

On maximization of some functions of eigenvalues of nonnegative definite matrices

K. Filipiak¹ A. Markiewicz¹ R. Róžański²

¹Poznań University of Life Sciences, Poland

²The Higher Vocational State School in Gorzów Wlkp., Poland

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Notation

$$\mathbf{C} \in \mathcal{M}_v^{\geq}$$
$$\mathbf{C} = b\mathbf{I}_v - \frac{1}{b}\mathbf{S}^T\mathbf{S}, \quad b \in \mathbb{N}$$

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$$\mathbf{S}\mathbf{1}_v = \mathbf{S}^T\mathbf{1}_v = b\mathbf{1}_v$$

Problems

$$0 = \lambda_0(\mathbf{C}) \leq \lambda_1(\mathbf{C}) \leq \dots \leq \lambda_{v-1}(\mathbf{C})$$

E-optimality

MAXIMIZATION OF $\lambda_1(\mathbf{C})$

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$$0 = \lambda_0(\mathbf{C}) \leq \lambda_1(\mathbf{C}) \leq \dots \leq \lambda_{v-1}(\mathbf{C})$$

E-optimality

MAXIMIZATION OF $\lambda_1(\mathbf{C})$

D-optimality

MAXIMIZATION OF $\prod_{i=1}^{v-1} \lambda_i(\mathbf{C})$

Special classes for $b = v - 2$ and $b = v$

$\overline{\mathcal{P}}_v$ - the class of derangement matrices of order v

$$b = v - 2$$

$$\tilde{\mathcal{B}} = \{\mathbf{P} : \mathbf{S} = \mathbf{1}_v \mathbf{1}_v^T - \mathbf{I}_v - \mathbf{P}, \mathbf{P} \in \overline{\mathcal{P}}_v\}$$

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$$\hat{\mathcal{B}} = \{\mathbf{P} : \mathbf{S} = \mathbf{1}_v \mathbf{1}_v^T - \mathbf{I}_v + \mathbf{P}, \mathbf{P} \in \overline{\mathcal{P}}_v\}$$

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$$b = v$$

$$\mathbf{S} = \begin{pmatrix} 0 & 2 & 1 & 1 & 1 & 1 \\ 1 & 0 & 2 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 2 \\ 1 & 1 & 1 & 0 & 2 & 1 \\ 2 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 2 & 1 & 0 \end{pmatrix}$$

Special classes

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$$b = v$$

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Special classes

$$\mathbf{S} \in \tilde{\mathcal{B}}$$

$$\mathbf{C} = \frac{v^2 - 4v + 2}{v - 2} \mathbf{I}_v - \frac{1}{v - 2} (\mathbf{P} + \mathbf{P}^T) - \frac{v - 4}{v - 2} \mathbf{1}_v^T \mathbf{1}_v$$

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$\mathbf{1}_v$ – the eigenvector associated with 0 eigenvalue.

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E-optimality: $\text{MAX } \lambda_1(\bar{\mathbf{C}})$

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E-optimality: $\text{MAX } \lambda_1(\bar{\mathbf{C}})$

D-optimality: $\text{MAX } \det \bar{\mathbf{C}}$

Two cases

$\tilde{\mathcal{B}}$:

$$\mathbf{W} = (\nu - 2)\overline{\mathbf{C}} = \alpha\mathbf{I}_\nu - (\mathbf{P} + \mathbf{P}^T)$$

$\hat{\mathcal{B}}$:

$$\alpha > 2$$

$$\mathbf{V} = \nu\overline{\mathbf{C}} = \alpha\mathbf{I}_\nu + (\mathbf{P} + \mathbf{P}^T)$$

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E-optimality: $\text{MAX } \lambda_1(\mathbf{W})$ ($\text{MAX } \lambda_1(\mathbf{V})$)

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E-optimality: $\text{MAX } \lambda_1(\mathbf{W})$ ($\text{MAX } \lambda_1(\mathbf{V})$)

D-optimality: $\text{MAX } \det \mathbf{W}$ ($\text{MAX } \det \mathbf{V}$)

Permutation matrices

$$\mathbf{H}_v = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 0 & 1 \\ 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 1 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 \end{pmatrix}$$

Permutation matrices

$$\mathbf{H}_v = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 0 & 1 \\ 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 1 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 \end{pmatrix}$$

$\mathbf{P} = \mathbf{H}_v$ – irreducible matrix

Permutation matrices

$$\mathbf{H}_v = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 0 & 1 \\ 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 1 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 \end{pmatrix}$$

$\mathbf{P} = \mathbf{H}_v$ – irreducible matrix

$\mathbf{P} = \text{diag}(\mathbf{H}_{v_1} : \mathbf{H}_{v_2}),$

Permutation matrices

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$\mathbf{P} = \mathbf{H}_v$ – irreducible matrix

$\mathbf{P} = \text{diag}(\mathbf{H}_{v_1} : \mathbf{H}_{v_2})$, $\mathbf{P} = \text{diag}(\mathbf{H}_{v_1} : \mathbf{H}_{v_2} : \mathbf{H}_{v_3})$,

Permutation matrices

$$\mathbf{H}_v = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 0 & 1 \\ 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 1 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 \end{pmatrix}$$

$\mathbf{P} = \mathbf{H}_v$ – irreducible matrix

$\mathbf{P} = \text{diag}(\mathbf{H}_{v_1} : \mathbf{H}_{v_2})$, $\mathbf{P} = \text{diag}(\mathbf{H}_{v_1} : \mathbf{H}_{v_2} : \mathbf{H}_{v_3})$, ...

– reducible matrices

E-optimality

$$\mathbf{W} = \begin{pmatrix} \alpha & -1 & 0 & 0 & 0 & 0 & -1 \\ -1 & \alpha & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & \alpha & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & \alpha & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & \alpha & -1 \\ -1 & 0 & 0 & 0 & 0 & -1 & \alpha \end{pmatrix}$$

E-optimality

$$\mathbf{W} = \begin{pmatrix} \alpha & -1 & 0 & 0 & 0 & 0 & -1 \\ -1 & \alpha & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & \alpha & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & \alpha & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & \alpha & -1 \\ -1 & 0 & 0 & 0 & 0 & -1 & \alpha \end{pmatrix}$$

$$\mathbf{W} = \left(\begin{array}{cccc|ccc} \alpha & -1 & 0 & -1 & 0 & 0 & 0 \\ -1 & \alpha & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & 0 & 0 & 0 \\ -1 & 0 & -1 & \alpha & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \alpha & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & \alpha & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & \alpha \end{array} \right)$$

E-optimality

$$\mathbf{W} = \begin{pmatrix} \alpha & -1 & 0 & 0 & 0 & 0 & -1 \\ -1 & \alpha & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & \alpha & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & \alpha & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & \alpha & -1 \\ -1 & 0 & 0 & 0 & 0 & -1 & \alpha \end{pmatrix}$$

$\lambda_1(\mathbf{W})$

$$\mathbf{W} = \left(\begin{array}{cccc|ccc} \alpha & -1 & 0 & -1 & 0 & 0 & 0 \\ -1 & \alpha & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & 0 & 0 & 0 \\ -1 & 0 & -1 & \alpha & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \alpha & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & \alpha & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & \alpha \end{array} \right)$$

E-optimality

$$\mathbf{W} = \begin{pmatrix} \alpha & -1 & 0 & 0 & 0 & 0 & -1 \\ -1 & \alpha & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & \alpha & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & \alpha & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & \alpha & -1 \\ -1 & 0 & 0 & 0 & 0 & -1 & \alpha \end{pmatrix}$$

$\lambda_1(\mathbf{W})$

$$\mathbf{W} = \begin{pmatrix} \alpha & -1 & 0 & -1 & | & 0 & 0 & 0 \\ -1 & \alpha & -1 & 0 & | & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & | & 0 & 0 & 0 \\ -1 & 0 & -1 & \alpha & | & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & | & \alpha & -1 & -1 \\ 0 & 0 & 0 & 0 & | & -1 & \alpha & -1 \\ 0 & 0 & 0 & 0 & | & -1 & -1 & \alpha \end{pmatrix}$$

$\lambda_1(\mathbf{W}) = \min(\lambda_1(\mathbf{W}_1), \lambda_1(\mathbf{W}_2))$

$$\tilde{\mathcal{B}} : \quad \mathbf{W} = \alpha \mathbf{I}_v - (\mathbf{P} + \mathbf{P}^T)$$

$$\mu_k(\mathbf{H}_v + \mathbf{H}_v^T) = 2 \cos \frac{2k\pi}{v}, \quad k = 0, 1, 2, \dots, v-1$$

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$$\mathbf{P} = \mathbf{H}_v:$$

$$\mu_k(\mathbf{W}) = \alpha - 2 \cos \frac{2k\pi}{v}, \quad k = 0, 1, 2, \dots, v-1$$

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$$\mathbf{P} = \text{diag}(\mathbf{H}_{v_1} : \mathbf{H}_{v_2}):$$

$$\mu_k(\mathbf{W}) = \begin{cases} \alpha - 2 \cos \frac{2k\pi}{v_1}, & k = 0, 1, 2, \dots, v_1 - 1 \\ \alpha - 2 \cos \frac{2k\pi}{v_2}, & k = 0, 1, 2, \dots, v_2 - 1 \end{cases}$$

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$$\lambda_1(\mathbf{W}) = \mu_1(\mathbf{W}) - \text{if } \mathbf{P} = \mathbf{H}_v \text{ (irreducible)}$$

$$\tilde{\mathcal{B}} : \quad \mathbf{W} = \alpha \mathbf{I}_v - (\mathbf{P} + \mathbf{P}^T)$$

$$\mu_k(\mathbf{H}_v + \mathbf{H}_v^T) = 2 \cos \frac{2k\pi}{v}, \quad k = 0, 1, 2, \dots, v-1$$

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$$\lambda_1(\mathbf{W}) = \mu_0(\mathbf{W}) - \text{if } \mathbf{P} \text{ is reducible}$$

$$\tilde{\mathcal{B}} : \quad \mathbf{W} = \alpha \mathbf{I}_v - (\mathbf{P} + \mathbf{P}^T)$$

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Theorem 1

Let $\overline{\mathcal{P}}_v$ be the set of permutation, derangement matrices of order v . The matrix $\mathbf{P} \in \overline{\mathcal{P}}_v$ that maximizes $\lambda_1(\mathbf{W})$ over all matrices of the form $\mathbf{W} = \alpha \mathbf{I}_v - (\mathbf{P} + \mathbf{P}^T)$, $\alpha > 2$, is permutationally similar to the matrix \mathbf{H}_v .

E-optimality

$$\mathbf{V} = \begin{pmatrix} \alpha & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & \alpha & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & \alpha & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \alpha & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & \alpha & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & \alpha & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & \alpha \end{pmatrix}$$

E-optimality

$$\mathbf{V} = \begin{pmatrix} \alpha & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & \alpha & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & \alpha & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \alpha & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & \alpha & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & \alpha & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & \alpha \end{pmatrix}$$

$$\mathbf{V} = \left(\begin{array}{cccc|ccc} \alpha & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & \alpha & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & \alpha & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & \alpha & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \alpha & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & \alpha & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & \alpha \end{array} \right)$$

E-optimality

$$\mathbf{V} = \begin{pmatrix} \alpha & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & \alpha & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & \alpha & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \alpha & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & \alpha & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & \alpha & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & \alpha \end{pmatrix}$$

$\lambda_1(\mathbf{V})$

$$\mathbf{V} = \left(\begin{array}{cccc|ccc} \alpha & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & \alpha & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & \alpha & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & \alpha & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \alpha & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & \alpha & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & \alpha \end{array} \right)$$

E-optimality

$$\mathbf{V} = \begin{pmatrix} \alpha & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & \alpha & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & \alpha & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \alpha & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & \alpha & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & \alpha & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & \alpha \end{pmatrix}$$

$$\lambda_1(\mathbf{V})$$

$$\mathbf{V} = \left(\begin{array}{cccc|ccc} \alpha & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & \alpha & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & \alpha & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & \alpha & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \alpha & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & \alpha & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & \alpha \end{array} \right)$$

$$\lambda_1(\mathbf{V}) = \min(\lambda_1(\mathbf{V}_1), \lambda_1(\mathbf{V}_2))$$

$$\hat{\mathcal{B}} : \quad \mathbf{V} = \alpha \mathbf{I}_v + (\mathbf{P} + \mathbf{P}^T)$$

$$\mu_k(\mathbf{H}_v + \mathbf{H}_v^T) = 2 \cos \frac{2k\pi}{v}, \quad k = 0, 1, 2, \dots, v-1$$

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$$\mathbf{P} = \mathbf{H}_v:$$

$$\mu_k(\mathbf{W}) = \alpha + 2 \cos \frac{2k\pi}{v}, \quad k = 0, 1, 2, \dots, v-1$$

$$\widehat{\mathcal{B}} : \quad \mathbf{V} = \alpha \mathbf{I}_v + (\mathbf{P} + \mathbf{P}^T)$$

$$\mu_k(\mathbf{H}_v + \mathbf{H}_v^T) = 2 \cos \frac{2k\pi}{v}, \quad k = 0, 1, 2, \dots, v-1$$

$$\mathbf{P} = \mathbf{H}_v:$$

$$\mu_k(\mathbf{W}) = \alpha + 2 \cos \frac{2k\pi}{v}, \quad k = 0, 1, 2, \dots, v-1$$

$$\mathbf{P} = \text{diag}(\mathbf{H}_{v_1} : \mathbf{H}_{v_2}):$$

$$\mu_k(\mathbf{W}) = \begin{cases} \alpha + 2 \cos \frac{2k\pi}{v_1}, & k = 0, 1, 2, \dots, v_1 - 1 \\ \alpha + 2 \cos \frac{2k\pi}{v_2}, & k = 0, 1, 2, \dots, v_2 - 1 \end{cases}$$

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Theorem 2

Let $\overline{\mathcal{P}}_\nu$ be the set of permutation, derangement matrices of order ν . The matrix $\mathbf{P} \in \overline{\mathcal{P}}_\nu$ that maximizes $\lambda_1(\mathbf{V})$ over all matrices of the form $\mathbf{V} = \alpha \mathbf{I}_\nu + (\mathbf{P} + \mathbf{P}^T)$, $\alpha > 2$, is permutationally similar to the matrix

- (i) \mathbf{H}_ν if $\nu = 2, 7$;
- (ii) $\mathbf{I}_2 \otimes \mathbf{H}_2$ or \mathbf{H}_4 if $\nu = 4$;
- (iii) $\mathbf{I}_m \otimes \mathbf{H}_3$ if $\nu = 3m$, $m \in \mathbb{N}$;
- (iv) $\text{diag}(\mathbf{I}_i \otimes \mathbf{H}_3, \mathbf{I}_j \otimes \mathbf{H}_5)$ if $\nu = 5$ or $\nu \geq 8$ and $\nu \neq 3m$, $m \in \mathbb{N}$, with $\nu = 3i + 5j$ for some $i \in \mathbb{N} \cup \{0\}$, $j \in \mathbb{N}$.

D-optimality

$$\mathbf{W} = \begin{pmatrix} \alpha & -1 & 0 & 0 & 0 & 0 & -1 \\ -1 & \alpha & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & \alpha & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & \alpha & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & \alpha & -1 \\ -1 & 0 & 0 & 0 & 0 & -1 & \alpha \end{pmatrix}$$

D-optimality

$$W = \begin{pmatrix} \alpha & -1 & 0 & 0 & 0 & 0 & -1 \\ -1 & \alpha & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & \alpha & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & \alpha & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & \alpha & -1 \\ -1 & 0 & 0 & 0 & 0 & -1 & \alpha \end{pmatrix}$$

$$W = \left(\begin{array}{cccc|ccc} \alpha & -1 & 0 & -1 & 0 & 0 & 0 \\ -1 & \alpha & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & 0 & 0 & 0 \\ -1 & 0 & -1 & \alpha & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \alpha & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & \alpha & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & \alpha \end{array} \right)$$

D-optimality

$$\mathbf{W} = \begin{pmatrix} \alpha & -1 & 0 & 0 & 0 & 0 & -1 \\ -1 & \alpha & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & \alpha & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & \alpha & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & \alpha & -1 \\ -1 & 0 & 0 & 0 & 0 & -1 & \alpha \end{pmatrix}$$

det \mathbf{W}

$$\mathbf{W} = \left(\begin{array}{cccc|ccc} \alpha & -1 & 0 & -1 & 0 & 0 & 0 \\ -1 & \alpha & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & 0 & 0 & 0 \\ -1 & 0 & -1 & \alpha & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \alpha & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & \alpha & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & \alpha \end{array} \right)$$

D-optimality

$$\mathbf{W} = \begin{pmatrix} \alpha & -1 & 0 & 0 & 0 & 0 & -1 \\ -1 & \alpha & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & \alpha & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & \alpha & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & \alpha & -1 \\ -1 & 0 & 0 & 0 & 0 & -1 & \alpha \end{pmatrix}$$

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$$\mathbf{W} = \left(\begin{array}{cccc|ccc} \alpha & -1 & 0 & -1 & 0 & 0 & 0 \\ -1 & \alpha & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \alpha & -1 & 0 & 0 & 0 \\ -1 & 0 & -1 & \alpha & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \alpha & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & \alpha & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & \alpha \end{array} \right)$$

$\det \mathbf{W} = \det \mathbf{W}_1 \cdot \det \mathbf{W}_2$

$$\mathbf{W} = \alpha \mathbf{I}_v - (\mathbf{P} + \mathbf{P}^T)$$

Determinant of tridiagonal matrix with corners
(Molinari, 2008):

$$\det(\alpha \mathbf{I}_v - (\mathbf{H}_v + \mathbf{H}_v^T)) = -2 + \text{tr} \left[\left(\begin{array}{cc} \alpha & -1 \\ 1 & 0 \end{array} \right)^v \right]$$

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$$x = \lambda_0 \left[\left(\begin{array}{cc} \alpha & -1 \\ 1 & 0 \end{array} \right) \right] = \frac{\alpha - \sqrt{\alpha^2 - 4}}{2}, \quad x \in (0, \frac{1}{2})$$

$$y = \lambda_1 \left[\left(\begin{array}{cc} \alpha & -1 \\ 1 & 0 \end{array} \right) \right] = \frac{\alpha + \sqrt{\alpha^2 - 4}}{2} = \frac{1}{x}, \quad y \in (\alpha - \frac{1}{2}, \alpha)$$

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$$-2 + x^v + y^v \geq (-2 + x^{v_1} + y^{v_1})(-2 + x^{v_2} + y^{v_2})$$

Theorem 3

Let $\overline{\mathcal{P}}_\nu$ be the set of permutation, derangement matrices of order ν . The matrix $\mathbf{P} \in \overline{\mathcal{P}}_\nu$ that maximizes $\det \mathbf{W}$ over all matrices of the form $\mathbf{W} = \alpha \mathbf{I}_\nu - (\mathbf{P} + \mathbf{P}^T)$, $\alpha > 2$, is permutationally similar to the matrix \mathbf{H}_ν .

$$\mathbf{V} = \alpha \mathbf{I}_v + (\mathbf{P} + \mathbf{P}^T)$$

Determinant of tridiagonal matrix with corners
(Molinari, 2008):

$$\det(\alpha \mathbf{I}_v + (\mathbf{H}_v + \mathbf{H}_v^T)) = 2 \cdot (-1)^{v+1} + \text{tr} \left[\begin{pmatrix} \alpha & -1 \\ 1 & 0 \end{pmatrix}^v \right]$$

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Determinant of tridiagonal matrix with corners
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$$x = \lambda_0 \left[\begin{pmatrix} \alpha & -1 \\ 1 & 0 \end{pmatrix} \right] = \frac{\alpha - \sqrt{\alpha^2 - 4}}{2}, \quad x \in (0, \frac{1}{2})$$

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$$\mathbf{V} = \alpha \mathbf{I}_v + (\mathbf{P} + \mathbf{P}^T)$$

$$\det(\alpha \mathbf{I}_v + (\mathbf{H}_v + \mathbf{H}_v^T)) = \begin{cases} -2 + x^v + y^v, & v \text{ even} \\ 2 + x^v + y^v, & v \text{ odd} \end{cases}$$

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$\mathbf{P} = \text{diag}(\mathbf{H}_{v_1} : \mathbf{H}_{v_2}), v_i - \text{odd}:$

$$-2 + x^v + y^v \leq (2 + x^{v_1} + y^{v_1})(2 + x^{v_2} + y^{v_2})$$

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$\mathbf{P} = \text{diag}(\mathbf{H}_{v_1} : \mathbf{H}_{v_2})$, v_1 - odd, v_2 - even:

$$2 + x^v + y^v \leq (2 + x^{v_1} + y^{v_1})(-2 + x^{v_2} + y^{v_2})$$

Theorem 4

Let $\overline{\mathcal{P}}_v$ be the set of permutation, derangement matrices of order v . The matrix $\mathbf{P} \in \overline{\mathcal{P}}_v$ that maximizes $\det \mathbf{V}$ over all matrices of the form $\mathbf{V} = \alpha \mathbf{I}_v + (\mathbf{P} + \mathbf{P}^T)$, $\alpha > 2$, is permutationally similar to the matrix

- (i) $\mathbf{I}_m \otimes \mathbf{H}_3$ if $v = 3m$, $m \in \mathbb{N}$;
- (ii) $\text{diag}(\mathbf{I}_m \otimes \mathbf{H}_3, \mathbf{H}_4)$ if $v = 3m + 4$, $m \in \mathbb{N} \cup \{0\}$;
- (iii) $\text{diag}(\mathbf{I}_m \otimes \mathbf{H}_3, \mathbf{H}_5)$ if $v = 3m + 5$, $m \in \mathbb{N} \cup \{0\}$.

Experiment

- v - number of treatments

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- v - number of treatments
- bk - number of units

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- k - number of units in each block (block size)

Experiment

- v - number of treatments
- bk - number of units
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- $\mathcal{D}_{v,b,k}$ - the class of block designs

Interference model

Interference model

$$\mathbf{y} = \mathbf{T}_d\boldsymbol{\tau} + \mathbf{L}_d\boldsymbol{\lambda} + \mathbf{B}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

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- \mathbf{y} - vector of observations

Interference model

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- \mathbf{y} - vector of observations
- $\boldsymbol{\tau}$ - vector of treatment effects

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- \mathbf{T}_d - the design matrix of treatment effects
- \mathbf{L}_d - the design matrix of left neighbor effects
- $\mathbf{B} = \mathbf{I}_b \otimes \mathbf{1}_k$ - the design matrix of block effects

Interference model

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$$\mathbf{L}_d = (\mathbf{I}_b \otimes \mathbf{H}_k) \mathbf{T}_d$$

Interference model

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$$\mathbf{y} = \mathbf{T}_d \boldsymbol{\tau} + \mathbf{L}_d \boldsymbol{\lambda} + \mathbf{B} \boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

$$\mathbf{L}_d = (\mathbf{I}_b \otimes \mathbf{H}_k) \mathbf{T}_d$$

$$\mathbf{H}_k = \begin{pmatrix} \mathbf{0}'_{k-1} & 1 \\ \mathbf{I}_{k-1} & \mathbf{0}_{k-1} \end{pmatrix} = \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \end{pmatrix}$$

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$$\mathbf{y} = \mathbf{T}_d \boldsymbol{\tau} + \mathbf{L}_d \boldsymbol{\lambda} + \mathbf{B} \boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

$$\mathbf{L}_d = (\mathbf{I}_b \otimes \mathbf{H}_k) \mathbf{T}_d$$

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\mathbf{H}_k - the circular incidence matrix

Information matrix for the estimation of treatment effects

$$\mathbf{U}_d = \left(\begin{array}{c|cc} \mathbf{T}_d^T \mathbf{T}_d & \mathbf{T}_d^T \mathbf{L}_d & \mathbf{T}_d^T \mathbf{B} \\ \hline \mathbf{L}_d^T \mathbf{T}_d & \mathbf{L}_d^T \mathbf{L}_d & \mathbf{L}_d^T \mathbf{B} \\ \mathbf{B}^T \mathbf{T}_d & \mathbf{B}^T \mathbf{L}_d & \mathbf{B}^T \mathbf{B} \end{array} \right)$$

Information matrix for the estimation of treatment effects

$$\mathbf{U}_d = \left(\begin{array}{c|cc} \mathbf{T}_d^T \mathbf{T}_d & \mathbf{T}_d^T \mathbf{L}_d & \mathbf{T}_d^T \mathbf{B} \\ \hline \mathbf{L}_d^T \mathbf{T}_d & \mathbf{L}_d^T \mathbf{L}_d & \mathbf{L}_d^T \mathbf{B} \\ \mathbf{B}^T \mathbf{T}_d & \mathbf{B}^T \mathbf{L}_d & \mathbf{B}^T \mathbf{B} \end{array} \right) = \left(\begin{array}{c|cc} \mathbf{R}_d & \mathbf{S}_d^T & \mathbf{N}_d \\ \hline \mathbf{S}_d & \mathbf{R}_d & \mathbf{N}_d \\ \mathbf{N}_d^T & \mathbf{N}_d^T & \mathbf{K} \end{array} \right)$$

Information matrix for the estimation of treatment effects

$$\mathbf{U}_d = \left(\begin{array}{c|cc} \mathbf{T}_d^T \mathbf{T}_d & \mathbf{T}_d^T \mathbf{L}_d & \mathbf{T}_d^T \mathbf{B} \\ \hline \mathbf{L}_d^T \mathbf{T}_d & \mathbf{L}_d^T \mathbf{L}_d & \mathbf{L}_d^T \mathbf{B} \\ \mathbf{B}^T \mathbf{T}_d & \mathbf{B}^T \mathbf{L}_d & \mathbf{B}^T \mathbf{B} \end{array} \right) = \left(\begin{array}{c|cc} \mathbf{R}_d & \mathbf{S}_d^T & \mathbf{N}_d \\ \hline \mathbf{S}_d & \mathbf{R}_d & \mathbf{N}_d \\ \mathbf{N}_d^T & \mathbf{N}_d^T & \mathbf{K} \end{array} \right)$$

$$\mathbf{R}_d = \text{diag}(r_1, \dots, r_v), \quad \mathbf{K} = k\mathbf{I}_b$$

Information matrix for the estimation of treatment effects

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$$\mathbf{R}_d = \text{diag}(r_1, \dots, r_v), \quad \mathbf{K} = k\mathbf{I}_b$$

$$\mathbf{C}_d = \left[\mathbf{U}_d / \left(\begin{array}{cc} \mathbf{R}_d & \mathbf{N}_d \\ \mathbf{N}_d^T & \mathbf{K} \end{array} \right) \right] = \mathbf{R}_d - \mathbf{S}_d^T \mathbf{R}_d \mathbf{S}_d -$$

$$- (\mathbf{N}_d - \mathbf{S}_d^T \mathbf{R}_d^{-1} \mathbf{N}_d) (\mathbf{K} - \mathbf{N}_d^T \mathbf{R}_d^{-1} \mathbf{N}_d)^{-1} (\mathbf{N}_d - \mathbf{S}_d^T \mathbf{R}_d^{-1} \mathbf{N}_d)^T$$

Example - Complete binary design

$$v = k = 4, \quad b = 2$$

$$d = \begin{pmatrix} A & B & C & D \\ A & C & B & D \end{pmatrix}$$

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Design - general case

$$\mathbf{N}_d \mathbf{1}_b = \begin{pmatrix} r_1 \\ \vdots \\ r_v \end{pmatrix},$$

$$\mathbf{N}_d^T \mathbf{1}_v = v \mathbf{1}_b$$

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$$\sum_{i=1}^v \sum_{j=1}^b n_{ij} = \sum_{i=1}^v \sum_{j=1}^v s_{ij} = bv$$

C_d of complete binary design

$$\mathbf{C}_d = \left[\mathbf{U}_d / \begin{pmatrix} \mathbf{R}_d & \mathbf{N}_d \\ \mathbf{N}_d^T & \mathbf{K} \end{pmatrix} \right] = \mathbf{R}_d - \mathbf{S}_d^T \mathbf{R}_d \mathbf{S}_d - \\ - (\mathbf{N}_d - \mathbf{S}_d^T \mathbf{R}_d^{-1} \mathbf{N}_d) (\mathbf{K} - \mathbf{N}_d^T \mathbf{R}_d^{-1} \mathbf{N}_d) - (\mathbf{N}_d - \mathbf{S}_d^T \mathbf{R}_d^{-1} \mathbf{N}_d)^T$$

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Binary design with $v = k$: $\mathbf{R}_d = b\mathbf{I}_v$

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Binary design with $v = k$: $\mathbf{R}_d = b\mathbf{I}_v$

$$\mathbf{C}_d = b\mathbf{I}_v - b^{-1}\mathbf{S}_d^T \mathbf{S}_d$$

E, D-optimality over $\mathcal{D}_{v,v-2,v}$

Theorem

If there exists design d^* with the left-neighboring matrix $\mathbf{S}_{d^*} = \mathbf{1}_v \mathbf{1}_v^T - \mathbf{I}_v - \mathbf{P}_{d^*}$, such that \mathbf{P}_{d^*} is permutationally similar to the matrix given in Theorem 1, then d^* is E-optimal over the class $\mathcal{D}_{v,v-2,v}$.

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If there exists design d^* with the left-neighboring matrix $\mathbf{S}_{d^*} = \mathbf{1}_v \mathbf{1}_v^T - \mathbf{I}_v - \mathbf{P}_{d^*}$, such that \mathbf{P}_{d^*} is permutationally similar to the matrix given in Theorem 1, then d^* is E-optimal over the class $\mathcal{D}_{v,v-2,v}$.

Theorem

If there exists design d^* with the left-neighboring matrix $\mathbf{S}_{d^*} = \mathbf{1}_v \mathbf{1}_v^T - \mathbf{I}_v + \mathbf{P}_{d^*}$, such that \mathbf{P}_{d^*} is permutationally similar to the matrix given in Theorem 3, then d^* is D-optimal over the class $\mathcal{D}_{v,v-2,v}$.

Theorem

If there exists design d^* with the left-neighboring matrix $\mathbf{S}_{d^*} = \mathbf{1}_v \mathbf{1}_v^T - \mathbf{I}_v - \mathbf{P}_{d^*}$, such that \mathbf{P}_{d^*} is permutationally similar to the matrix given in Theorem 2, then d^* is E-optimal over the class $\mathcal{D}_{v,v,v}$.

E, D-optimality over $\mathcal{D}_{v,v,v}$

Theorem

If there exists design d^* with the left-neighboring matrix $\mathbf{S}_{d^*} = \mathbf{1}_v \mathbf{1}_v^T - \mathbf{I}_v - \mathbf{P}_{d^*}$, such that \mathbf{P}_{d^*} is permutationally similar to the matrix given in Theorem 2, then d^* is E-optimal over the class $\mathcal{D}_{v,v,v}$.

Theorem

If there exists design d^* with the left-neighboring matrix $\mathbf{S}_{d^*} = \mathbf{1}_v \mathbf{1}_v^T - \mathbf{I}_v + \mathbf{P}_{d^*}$, such that \mathbf{P}_{d^*} is permutationally similar to the matrix given in Theorem 4, then d^* is D-optimal over the class of all equireplicated designs.

Main References

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