

# Supplementary Material for "Compound optimality criteria and graphical tools for designs for prediction"

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## 1 Introduction

In this file we show some of the designs constructed in Example 2 (that were not shown in the paper for the sake of saving space) and additional graphs for evaluating prediction properties of the designs for both examples of the paper.

## 2 Example 1

Figures A-L show prediction capability of designs in Example 1.

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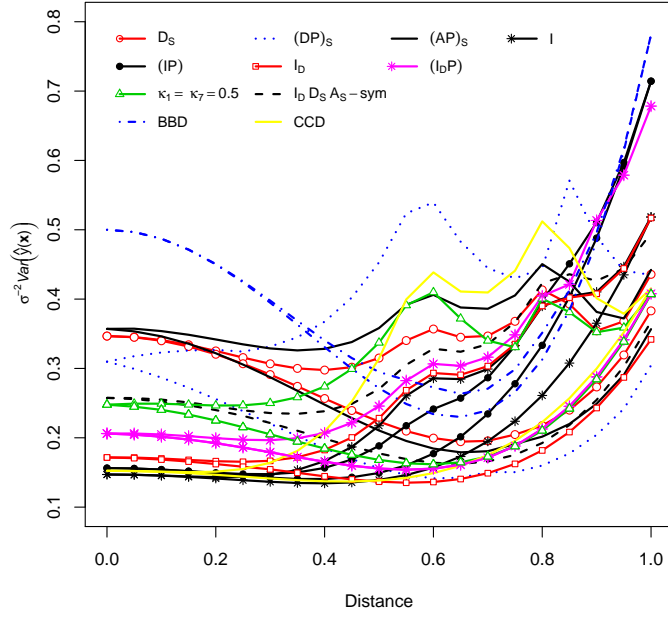


Figure A: VDG for point predictions vs. distance from the centre of designs in Example 1.

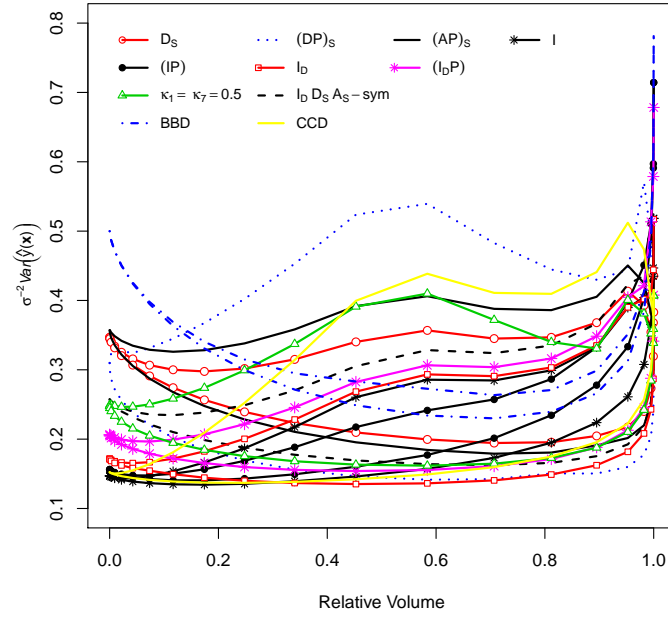


Figure B: VDG for point predictions vs. relative volume of the region of designs in Example 1.

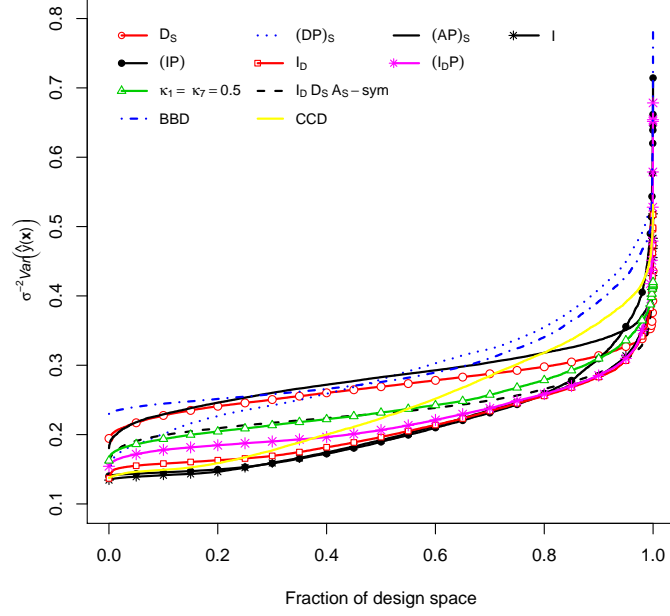


Figure C: FDS plots for point predictions of designs in Example 1.

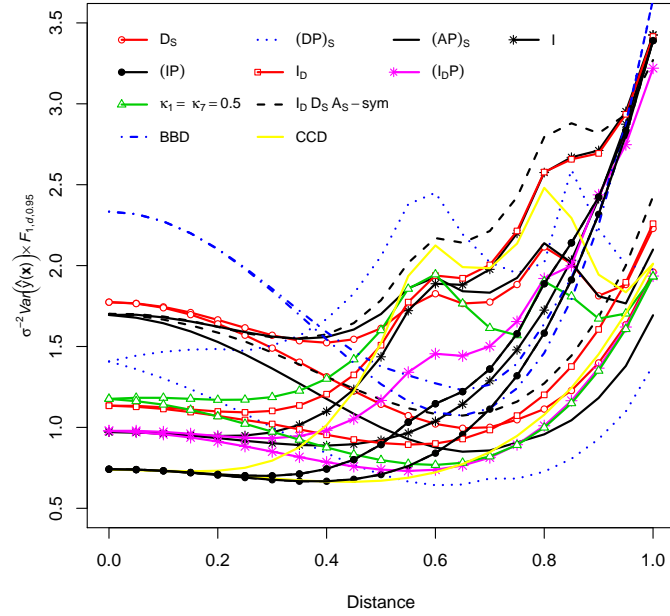


Figure D: VDG for interval predictions vs. distance from the centre of designs in Example 1.

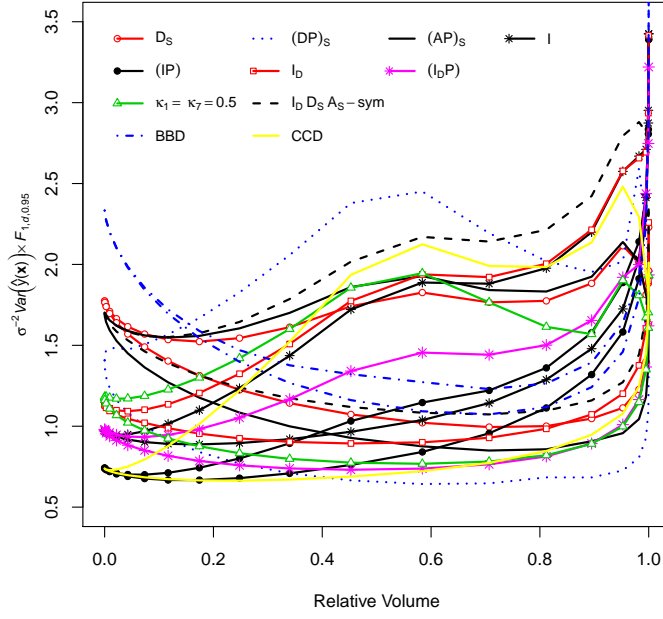


Figure E: VDG for interval predictions vs. relative volume of the region of designs in Example 1.

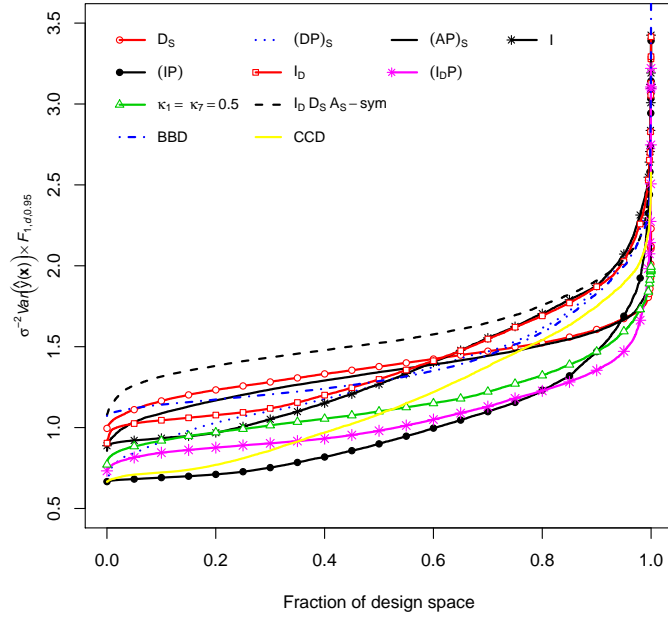


Figure F: FDS plots for interval predictions of designs in Example 1.

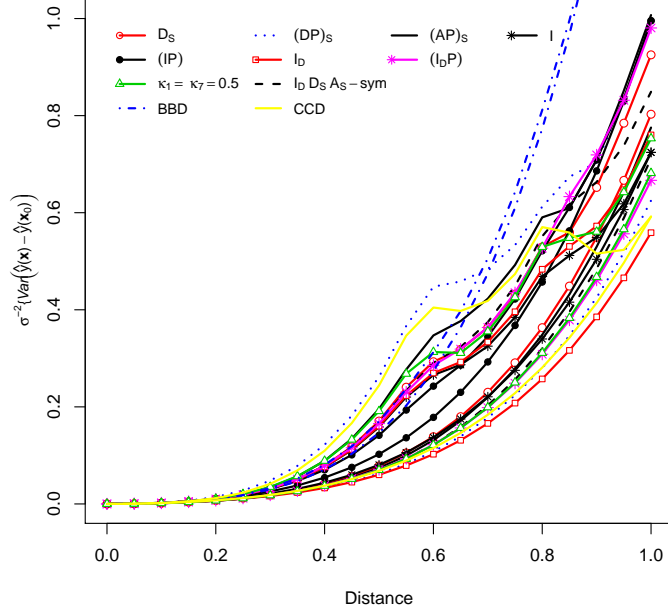


Figure G: DVDG for point predictions vs. distance from the centre of designs in Example 1.

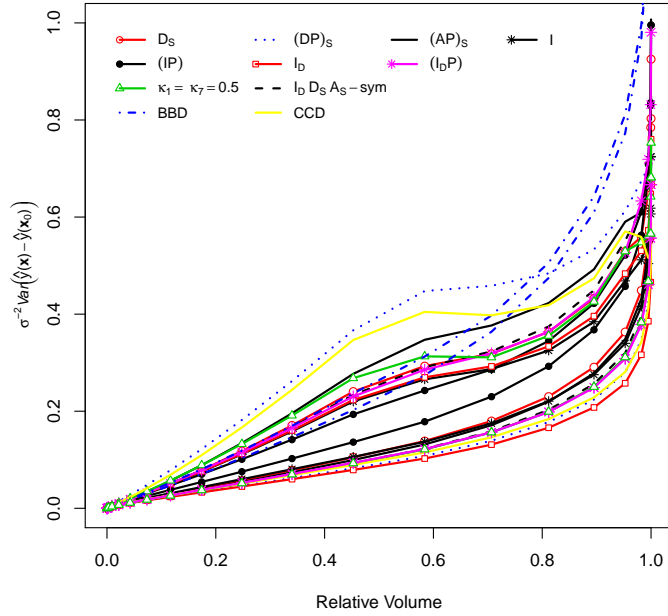


Figure H: DVDG for point predictions vs. relative volume of the region of designs in Example 1.

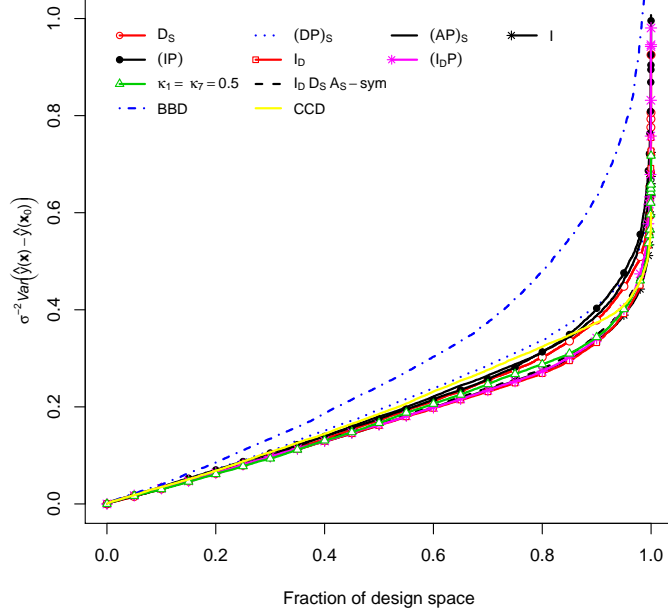


Figure I: DFDS plots for point predictions of designs in Example 1.

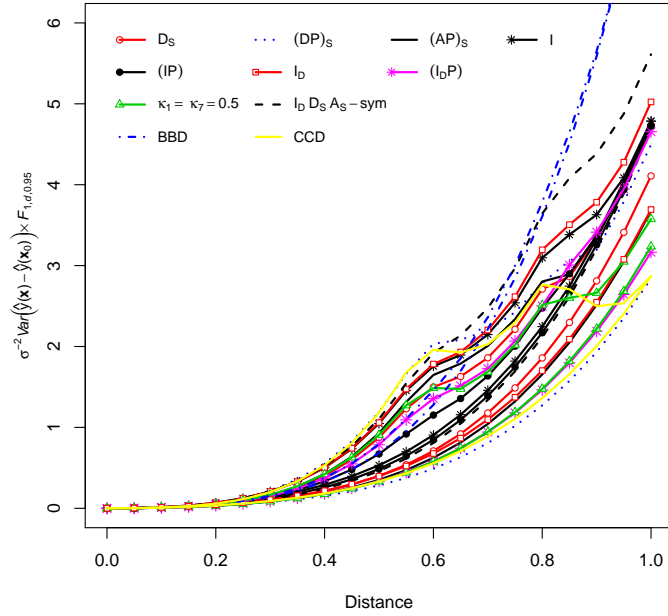


Figure J: DVDG for interval predictions vs. distance from the centre of designs in Example 1.

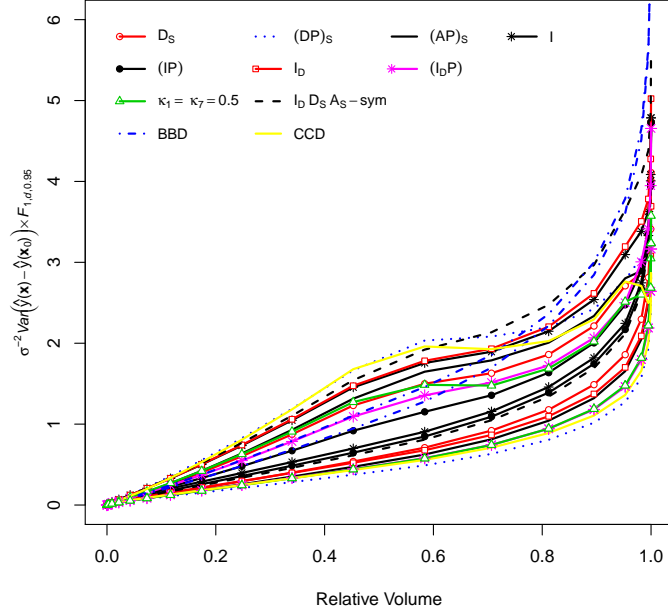


Figure K: DVDG for interval predictions vs. relative volume of the region of designs in Example 1.

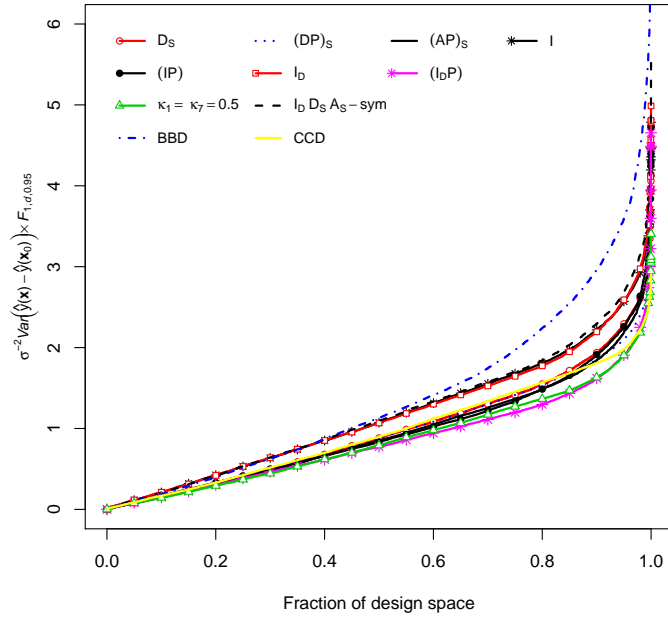


Figure L: DFDS plots for interval predictions of designs in Example 1.

### 3 Example 2

Tables A-C show designs 1, 2, 3, 4, 5, 7, 8, 9, 10 constructed for Example 2. Design 11 is similar to a CCD (design 6) except that it includes the four factorial points duplicated shown in Table D, the centre point is replicated four times and includes the axial pair for only one factor ( $X_3$ ), while for the other factors it includes only one axial point.

Table A: Alternative designs for Example 2 ( $n = 30$ ,  $q = 5$ ,  $p = 21$  in spherical region)

1 $D_S/I$					Design 2 $(DP)_S$					3 $A_S$				
$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$
-1.12	1.12	-1.12	0	-1.12	-1.29	-1.29	0	1.29	0	0	-1.12	1.12	-1.12	-1.12
-1.12	1.12	1.12	0	-1.12	-1.29	-1.29	0	-1.29	0	0	-1.12	1.12	1.12	-1.12
1.12	1.12	-1.12	0	-1.12	-1.29	1.29	0	-1.29	0	0	1.12	1.12	-1.12	-1.12
1.12	1.12	1.12	0	-1.12	-1.29	1.29	0	1.29	0	0	1.12	1.12	1.12	-1.12
-1.29	1.29	0	0	1.29	-1.29	1.29	0	1.29	0	1.29	-1.29	-1.29	0	0
1.29	1.29	0	0	1.29	1.29	-1.29	-1.29	0	0	1.29	-1.29	1.29	0	0
-1.29	0	-1.29	1.29	0	1.29	1.29	-1.29	0	0	1.29	1.29	-1.29	0	0
-1.29	0	1.29	1.29	0	1.29	1.29	-1.29	0	0	1.29	1.29	1.29	0	0
1.29	0	-1.29	1.29	0	1.29	0	1.29	1.29	0	-1.29	-1.29	0	-1.29	0
1.29	0	1.29	1.29	0	1.29	0	1.29	-1.29	0	-1.29	-1.29	0	1.29	0
-1.29	0	0	-1.29	-1.29	1.29	0	1.29	1.29	0	-1.29	1.29	0	-1.29	0
-1.29	0	0	-1.29	1.29	0	-1.29	1.29	0	-1.29	-1.29	1.29	0	1.29	0
1.29	0	0	-1.29	-1.29	0	-1.29	1.29	0	1.29	-1.29	0	-1.29	0	-1.29
1.29	0	0	-1.29	1.29	0	-1.29	1.29	0	1.29	-1.29	0	-1.29	0	1.29
0	-1.29	-1.29	-1.29	0	0	1.29	1.29	0	-1.29	-1.29	0	1.29	0	-1.29
0	-1.29	1.29	-1.29	0	0	1.29	1.29	0	1.29	-1.29	0	1.29	0	1.29
0	1.29	-1.29	-1.29	0	0	1.29	1.29	0	1.29	1.29	0	0	-1.29	-1.29
0	1.29	1.29	-1.29	0	0	0	-1.29	-1.29	-1.29	1.29	0	0	-1.29	1.29
0	-1.29	-1.29	0	-1.29	0	0	-1.29	-1.29	1.29	1.29	0	0	1.29	-1.29
0	-1.29	1.29	0	-1.29	0	0	-1.29	-1.29	-1.29	1.29	0	0	1.29	1.29
-1.58	-1.58	0	0	0	0	0	-1.29	1.29	1.29	0	-1.29	-1.29	0	-1.29
1.58	-1.58	0	0	0	0	0	-1.29	1.29	-1.29	0	1.29	-1.29	0	-1.29
0	-1.58	0	1.58	0	0	0	-1.29	-1.29	1.29	0	0	1.29	-1.29	1.29
0	1.58	0	1.58	0	-1.58	0	-1.58	0	0	0	0	1.29	1.29	1.29
0	-1.58	0	0	1.58	-1.58	0	1.58	0	0	0	-1.58	0	0	1.58
0	0	-1.58	0	1.58	-1.58	0	1.58	0	0	0	1.58	0	0	1.58
0	0	1.58	0	1.58	1.58	0	0	0	-1.58	0	0	-1.58	-1.58	0
0	0	0	1.58	-1.58	1.58	0	0	0	1.58	0	0	-1.58	1.58	0
0	0	0	1.58	1.58	1.58	0	0	0	1.58	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0



Table B: Alternative designs for Example 2 ( $n = 30$ ,  $q = 5$ ,  $p = 21$  in spherical region)

4 ( $AP$ ) <sub>S</sub>					Design 5 ( $IP$ )					7 ( $IDP$ )				
$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$
-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	-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	-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	-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	-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
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	-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	-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	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	-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
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	1.12	-1.12	1.12	-1.12
1.12	1.12	-1.12	0	-1.12	1	1	1	1	1	0	1.12	-1.12	1.12	-1.12
1.12	1.12	-1.12	0	-1.12	-1.12	1.12	-1.12	0	-1.12	2.24	0	0	0	0
2.24	0	0	0	0	-1.12	1.12	-1.12	0	-1.12	0	-2.24	0	0	0
0	-2.24	0	0	0	0	-1.12	-1.12	-1.12	-1.12	0	0	2.24	0	0
0	0	2.24	0	0	0	-1.12	-1.12	-1.12	-1.12	0	0	0	2.24	0
0	0	0	-2.24	0	2.24	0	0	0	0	0	0	0	0	2.24
0	0	0	0	2.24	0	2.24	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	-2.24	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	-2.24	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	2.24	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table C: Alternative designs for Example 2 ( $n = 30$ ,  $q = 5$ ,  $p = 21$  in spherical region)

8					Design					10				
$\kappa_1 = .3; \kappa_7 = .7$					$\kappa_1 = .1; \kappa_7 = .9$					$\kappa_0 = .9; \kappa_8 = .1$				
$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$	$X_1$	$X_2$	$X_3$	$X_4$	$X_5$
1.12	-1.12	1.12	1.12	0	-1	-1	-1	1	-1	-1.29	-1.29	-1.29	0	0
1.12	1.12	1.12	1.12	0	-1	-1	1	1	1	-1.29	-1.29	1.29	0	0
1.12	-1.12	-1.12	0	1.12	-1	1	-1	1	1	-1.29	1.29	-1.29	0	0
1.12	1.12	-1.12	0	1.12	-1	1	1	1	-1	-1.29	1.29	1.29	0	0
-1.29	-1.29	-1.29	0	0	-1	1	1	-1	1	1.29	-1.29	0	0	-1.29
-1.29	-1.29	1.29	0	0	1	-1	-1	-1	-1	1.29	-1.29	0	0	-1.29
-1.29	1.29	-1.29	0	0	1	-1	1	-1	1	1.29	-1.29	0	0	1.29
-1.29	1.29	1.29	0	0	1	1	-1	-1	1	1.29	-1.29	0	0	1.29
-1.29	0	0	-1.29	-1.29	1	1	1	1	1	1.29	1.29	0	0	-1.29
-1.29	0	0	-1.29	1.29	1	1	1	-1	-1	1.29	1.29	0	0	1.29
-1.29	0	0	1.29	-1.29	-1.29	-1.29	0	-1.29	0	-1.29	0	0	-1.29	1.29
-1.29	0	0	1.29	1.29	1.29	-1.29	0	1.29	0	-1.29	0	0	1.29	-1.29
-1.29	0	0	1.29	1.29	-1.29	0	-1.29	-1.29	0	-1.29	0	0	1.29	1.29
1.29	0	-1.29	0	-1.29	1.29	0	-1.29	1.29	0	-1.29	0	0	-1.29	-1.29
1.29	0	1.29	-1.29	0	-1.29	0	0	-1.29	-1.29	1.29	0	-1.29	-1.29	0
0	-1.58	0	-1.58	0	1.29	0	0	1.29	-1.29	1.29	0	-1.29	1.29	0
0	1.58	0	-1.58	0	0	-1.29	-1.29	0	1.29	1.29	0	1.29	-1.29	0
0	-1.58	0	0	-1.58	0	-1.29	1.29	0	-1.29	1.29	0	1.29	-1.29	0
0	1.58	0	0	-1.58	0	1.29	-1.29	0	-1.29	1.29	0	1.29	1.29	0
0	0	-1.58	-1.58	0	-2.24	0	0	0	0	0	-1.58	0	-1.58	0
0	0	-1.58	1.58	0	0	2.24	0	0	0	0	-1.58	0	1.58	0
0	0	-1.58	1.58	0	0	0	2.24	0	0	0	1.58	0	-1.58	0
0	0	1.58	0	-1.58	0	0	0	2.24	0	0	1.58	0	1.58	0
0	0	1.58	0	1.58	0	0	0	0	2.24	0	0	-1.58	0	-1.58
0	0	1.58	0	1.58	0	0	0	0	0	0	0	-1.58	0	1.58
0	0	0	0	0	0	0	0	0	0	0	0	1.58	0	-1.58
0	0	0	0	0	0	0	0	0	0	0	0	1.58	0	1.58
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D: Points from the  $2^5$  that are duplicated in Design 11 (Table 3)

$X_1$	$X_2$	$X_3$	$X_4$	$X_5$
-1	-1	1	1	1
-1	1	-1	1	1
-1	1	1	1	-1
1	-1	1	-1	1

Figures M-X show prediction capability of designs in Example 2.

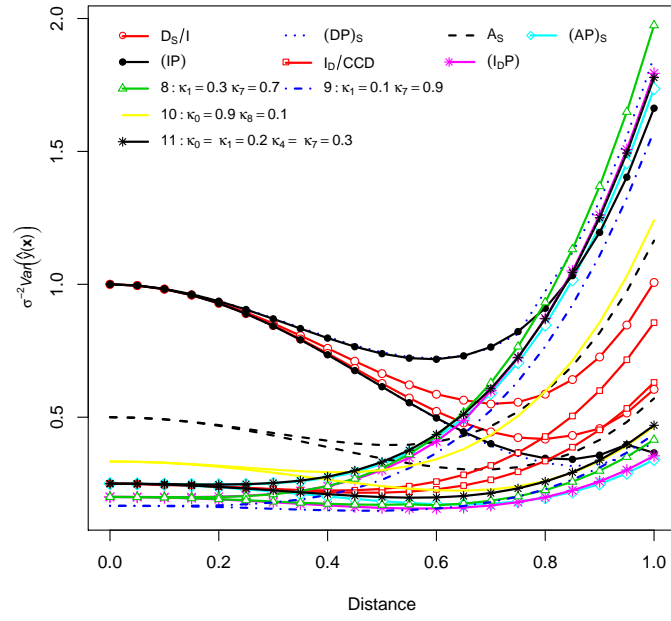


Figure M: VDG for point predictions vs. distance from the centre of designs in Example 2.

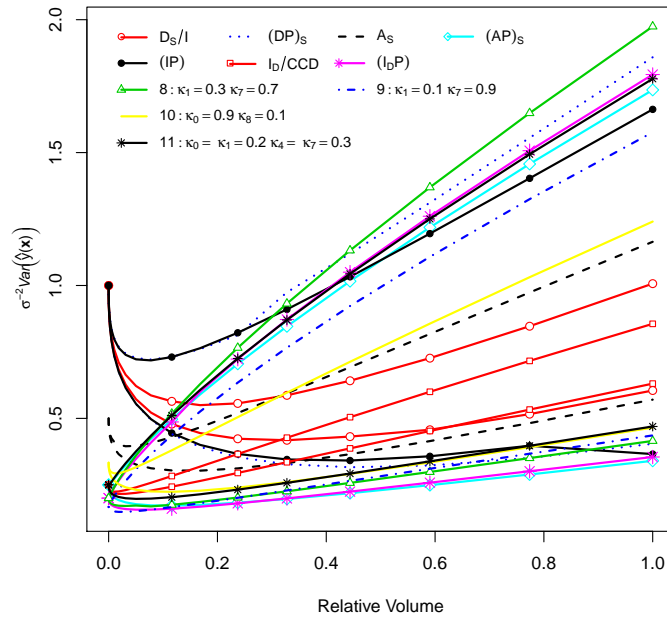


Figure N: VDG for point predictions vs. relative volume of the region of designs in Example 2.

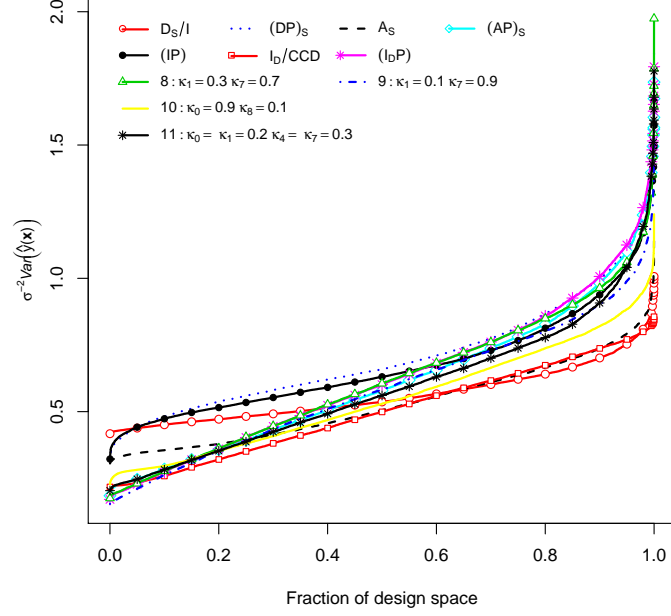


Figure O: FDS plots for point predictions of designs in Example 2.

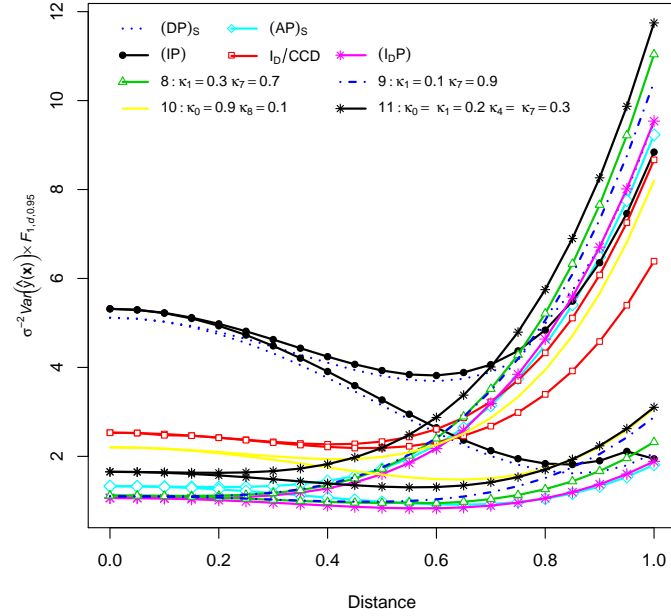


Figure P: VDG for interval predictions vs. distance from the centre of designs in Example 2.

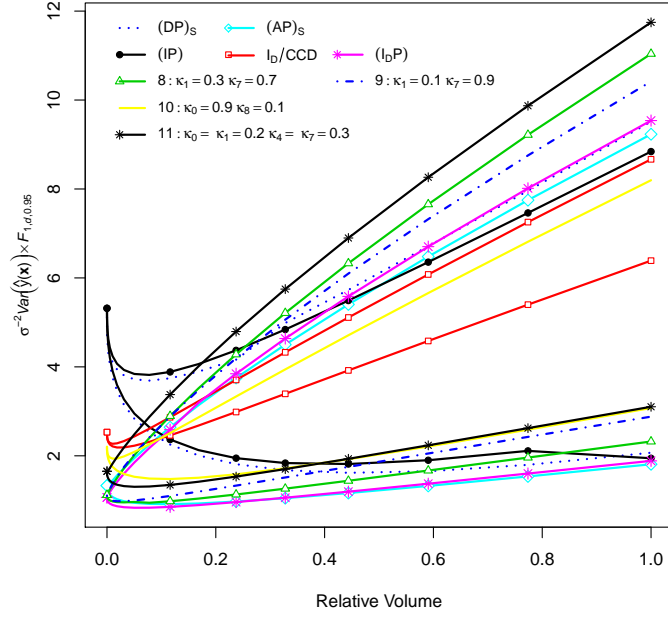


Figure Q: VDG for interval predictions vs. relative volume of the region of designs in Example 2.

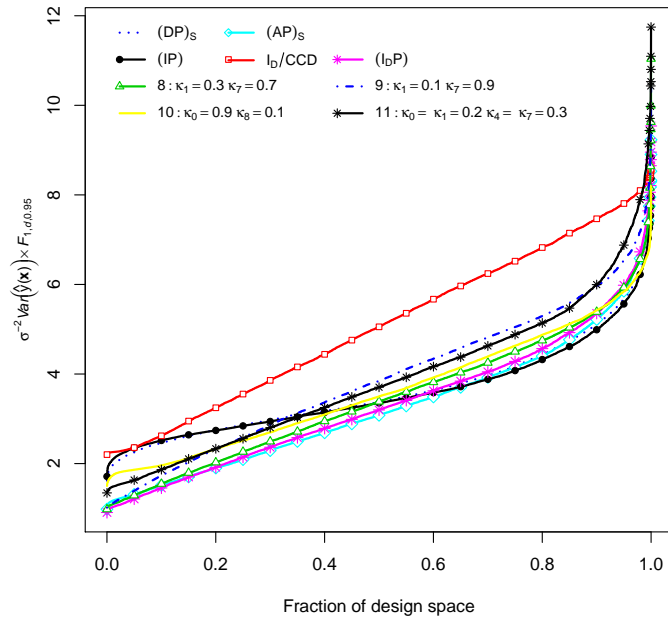


Figure R: FDS plots for interval predictions of designs in Example 2.

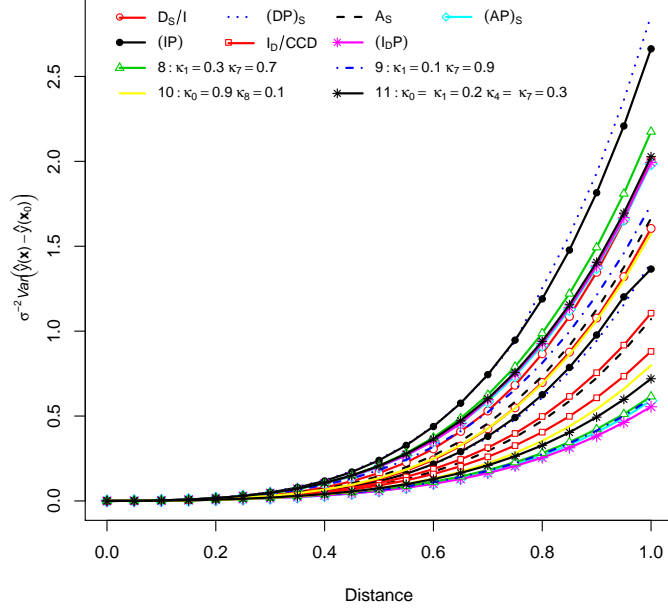


Figure S: DVDG for point predictions vs. distance from the centre of designs in Example 2.

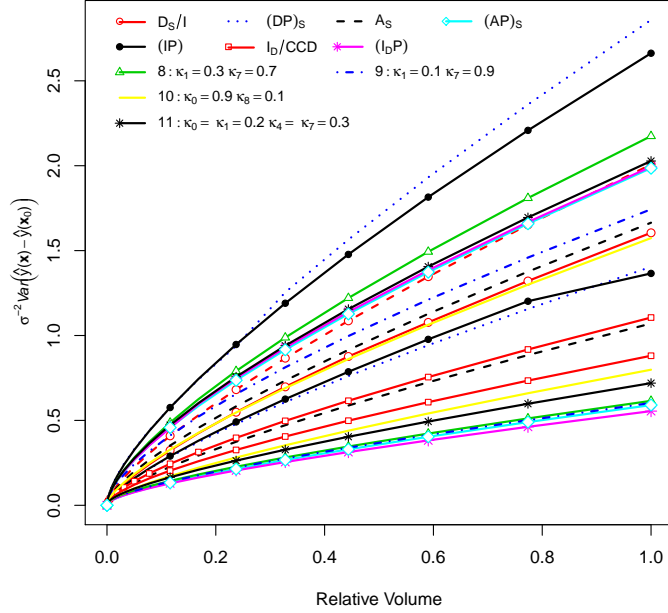


Figure T: DVDG for point predictions vs. relative volume of the region of designs in Example 2.

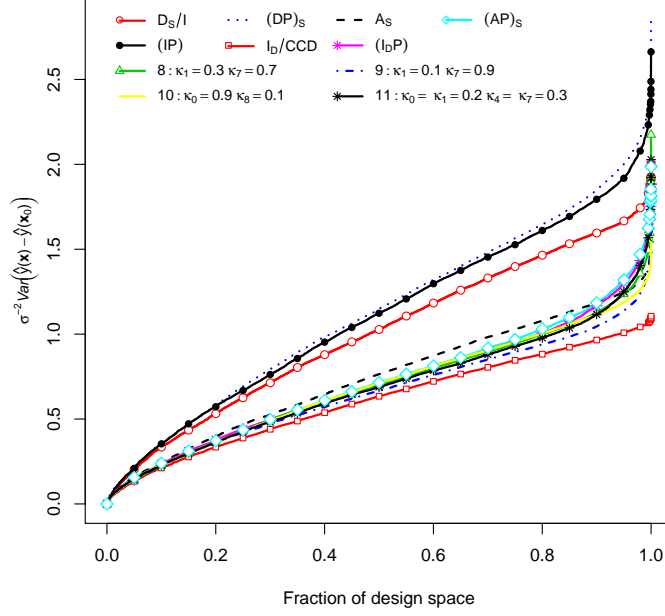


Figure U: DFDS plots for point predictions of designs in Example 2.

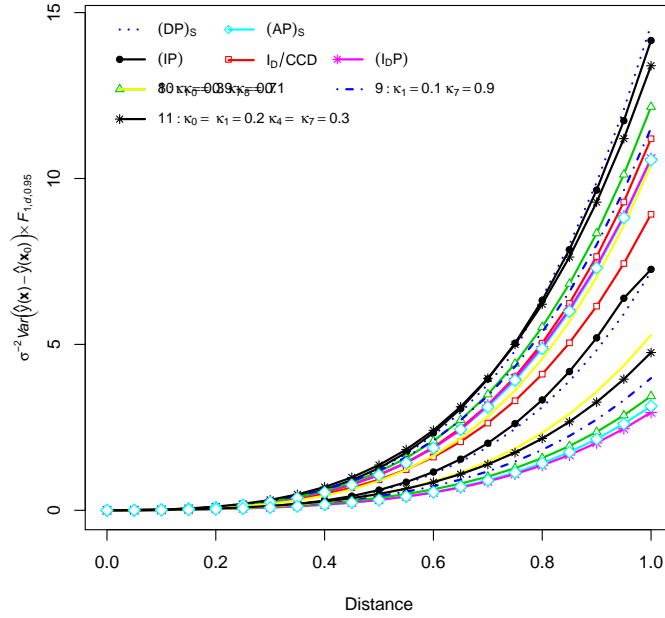


Figure V: DVDG for interval predictions vs. distance from the centre of designs in Example 2.

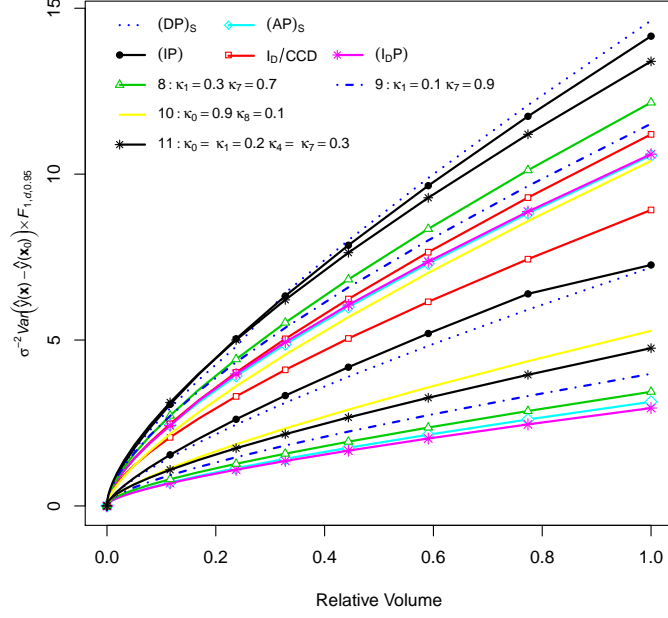


Figure W: DVDG for interval predictions vs. relative volume of the region of designs in Example 2.

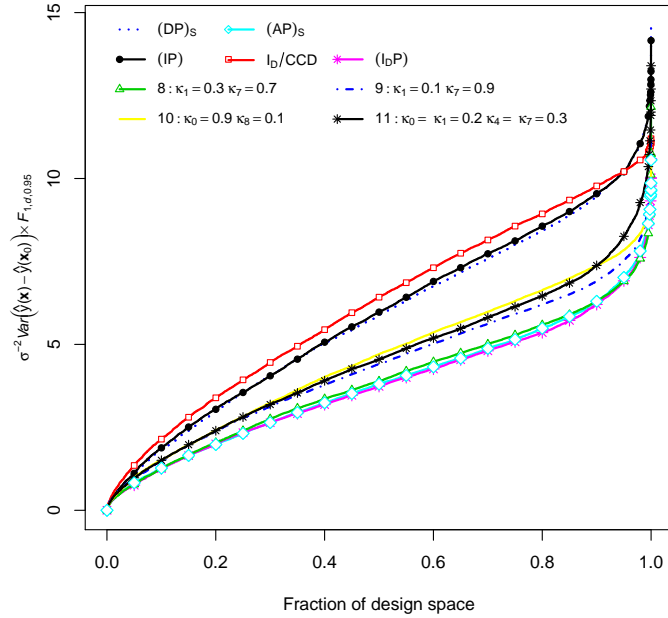


Figure X: DFDS plots for interval predictions of designs in Example 2.