# DP-Optimality in Terms of Multiple Criteria and its Application to the Split-Plot Design

Yongtao Cao , *Indiana University of Pennsylvania*

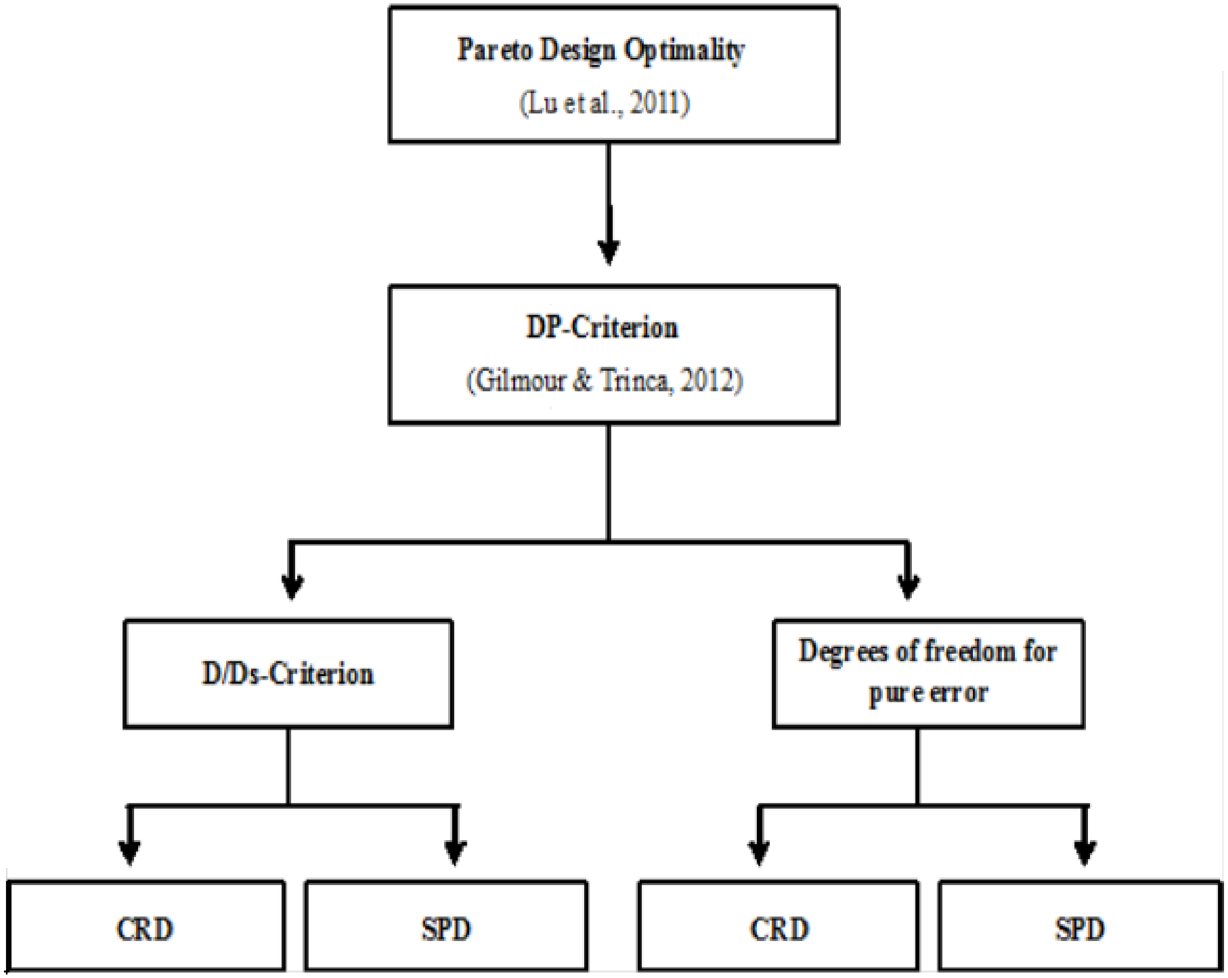
Shaun S. Wulff , *University of Wyoming*

Timothy J. Robinson , *University of Wyoming*

***Cao et al. (2017a)* Journal of Quality Technology 49(1):27-45**

DOI: 10.1080/00224065.2017.11918183

# 0. Introduction



# 0. Introduction

## 1. Pareto Optimality

**(a)** Definitions **(Lu et al., 2012)**

**(b)** Algorithm **(Cao et al., 2017a), (Cao et al., 2017b)**

## 2. DP-Optimality for CRD

**(a)** Defintions **(Gilmour and Trinca, 2012), (Cao et al., 2017a)**

**(b)** Examples **(Cao et al., 2017a)**

## 3. DP-Optimality for SPD

**(a)** Definitions **(Cao et al., 2017a)**

**(b)** Examples **(Cao et al., 2017a)**

## 4. Conclusion

# 1. Pareto Optimality (Definitions)

**(Lu et al., 2012)**

Consider $c$ multiple criteria to be maximized and a design $\xi$ from design space $\Xi$.

$$\mathbf{f}(\xi) = (f_1(\xi), f_2(\xi), ..., f_c(\xi)),\ \xi \in \Xi$$

A design $\xi^*$ *dominates* a design $\xi$ $(\xi^* \succ \xi)$ provided

**(d-1)** $f_i(\xi^*) \geq f_i(\xi)$ for all $i \in \{1, 2, ..., c\}$

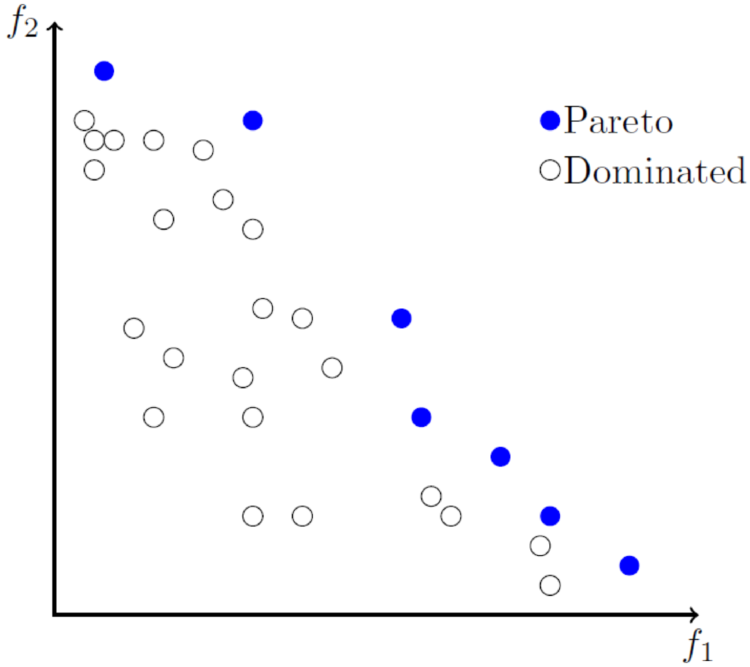
**(d-2)** $f_i(\xi^*) > f_i(\xi)$ for some $i \in \{1, 2, ..., c\}$

*pareto optimal* ***set*** $\mathcal{P} = \{\xi \in \Xi :\ \xi^* \nsucc \xi$ for any $\xi^* \in \Xi\}$

*pareto front* $\mathcal{PF} = \{\mathbf{f}(\xi) :\ \xi \in \mathcal{P}\}$

# 1. Pareto Optimality (Definitions)

$$c = 2\ ,\ \ \mathbf{f}(\xi) = (f_1(\xi), f_2(\xi))$$




*pareto optimal set* $\boldsymbol{\mathcal{P}} = \{\xi \in \Xi :\ \xi^* \not\succ \xi \text{ for any } \xi^* \in \Xi\,\}$

*pareto front* $\boldsymbol{\mathcal{PF}} = \{\mathbf{f}(\xi) :\ \xi \in \boldsymbol{\mathcal{P}}\,\}$

# 1. Pareto Optimality (Algorithm)

**(Cao et al., 2017a), (Cao et al., 2017b)**

**1.** Randomly generate design $\xi_1$. Initialize $\xi_1 \in \mathcal{P}_1^0$ and $\mathbf{f}(\xi_1) \in \mathcal{PF}_1^0$.

**2. Pareto Coordinate Exchange (PCE) Operator**

**2.a** Perform *coordinate* exchanges on $\xi_1$ to produce new designs $\xi_1^*$.

**2.b** Compare $\xi_1, \xi_1^*$, and any $\xi_1^0 \in \mathcal{P}_1^0$ using (d-1) and (d-2) to update $\mathcal{P}_1^0$ and $\mathcal{PF}_1^0$.

**3. Enhanced Elitism (EE) Operator**

**3.a** Perform PCE operator on all $\xi_1^0 \in \mathcal{P}_1^0$. Use (d-1) and (d-2) to obtain $\mathcal{P}_1^1$ and $\mathcal{PF}_1^1$.

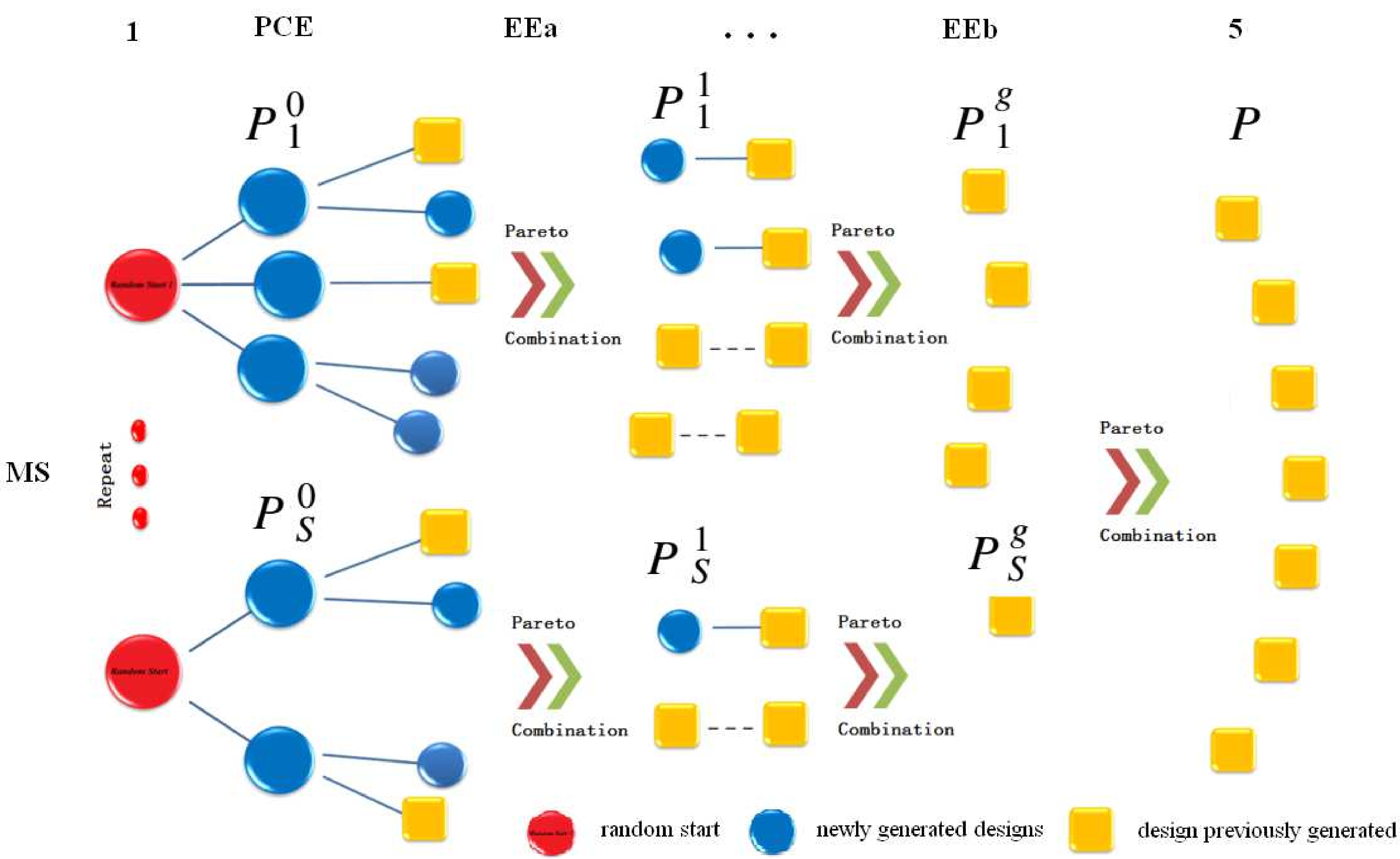
**3.b** Repeat Step 3.a $g$ times until $\mathcal{P}_1^g = \mathcal{P}_1^{g-1}$, and set $\mathcal{P}_1 = \mathcal{P}_1^g$ and $\mathcal{PF}_1 = \mathcal{PF}_1^g$.

**4. Multi-Start (MS) Operator.**

Repeat steps 1-3 for different random starting designs to obtain $\mathcal{P}_2, ..., \mathcal{P}_s$ , $\mathcal{PF}_2, ..., \mathcal{PF}_s$ .

**5.** Use (d-1) and (d-2) to determine $\mathcal{P}$ from the Pareto sets $\mathcal{P}_1, ..., \mathcal{P}_s$. Form $\mathcal{PF}$ from $\mathcal{P}$.

# 1. Pareto Optimality (Algorithm)



# 2. DP-Optimality CRD (Definitions)

**CRD** $\mathbb{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbb{E}$ , $\mathbf{X} = (\mathbf{1}, \mathbf{F}, \mathbf{F} \bullet \mathbf{F}, \mathbf{F} \ominus \mathbf{F})$ , $p = 1 + 2m_f + m_f(m_f - 1)/2$

- Design objective is to optimally select the levels or entries in $\mathbf{F}_{n \times m_f}$.

**Criteria** $|\text{Cov}(\widehat{\mathbb{B}}_{\mathbf{I}})| = (\boldsymbol{\sigma}^{\mathbf{2}})^p |\mathbf{X}'\mathbf{X}|^{-1} \propto D^{-1} = (\text{D-criterion})^{-1}$

- Global measure of overall precision in the estimation of regression model parameters.

→ minimize volume of joint confidence region for $\boldsymbol{\beta}$

→ maximize power of joint hypothesis test for $\boldsymbol{\beta}$

★ Need sufficient degrees of freedom (df) for estimating the unknown → $\boldsymbol{\sigma}^{\mathbf{2}}$.

( How is $\sigma^2$ to be estimated? )

## 2. DP-Optimality CRD (Definitions)

- Some argue $\sigma^2$ is best estimated based upon *pure error* (replicates).

  → Experiments should be designed to have sufficient number of df for pure error.

**Pure Error (Robinson and Anderson-Cook, 2011)**

(1) allows for testing lack-of-fit.

(2) provides degrees of freedom for error (even in saturated designs).

(3) produces variance estimates that are not model dependent.

**(Gilmour and Trinca, 2012)**

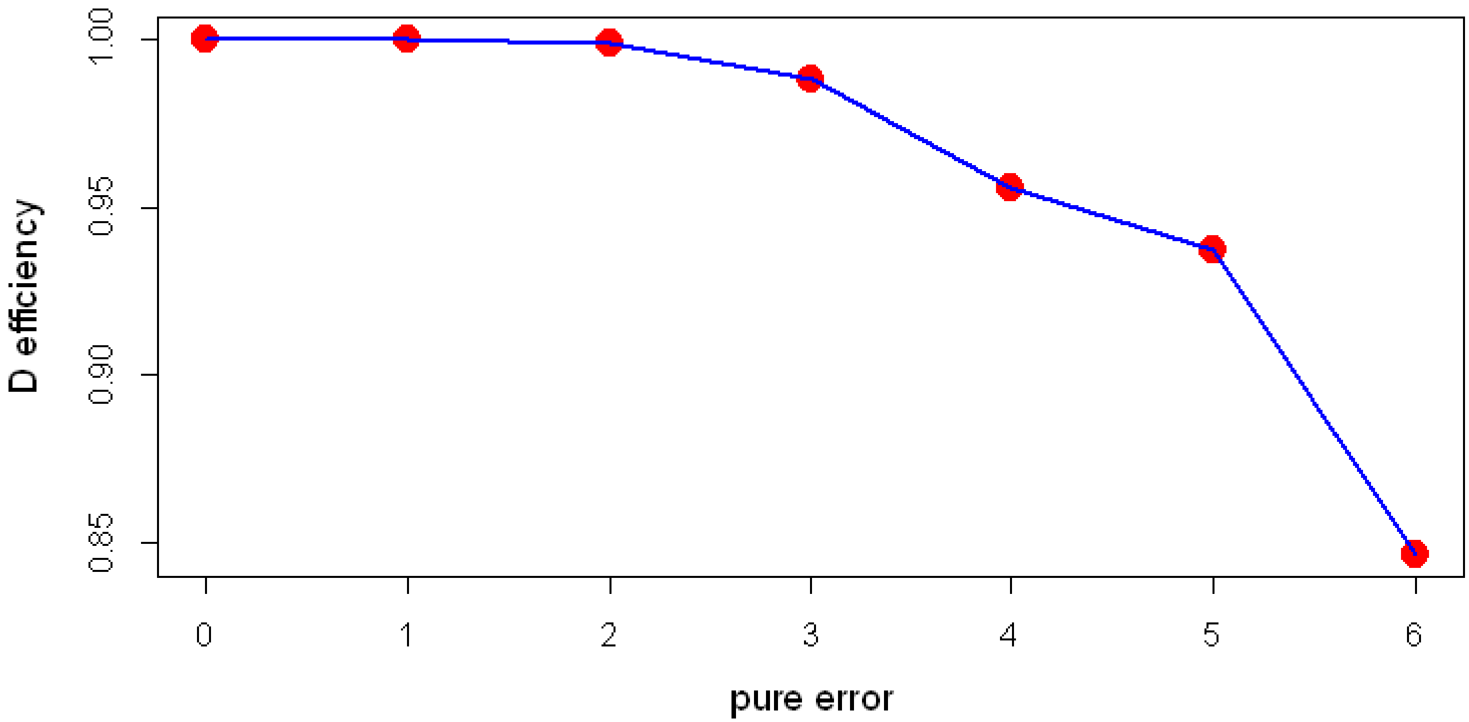
$DP = (F_{p,\boldsymbol{r},1-\alpha})^p |\mathbf{X}'\mathbf{X}|^{-1} \propto$ (volume of joint confidence region for $\boldsymbol{\beta}$, $\sigma^2$ unknown)$^2$

→ $\boldsymbol{DP}^{\text{CRD}} = (|\mathbf{X}'\mathbf{X}|, \text{df}_{\text{PE}}(\text{CRD}))$ , $\text{df}_{\text{PE}}(\text{CRD}) = \boldsymbol{r} =$ # replicate design runs

## 2. DP-Optimality CRD (Examples)

**CRD1. Three factors in 16 runs (Gilmour and Trinca, 2012).** $p = 10$

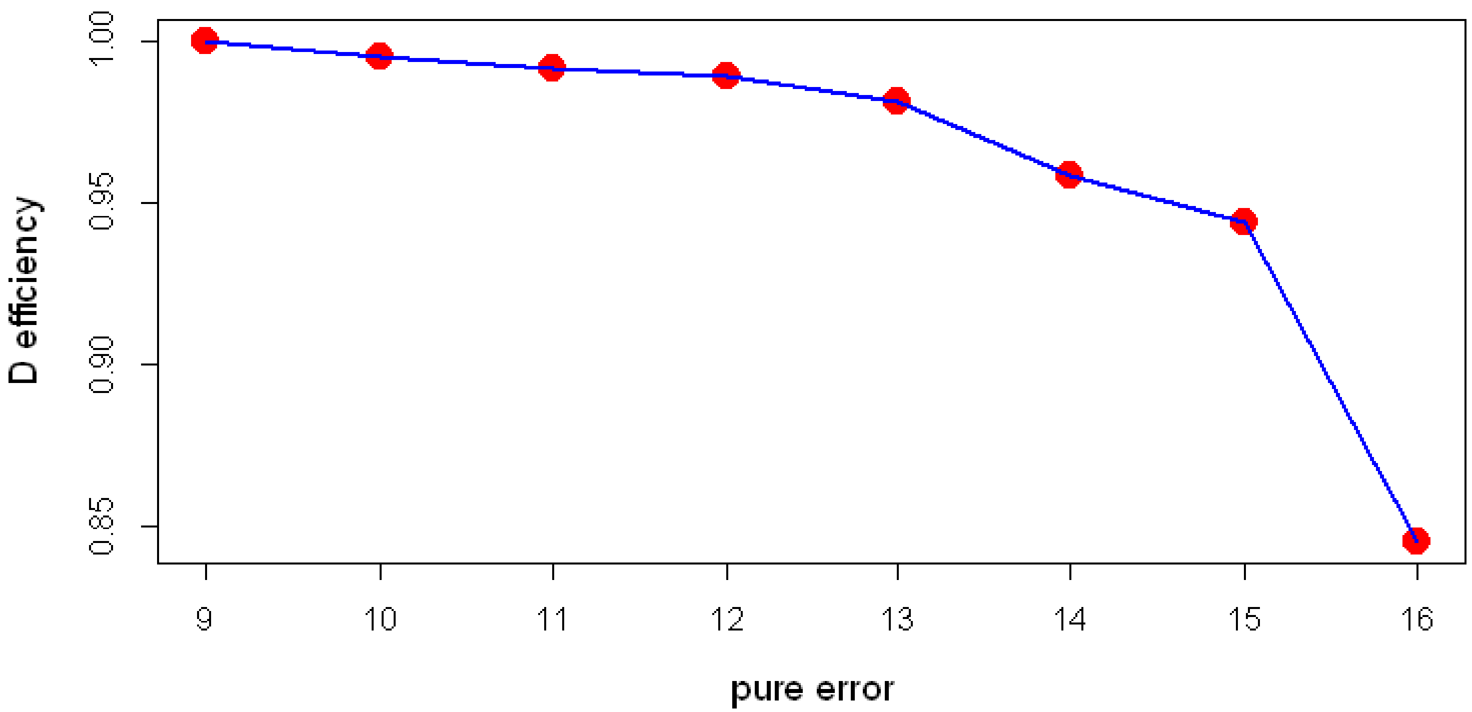
| CRD1 | 1 | GTD1 | 3 | 4 | 5 | GTD2 | GTD3 |
|---|---|---|---|---|---|---|---|
| df(PE, LoF) | (0, 6) | (1, 5) | (2, 4) | (3, 3) | (4, 2) | (5, 1) | (6, 0) |
| D-eff | 1.0000 | 0.9995 | 0.9988 | 0.9881 | 0.9558 | 0.9371 | 0.8464 |



## 2. DP-Optimality CRD (Examples)

**CRD2. Three factors in 26 runs (Gilmour and Trinca, 2012).** $p = 10$

| CRD2 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| df(PE, LoF) | (9, 7) | (10, 6) | (11, 5) | (12, 4) | (13, 3) | (14, 2) | (15, 1) | (16, 0) |
| D-eff | 1.0000 | 0.9948 | 0.9916 | 0.9892 | 0.9809 | 0.9582 | 0.9441 | 0.8451 |



# 2. DP-Optimality CRD  (Extension)

EPCEA for D-opt VS Pure error df CRD: 3f3l

Number of Random Starts:

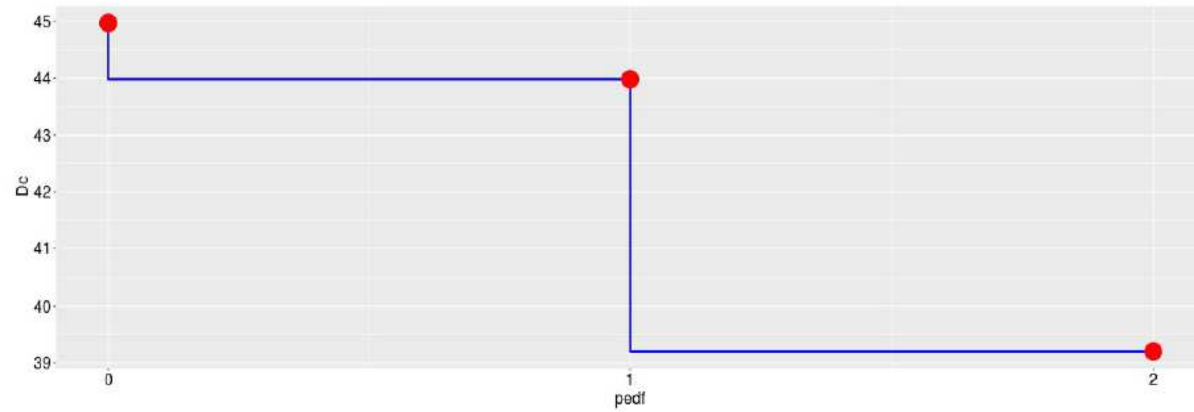
5 — 200

2 22 42 62 82 102 122 142 162 182 200

Number of Runs:

7 — 12 — 27

7 9 11 13 15 17 19 21 23 25 27




**https://ycao.shinyapps.io/EPCEA/**

(preliminary version)

Show 25 entries

Search:

| x1 | x2 | x3 | x1 | x2 | x3 | x1 | x2 | x3 |
|---|---|---|---|---|---|---|---|---|
| -1 | -1 | 1 | -1 | -1 | 1 | -1 | -1 | 1 |
| -1 | -1 | -1 | -1 | 1 | -1 | -1 | 1 | -1 |
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 0 | 1 | -1 | 1 | 1 | -1 | 1 | 1 | -1 |
| -1 | 0 | 0 | -1 | 0 | 0 | 1 | 0 | 0 |
| -1 | 1 | 1 | -1 | 1 | 1 | -1 | 1 | 1 |
| 0 | -1 | 0 | 0 | -1 | 0 | 0 | -1 | 0 |
| 1 | 0 | -1 | 1 | -1 | -1 | 1 | -1 | -1 |
| -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 |
| 1 | -1 | 1 | 1 | -1 | 1 | 1 | -1 | 1 |
| 0 | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 1 |
| -1 | 0 | 0 | -1 | 0 | 0 | -1 | 0 | 0 |
| x1 | x2 | x3 | x1 | x2 | x3 | x1 | x2 | x3 |

## 3. DP-Optimality SPD (Definitions)

**SPD** $\mathbb{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbb{G} + \mathbb{E}$ , $\mathbf{X} = (\mathbf{1}, \mathbf{W}, \mathbf{W} \bullet \mathbf{W}, \mathbf{W} \ominus \mathbf{W}, \mathbf{S}, \mathbf{S} \bullet \mathbf{S}, \mathbf{S} \ominus \mathbf{S}, \mathbf{W} \odot \mathbf{S})$

- $p = 1 + 2m_w + \frac{1}{2}m_w(m_w - 1) + 2m_s + \frac{1}{2}m_s(m_s - 1) + m_w m_s$
- Design objective is to optimally select the entries in $\mathbf{W}_{n \times m_w}$, $\mathbf{S}_{n \times m_s}$.
- $\mathbf{Z} = \mathbf{I}_{n_w} \otimes \mathbf{1}_{n_s}$ → $n = n_w n_s$ (balanced SPD)

$$\text{Cov}(\mathbb{Y}) = \text{Cov}(\mathbf{Z}\mathbb{G} + \mathbb{E}) = \sigma_\gamma^2 \mathbf{Z}\mathbf{Z}' + \sigma_e^2 \mathbf{I} = \sigma_e^2(\eta \mathbf{Z}\mathbf{Z}' + \mathbf{I}) = \sigma_e^2 \mathbf{G}$$

**Criteria** $|\text{Cov}(\widehat{\mathbb{B}}_{\mathbf{G}})| = (\sigma_e^2)^p |\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}|^{-1} \propto D^{-1}$ (with $\sigma_e^2,\ \eta = \sigma_\gamma^2/\sigma_e^2$ known)

→ $\boldsymbol{DP}^{\text{SPD}} = (|\mathbf{X}'\mathbf{G}^{-1}\mathbf{X}|^{-1}, \text{df}_{\text{PE}}(\text{WP}), \text{df}_{\text{PE}}(\text{SP}))$

$\text{df}_{\text{PE}}(\text{WP}) = \text{rank}(\mathbf{Z}, \mathbf{T}) - \text{rank}(\mathbf{T}) = n_w - \boldsymbol{\theta}$ **T** matrix of treatment effects

$\text{df}_{\text{PE}}(\text{SP}) = n - \text{rank}(\mathbf{Z}, \mathbf{T}) = r - (n_w - \boldsymbol{\theta})$ $n_w - \boldsymbol{\theta} =$ # WP with replicate runs

## 3. DP-Optimality SPD (Examples)

**SPD1. 1 WP factor, 1 SP factor in 4 whole plots of size 2 (Macharia and Goos, 2010).**

$p = 6$

| SPD1 | MGD1 | | MGD2 | | 3 | |
|---|---|---|---|---|---|---|
| whole plot | $w$ | $s$ | $w$ | $s$ | $w$ | $s$ |
| 1 | -1 | -1 | -1 | -1 | -1 | -1 |
| | **-1** | **1** | -1 | 1 | -1 | 1 |
| 2 | **-1** | **1** | **0** | **-1** | **-1** | **0** |
| | -1 | 0 | **0** | **0** | **-1** | **0** |
| 3 | 0 | -1 | **0** | **-1** | **0** | **-1** |
| | 0 | 0 | **0** | **0** | **0** | **-1** |
| 4 | 1 | -1 | 1 | -1 | 1 | -1 |
| | 1 | 1 | 1 | 1 | 1 | 1 |
| $r$ | 1 | | 2 | | 2 | |
| $n_w - \theta$ | 1 | | 1 | | 0 | |
| D(1)-efficiency | **1.0000** | | 0.9352 | | 0.7787 | |
| df(wp)(PE, LOF) | (1,0) | | (1,0) | | (0,0) | |
| df(sp)(PE, LOF) | (0,1) | | (1,0) | | (2,0) | |
| **EED** | no | | yes | | yes | |

# 3. DP-Optimality SPD (Examples)

**SPD2. 2 WP factors, 1 SP factor in 9 whole plots of size 4 (Jones and Goos, 2012).**

| SPD2 | D(1)-eff | df(wp) (PE) | df(sp) (PE) | EED |
|---|---|---|---|---|
| **1** | 1.0000 | **1** | 14 | **no** |
| 2 | 0.9931 | 1 | 15 | no |
| **JGD** | 0.9872 | **1** | 15 | **yes** |
| | | | | |
| **3** | 0.9916 | **2** | 15 | no |
| 4 | 0.9889 | 2 | 16 | no |
| 5 | 0.9847 | 2 | 17 | no |
| 6 | 0.9769 | 2 | 18 | no |
| 7 | 0.9673 | 2 | 19 | no |
| 8 | 0.9498 | 2 | 20 | no |
| 9 | 0.4869 | 2 | 23 | no |

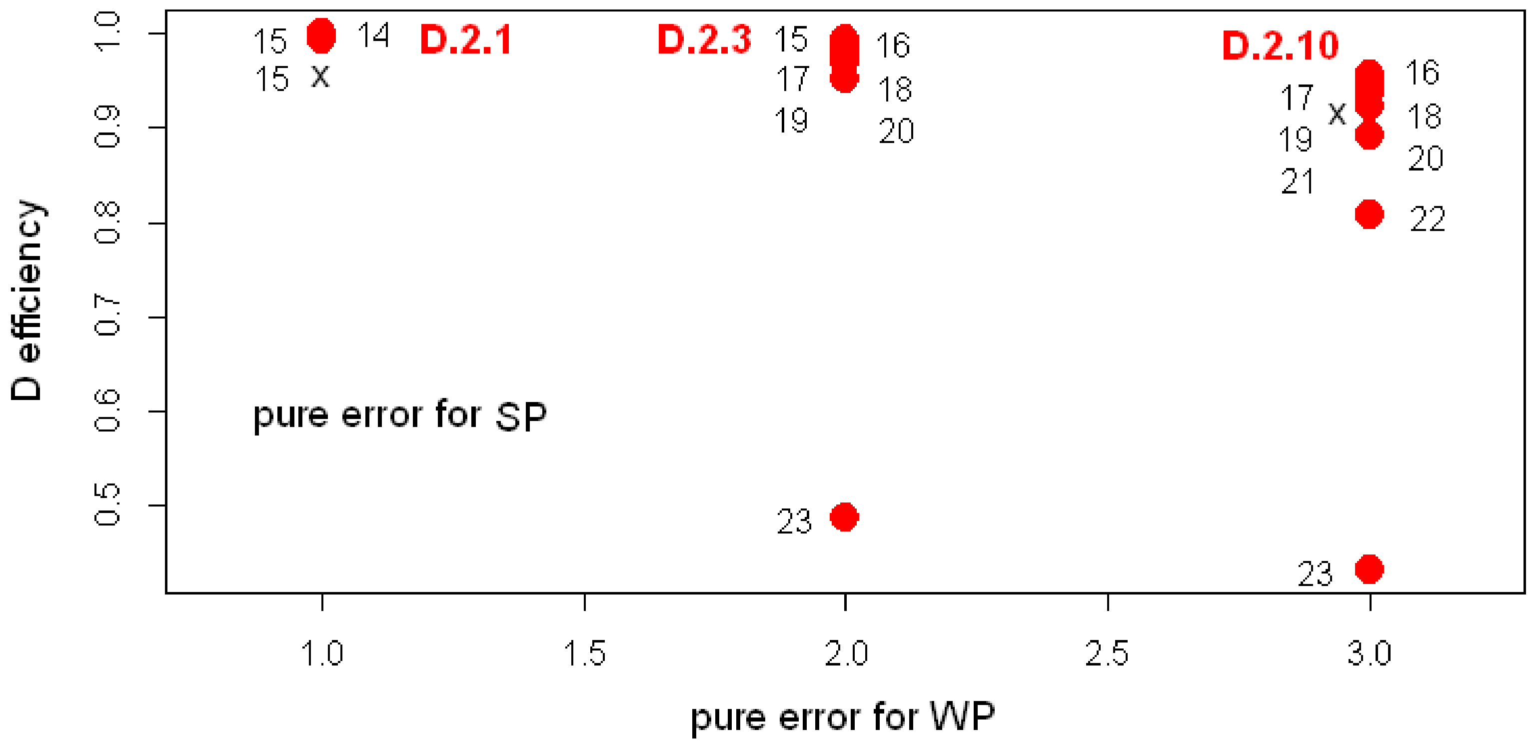
| SPD2 | D(1)-eff | df(wp) (PE) | df(sp) (PE) | EED |
|---|---|---|---|---|
| **10** | 0.9543 | **3** | 16 | no |
| 11 | 0.9522 | 3 | 17 | no |
| 12 | 0.9443 | 3 | 18 | no |
| 13 | 0.9346 | 3 | 19 | no |
| 14 | 0.9226 | 3 | 20 | no |
| 15 | 0.8924 | 3 | 21 | yes |
| 16 | 0.8078 | 3 | 22 | no |
| 17 | 0.4321 | 3 | 23 | yes |

$p = 10$

$$\text{df(wp)(PE)} + \text{df(wp)(LOF)} = 3\ ,\ \ \text{df(sp)(PE)} + \text{df(sp)(LOF)} = 23$$

## 3. DP-Optimality SPD (Examples)

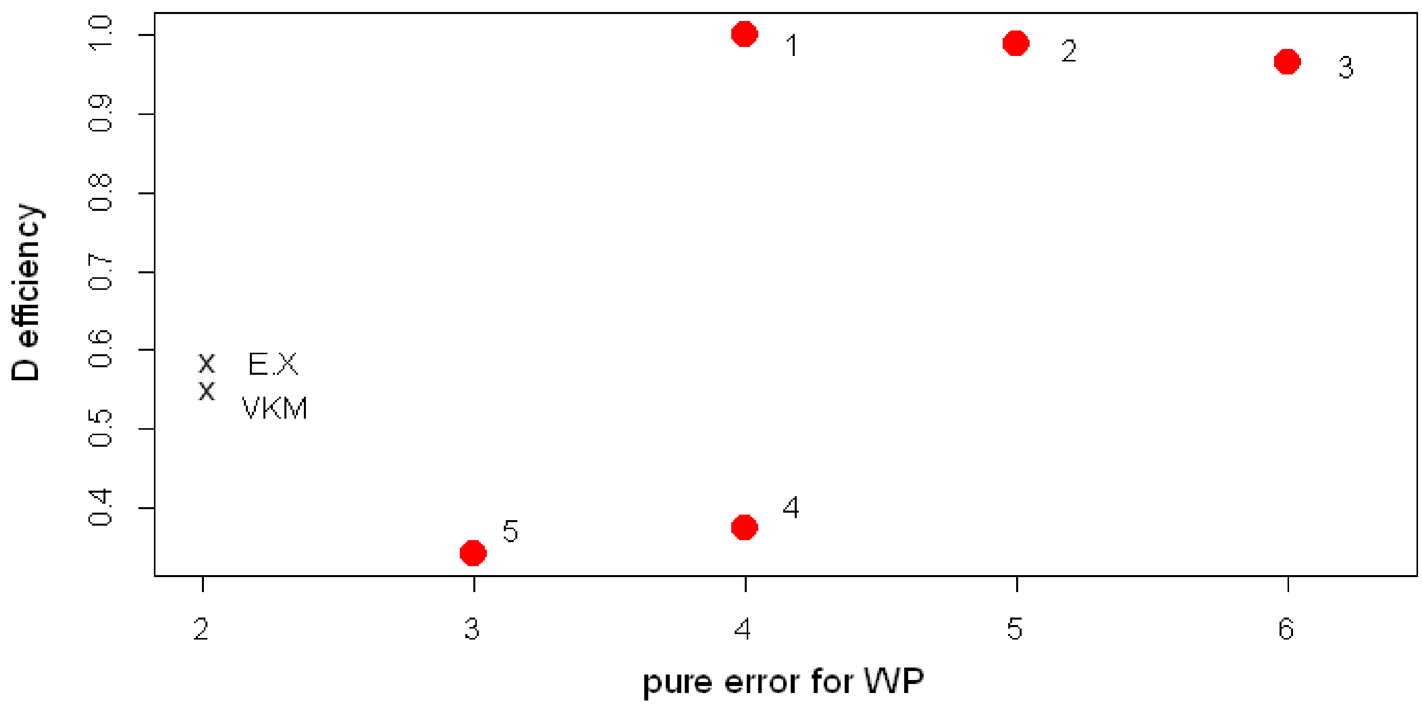
**SPD2. 2 WP factors, 1 SP factor in 9 whole plots of size 4 (Jones and Goos, 2012).**



# 3. DP-Optimality SPD (Examples)

**SPD3. 2 WP factors, 2 SP factors in 12 whole plots of size 4 (Vining et al., 2005).**

| SPD3 | 1 | 2 | 3 | 4 | 5 | EXD | VKMD |
|---|---|---|---|---|---|---|---|
| D(1)-efficiency | 1.0000 | 0.9880 | 0.9634 | 0.3742 | 0.3410 | 0.5904 | 0.5838 |
| df(wp)(PE, LOF) | (4,2) | (5,1) | (6,0) | (4,0) | (3,0) | (2,3) | (2,3) |
| EED | no | no | no | yes | yes | yes | yes |



## 3. DP-Optimality SPD (Extension)

**Orthogonal Subplot Designs (OSUB) $\sim$ EED (Parker et al., 2007)**

$\mathbf{0} = \mathbf{Z}'\mathbf{S} = \mathbf{Z}'(\mathbf{S} \ominus \mathbf{S}) \Rightarrow$ column sums of main effects, interactions 0 within WP

| SPD4 | D(1) | | 1 | | 2 | | 3 | | 4 | |
|---|---|---|---|---|---|---|---|---|---|---|
| whole plot | $w$ | $s$ | $w$ | $s$ | $w$ | $s$ | $w$ | $s$ | $w$ | $s$ |
| 1 | **1** | **1** | 1 | -1 | 1 | -1 | **1** | **0** | **-1** | **1** |
| | 1 | -1 | 1 | 1 | 1 | 1 | **1** | **0** | **-1** | **-1** |
| 2 | **-1** | **1** | **-1** | **1** | 0 | 1 | 1 | 1 | 1 | 1 |
| | -1 | -1 | **-1** | **-1** | 0 | -1 | 1 | -1 | 1 | -1 |
| 3 | **1** | **1** | **-1** | **1** | -1 | 1 | **0** | **0** | **-1** | **1** |
| | 1 | 0 | **-1** | **-1** | -1 | -1 | **0** | **0** | **-1** | **-1** |
| 4 | 0 | -1 | **-1** | **0** | **-1** | **0** | -1 | -1 | **-1** | **0** |
| | 0 | 0 | **-1** | **0** | **-1** | **0** | -1 | 1 | **-1** | **0** |
| 5 | **-1** | **1** | **0** | **0** | **0** | **0** | **-1** | **0** | 0 | -1 |
| | -1 | 0 | **0** | **0** | **0** | **0** | **-1** | **0** | 0 | 1 |
| D(1)-efficiency | 1.0000 | | 0.7777 | | 0.8320 | | 0.7777 | | 0.8201 | |
| $r = (n_w - \theta) + (r - n_w - \theta)$ | 2 = 2 + 0 | | 4 = 1 + 3 | | 2 = 0 + 2 | | 3 = 0 + 3 | | 3 = 1 + 2 | |
| OSUB, EED | no, no | | yes, yes | | yes, yes | | yes, yes | | yes, yes | |

## 4. Conclusion (Comments)

- **Pareto optimal designs**

→ Convenient for selecting optimal designs with respect to multiple criteria.

→ No need to specify complicated weightings to form a single design criterion.

→ Identifies the optimal design with respect to each criterion.

→ Trade-offs among the criteria can be investigated and balanced.

- **Future Research**

→ Improve computational efficiency of algorithms to incorporate numerous criteria.

→ Examine other traditional design criteria such as Ds, A, As, I.

→ Incorporate additional criteria related to statistical analyses.

# 4. Conclusion (References)


**Cao, Y.; Smucker, B.J.; and Robinson, T.J. (2017b)**. A Hybrid Elitist Pareto-based Coordinate Exchange Algorithm for Constructing Multi-Criteria Optimal Experimental Designs. *Statistics and Computing* 27, pp. 423-437.

**Gilmour, S.G. and Trinca, L.A. (2012)**. Optimum Design of Experiments for Statistical Inference. *Applied Statistics* 61, pp. 1-25.

**Jones, B. and Goos, P. (2012)**. An Algorithm for Finding D-Efficient Equivalent-Estimation Second-Order Split-Plot Designs. *Journal of Quality Technology* 44, pp. 363-374.

**Lu, L.; Anderson-Cook, C.M.; and Robinson, T.J. (2011)**. Optimization of Designed Experiments based on Multiple Criteria Utilizing a Pareto Frontier. *Technometrics* 61, pp. 353-365.

**Macharia, H. and Goos, P. (2010)**. D-Optimal and D-Efficient Equivalent-Estimation Second-Order Split-Plot Designs". *Journal of Quality Technology* 42, pp. 358-372.

**Parker, P.A.; Kowalski, S.M.; and Vining, G.G.** (2007). Construction of Balanced Equivalent Estimation Second-Order Split-Plot Designs. *Technometrics* 49, pp. 56-65.

**Vining, G.G.; Kowalski, S.M.; and Montgomery, D.C.** (2005). Response Surface Designs Within a Split-Plot Structure. *Journal of Quality Technology* 37, pp. 115-129.