmatrix} -\frac{c}{2} \\ \frac{c}{2} \\ \frac{c}{2} \\ 1-\frac{c}{2} \end{bmatrix} + s_{TT} \begin{bmatrix} \frac{c}{2} \\ 1-\frac{c}{2} \\ -\frac{c}{2} \\ \frac{c}{2} \end{bmatrix}
\end{aligned}
$$

$$= \begin{bmatrix} s_{RR} - \frac{c}{2}\left(s_{RR} - s_{TT} - (m_{RT} - m_{TR}) + 1\right) \\ s_{TT} + \frac{c}{2}\left(s_{RR} - s_{TT} - (m_{RT} - m_{TR}) + 1\right) \\ m_{RT} + \frac{c}{2}\left(s_{RR} - s_{TT} - (m_{RT} - m_{TR}) + 1\right) \\ m_{TR} - \frac{c}{2}\left(s_{RR} - s_{TT} - (m_{RT} - m_{TR}) + 1\right) \end{bmatrix},$$

if the sequence starts with R, and, similarly,

$$\begin{bmatrix} (\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2)^T \\ (\mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2)^T \end{bmatrix} \mathbf{1}_p$$

$$= \begin{bmatrix} s_{RR} - \frac{c}{2}\left(s_{RR} - s_{TT} - (m_{RT} - m_{TR}) - 1\right) \\ s_{TT} + \frac{c}{2}\left(s_{RR} - s_{TT} - (m_{RT} - m_{TR}) - 1\right) \\ m_{RT} + \frac{c}{2}\left(s_{RR} - s_{TT} - (m_{RT} - m_{TR}) - 1\right) \\ m_{TR} - \frac{c}{2}\left(s_{RR} - s_{TT} - (m_{RT} - m_{TR}) - 1\right) \end{bmatrix},$$

if the sequence starts with T.

Defining the parameters

$$s = s_{RR} + s_{TT}, \quad d_s = s_{RR} - s_{TT}$$

$$m = m_{RT} + m_{TR}, \quad d_m = m_{RT} - m_{TR},$$

we then get

$$G_z^{(2)} =$$

$$\frac{1}{p}\mathbf{1}_p^T \left[\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2,\, \mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2\right] \left[\mathbf{S}_z - c\mathbf{T}_z\mathbf{B}_2,\, \mathbf{M}_z + c\mathbf{T}_z\mathbf{B}_2\right]^T \mathbf{1}_p$$

$$= \frac{1}{p}\Big((\frac{s}{2} + \frac{d_s}{2} - \frac{c}{2}(d_s - d_m + 1))^2 + (\frac{s}{2} - \frac{d_s}{2} + \frac{c}{2}(d_s - d_m + 1))^2$$

$$
\begin{aligned}
& +(\frac{m}{2}+\frac{d_m}{2}+\frac{c}{2}(d_s-d_m+1))^2+(\frac{m}{2}-\frac{d_m}{2}-\frac{c}{2}(d_s-d_m+1))^2\Big) \\
= \quad & \frac{1}{2p}\Big(s^2+\big(d_s-c(d_s-d_m+1)\big)^2+m^2+\big(d_m+c(d_s-d_m+1)\big)^2\Big),
\end{aligned}
$$

if the sequence z starts with R. In the same way we get

$$
\begin{aligned}
& G_z^{(2)} = \\
& \frac{1}{2p}\Big(s^2+\big(d_s-c(d_s-d_m-1)\big)^2+m^2+\big(d_m+c(d_s-d_m-1)\big)^2\Big),
\end{aligned}
$$

if z starts with T.

To determine a minimum of $G_z^{(2)}$, we consider four cases.

Case 1: The sequence z starts with R and ends with R.

In this case $m_{RT} = m_{TR}$ and, therefore, $d_m = 0$. Hence,

$$
G_z^{(2)} = \frac{1}{2p}\Big(s^2+\big(d_s-c(d_s+1)\big)^2+m^2+\big(c(d_s+1)\big)^2\Big).
$$

Observe that

$$
\big(d_s-c(d_s+1)\big)^2+\big(c(d_s+1)\big)^2 = d_s^2(1-2c+2c^2)-d_s(2c-4c^2)+2c^2.
$$

Since d_s is an integer, we have $d_s \le d_s^2$. Making use of $0 < c < 1/2$, this implies that $-d_s(2c-4c^2) \ge -d_s^2(2c-4c^2)$ and, therefore,

$$
\big(d_s-c(d_s+1)\big)^2+\big(c(d_s+1)\big)^2 \ge d_s^2(1-4c+6c^2)+2c^2.
$$

Observing that $(1-4c+6c^2) = (1-2c)^2+2c^2 > 0$, we get that

$$
\big(d_s-c(d_s+1)\big)^2+\big(c(d_s+1)\big)^2 \ge 2c^2.
$$

Hence, we have shown that in Case 1

$$G_z^{(2)} \geq \frac{1}{2p}(s^2 + m^2 + 2c^2).$$

Case 2: The sequence z starts with R and ends with T.

In this case $m_{RT} = m_{TR} + 1$ and, therefore, $d_m = 1$. Hence,

$$G_z^{(2)} = \frac{1}{2p}\Big(s^2 + \big(d_s - cd_s\big)^2 + m^2 + \big(1 + cd_s\big)^2\Big).$$

Define $g = d_s + 1$. Then $d_s = g - 1$ and

$$\begin{aligned} &(d_s - cd_s)^2 + (1 + cd_s)^2 = (g-1)^2(1-c)^2 + (1 - c + cg)^2 \\ = \;\; & 2(1-c)^2 + g^2(1 - 2c + 2c^2) - g(2 - 6c + 4c^2). \end{aligned}$$

Because g is an integer and because $2 - 6c + 4c^2 = 2(1-c)(1-2c) \geq 0$ we conclude that $-g(2 - 6c + 4c^2) \geq -g^2(2 - 6c + 4c^2)$ and therefore that

$$(d_s - cd_s)^2 + (1 - cd_s)^2 \geq 2(1-c)^2 + g^2(4c - 1 - 2c^2).$$

Since $c = \frac{p}{2(p+1)}$ and $p \geq 2$, we have

$$4c - 1 - 2c^2 = \frac{p^2 - 2}{2p^2 + 4p + 2} > 0$$

and, therefore,

$$(d_s - cd_s)^2 + (1 - cd_s)^2 \geq 2(1-c)^2.$$

Note that $0 < c < 1/2$. Therefore, $2(1-c)^2 > 2c^2$ and we have shown that in Case 2

$$G_z^{(2)} > \frac{1}{2p}(s^2 + m^2 + 2c^2)$$

Case 3: The sequence starts with T and ends with R.

In this case $m_{TR} = m_{RT} + 1$ and therefore $d_m = -1$. This implies that

$$G_z^{(2)} \quad = \quad \frac{1}{2p}\Big(s^2 + \big(d_s - cd_s\big)^2 + m^2 + \big(-1 + cd_s\big)^2\Big),$$

If we define $\bar{d}_s = -d_s$, we see that

$$G_z^{(2)} = \frac{1}{2p}\Big(s^2 + \big(\bar{d}_s - c\bar{d}_s\big)^2 + m^2 + \big(1 + c\bar{d}_s\big)^2\Big).$$

Hence, we conclude in the same way as in Case 2, that in Case 3 we also have

$$G_z^{(2)} > \frac{1}{2p}(s^2 + m^2 + 2c^2).$$

Case 4: The sequence starts and ends with T.

In this case $m_{TR} = m_{RT}$ and therefore $d_m = 0$. This implies that

$$G_z^{(2)} \quad = \quad \frac{1}{2p}\Big(s^2 + \big(d_s - c(d_s - 1)\big)^2 + m^2 + \big(c(d_s - 1)\big)^2\Big),$$

Defining $\bar{d}_s = -d_s$, we see that

$$G_z^{(2)} = \frac{1}{2p}\Big(s^2 + \big(\bar{d}_s - c(\bar{d}_s + 1)\big)^2 + m^2 + \big(c(\bar{d}_s + 1)\big)^2\Big).$$

Hence, we conclude in the same way as in Case 1 that

$$G_z^{(2)} \geq \frac{1}{2p}(s^2 + m^2 + 2c^2).$$

Combining the four cases, we have shown for any sequence z that

$$G_z^{(2)} \geq \frac{1}{2p}(s^2 + m^2 + 2c^2).$$

Since $s+m = s_{RR}+s_{TT}+m_{RT}+m_{TR} = p-1$, we get $s^2+m^2 \geq \frac{1}{2}(p-1)^2$. Inserting $c = \frac{p}{2(p+1)}$, we hence have that

$$G_z^{(2)} \geq \frac{1}{4p}\big((p-1)^2 + \frac{p^2}{(p+1)^2}\big).$$

Combining the results for the three terms, we conclude for any $z \in Z_p$ that

$$\begin{aligned} G_z &\leq \frac{3p^3+4p^2-2p-4}{4(p+1)^2} - \frac{(p-1)^2 + \frac{p^2}{(p+1)^2}}{4p} - \frac{p-1}{4p} \\ &= \frac{3p^4+4p^3-2p^2-4p}{4p(p+1)^2} - \frac{p^4-p^2+1}{4p(p+1)^2} - \frac{(p-1)(p+1)^2}{4p(p+1)^2} \\ &= \frac{(2p+3)(p-1)}{4(p+1)}. \end{aligned}$$

This completes the proof of Proposition 10.