2D Linear Model Selection, f = 1/W^(1/2p), N = 100

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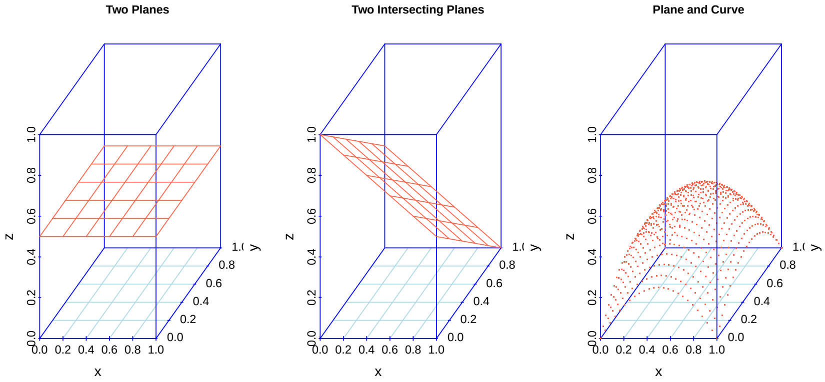
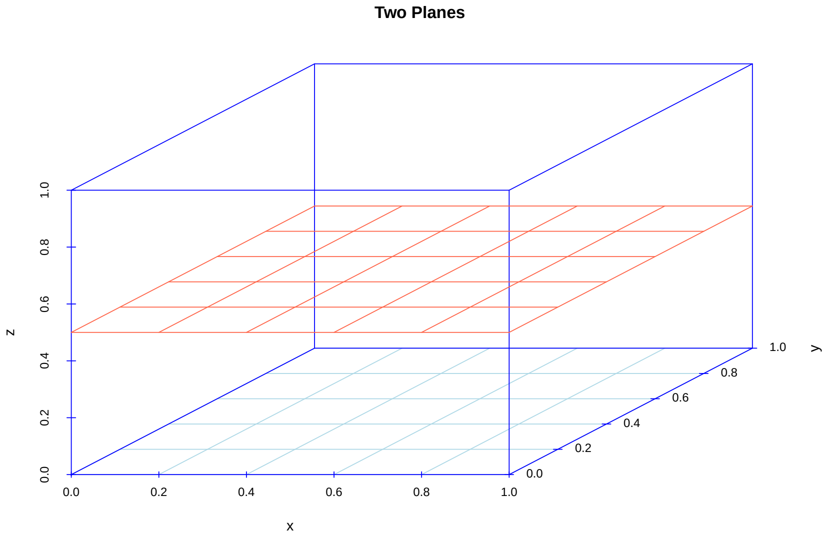
Experiments

Here I consider three examples in which two different models are compared:

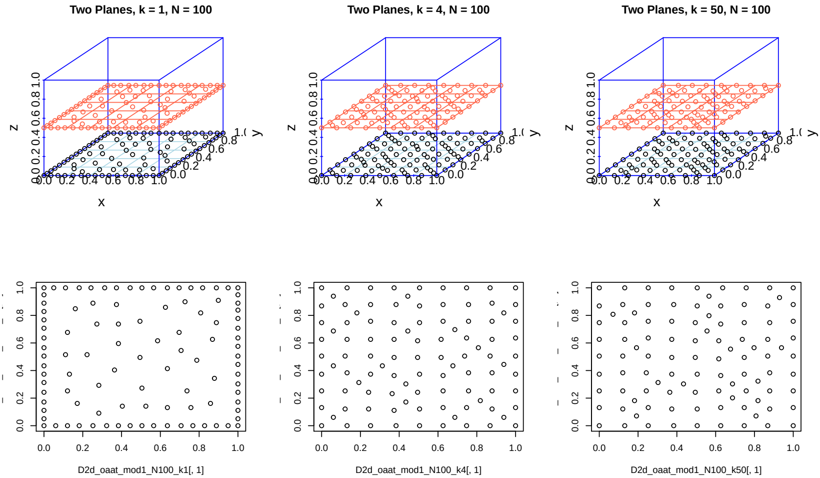


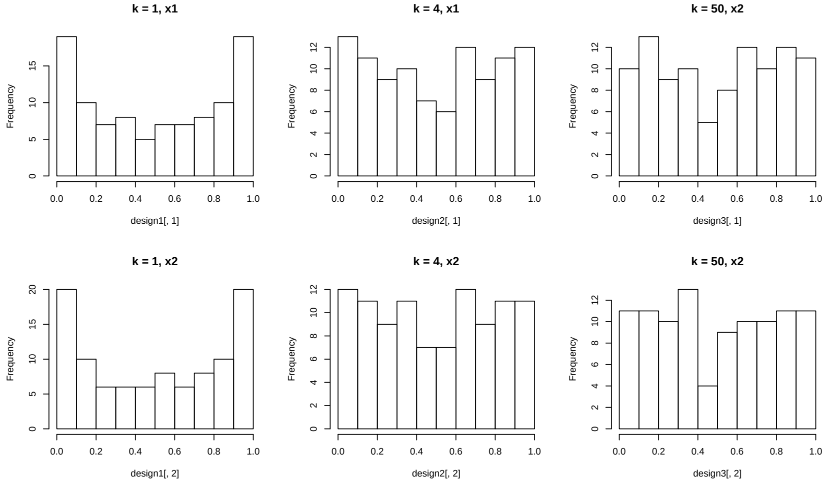
Example 1

Example 1

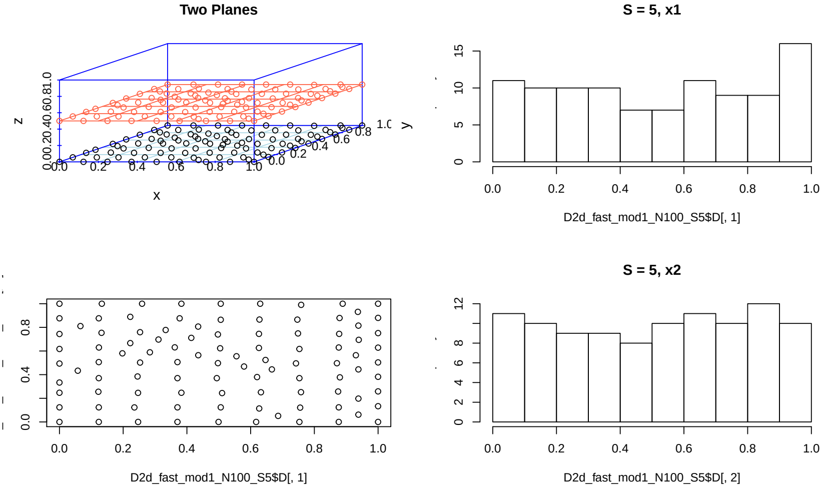


One-at-a-Time Algorithm, $k = 1, 4, 50$ and $N = 100$

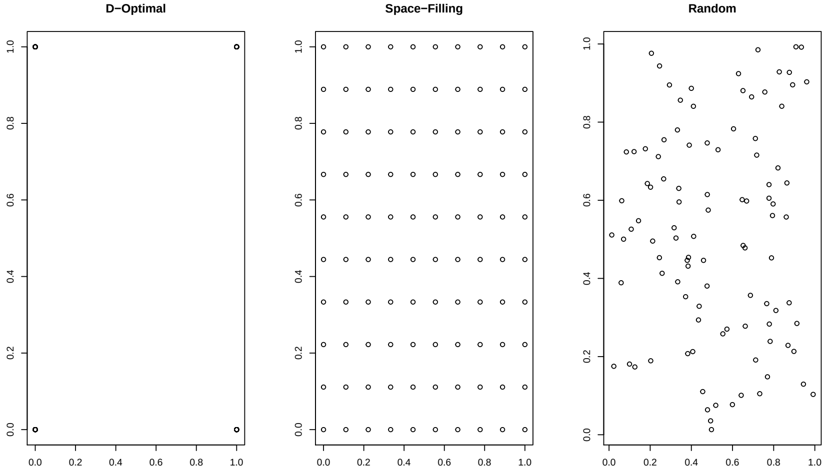


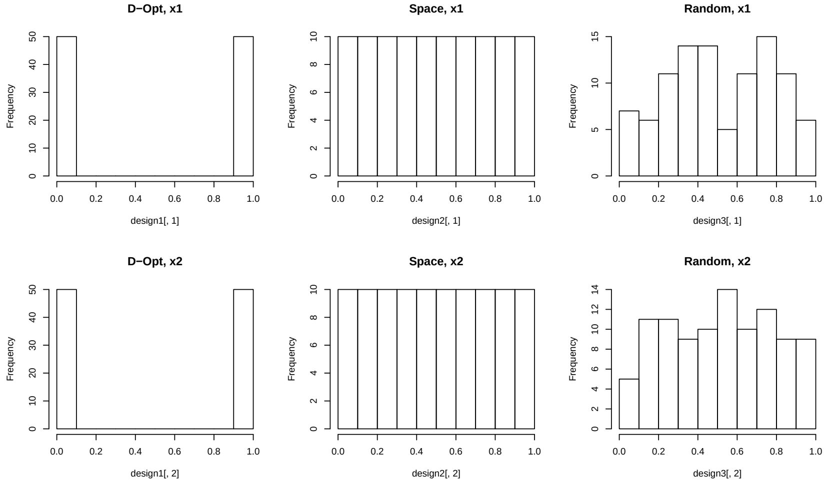

k = 1, x1
k = 4, x1
k = 50, x2
Frequency
design1[, 1]
design2[, 1]
design3[, 1]
k = 1, x2
k = 4, x2
k = 50, x2
design1[, 2]
design2[, 2]
design3[, 2]
0.0 0.2 0.4 0.6 0.8 1.0

Fast Algorithm, S = 5, N = 100



Other Designs, $N = 100$





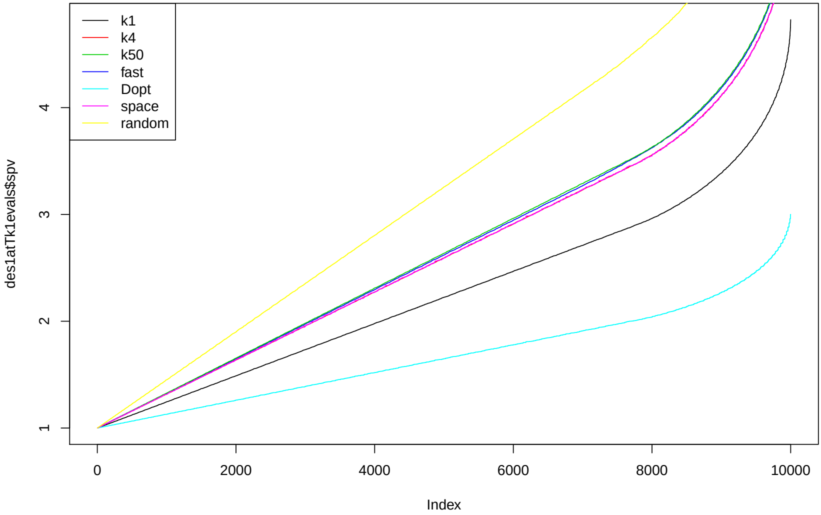
D−Opt, x1
Space, x1
Random, x1
D−Opt, x2
Space, x2
Random, x2
Frequency
design1[, 1]
design2[, 1]
design3[, 1]
design1[, 2]
design2[, 2]
design3[, 2]

Example 1 Evaluations, N = 100

	1atT,k=1	1atT,k=4	1atT,k=50	Fast,S=5	D-Opt	Space	Random
TPEx10e-3	44.139	47.279	47.95	47.871	Inf	46.919	61.259
Fast Crit	79.2	46.669	46.669	51.605	Inf	36	410.65
1atT Crit (k=4)	196.32	153.39	154.11	155.46	Inf	143.63	501.92
E[P(H0|Y,D)|H0,D]	1	0.999	0.998	0.999	1	1	1
E[P(H1|Y,D)|H0,D]	0.000245	0.000955	0.00162	0.00081	2.36e-05	0.000436	0.000234
E[BF01 | H0,D]	2.88e+14	4.85e+13	8.84e+13	9.94e+12	3.35e+14	1.22e+14	1.71e+13
E[P(H0|Y,D)|H1,D]	0.00011	2.1e-05	0.000131	0.000286	5.62e-05	0.000819	0.00109
E[P(H1|Y,D)|H1,D]	1	1	1	1	1	0.999	0.999
E[BF01|H1,D]	0.000111	2.1e-05	0.000132	0.000293	5.63e-05	0.000854	0.00121
V[B0|Y,X]	0.000791	0.000885	0.000902	0.000928	0.000588	0.000884	0.00106
V[B1|Y,X]	0.0013	0.00152	0.00156	0.0015	0.000803	0.00153	0.00189
V[B2|Y,X]	0.00128	0.00154	0.00156	0.00159	0.000803	0.00153	0.00186

Scaled Prediction Variance (SPV)

$$SPV = NV[\hat{y}(x_0)]/\sigma^2 = Nx_0'(X'X)^{-1}x_0$$

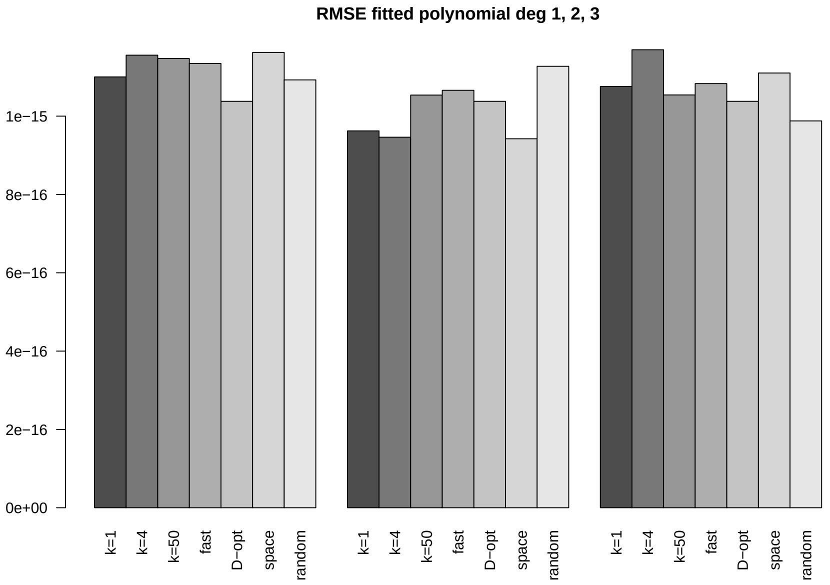


Empirical RMSE

(idea from “Bridging the Gap Between Space-Filling and Optimal Designs Design for Computer Experiments” dissertation by Kathryn Kennedy)

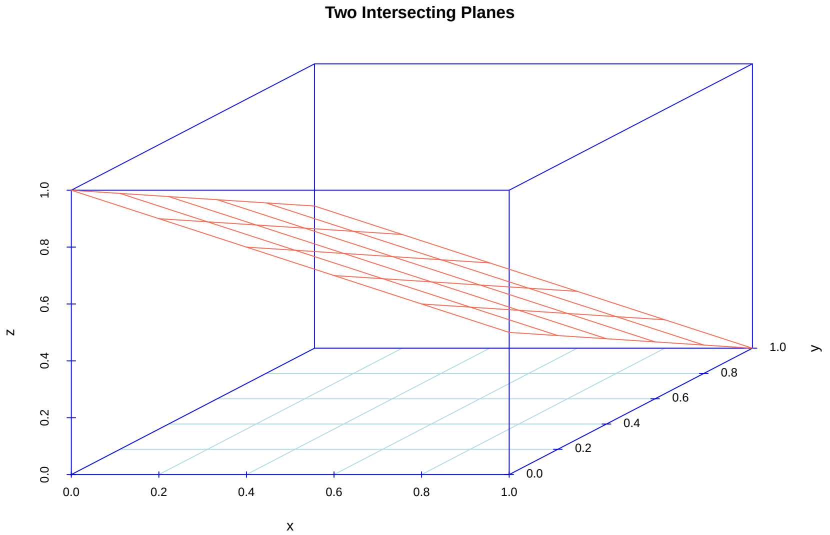
1. Create a hypothetical response variable using a test function (for my examples, I chooose the function given by H_1). (Should there be noise? Or is it supposed to be deterministic, like a computer experiment?)
2. “Analyze” the designs by fitting a polynomial (with no interaction terms). (A GP may also be used.)
3. Predict response variables for 10,000 test points (I chose them on a grid, but in her paper, she randomly chooses them from a uniform distribution) using the model created in step 2.
4. Calculate the residual error as the difference from the values determined by the test function.

Empirical RMSE

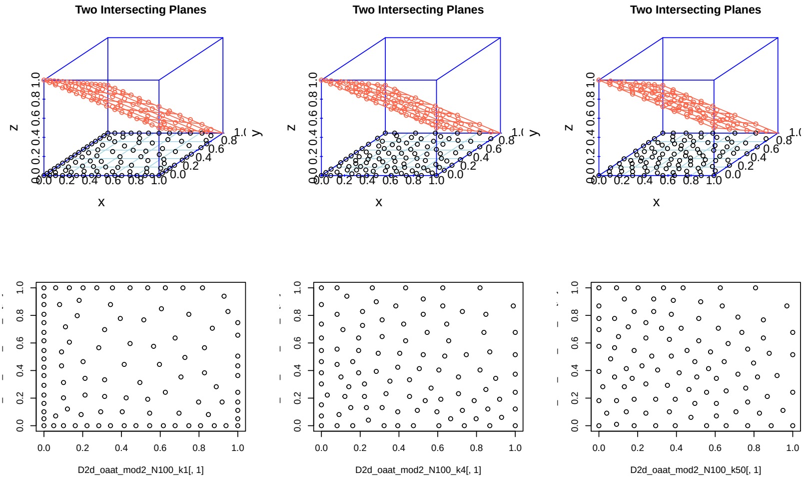


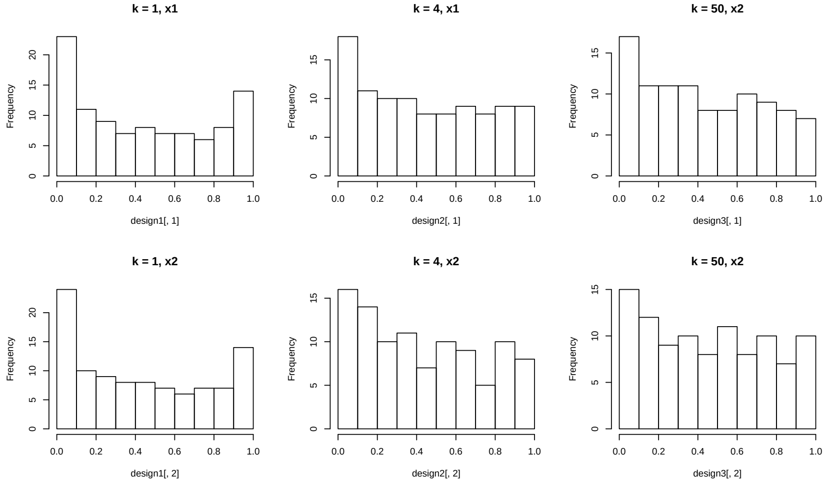
Example 2

Example 2

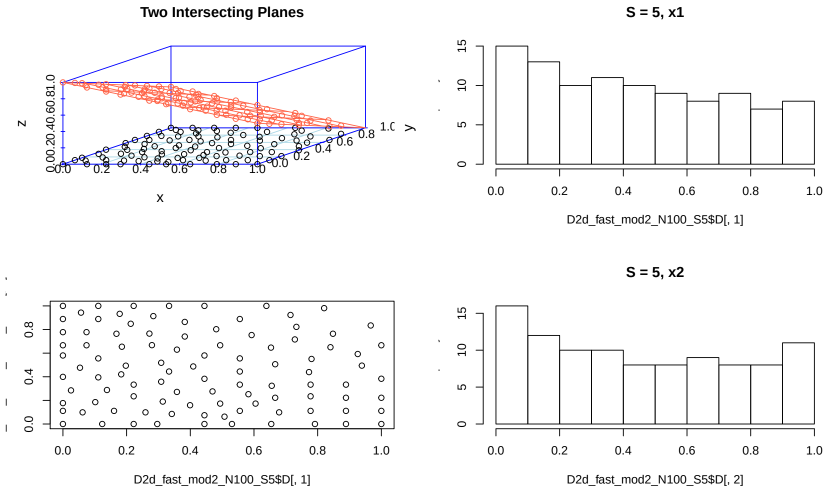

Two Intersecting Planes
z
1.0
0.8
0.6
0.4
0.2
0.0
x
0.0
0.2
0.4
0.6
0.8
1.0
y
0.0
0.2
0.4
0.6
0.8
1.0

One-at-a-Time Algorithm, $k = 1, 4, 50$ and $N = 100$




k = 1, x1
k = 4, x1
k = 50, x2
k = 1, x2
k = 4, x2
k = 50, x2
Frequency
design1[, 1]
design2[, 1]
design3[, 1]
design1[, 2]
design2[, 2]
design3[, 2]
0
5
10
15
20
0.0
0.2
0.4
0.6
0.8
1.0

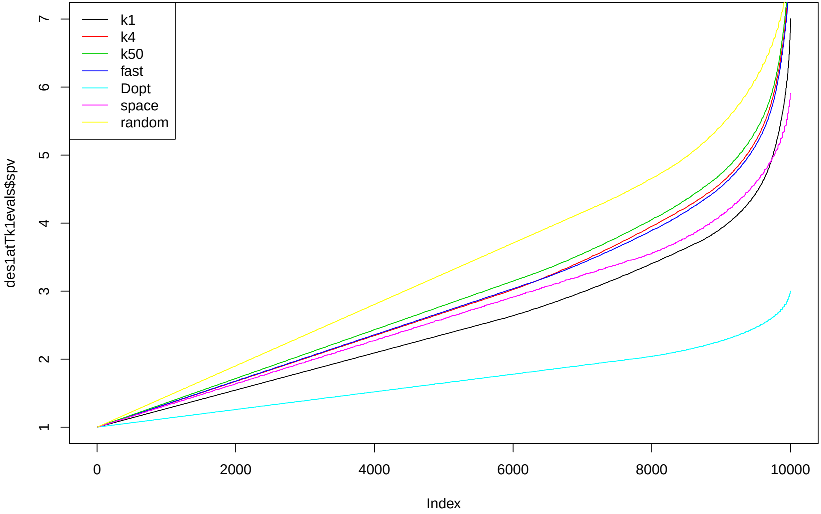
Fast Algorithm, S = 5, N = 100



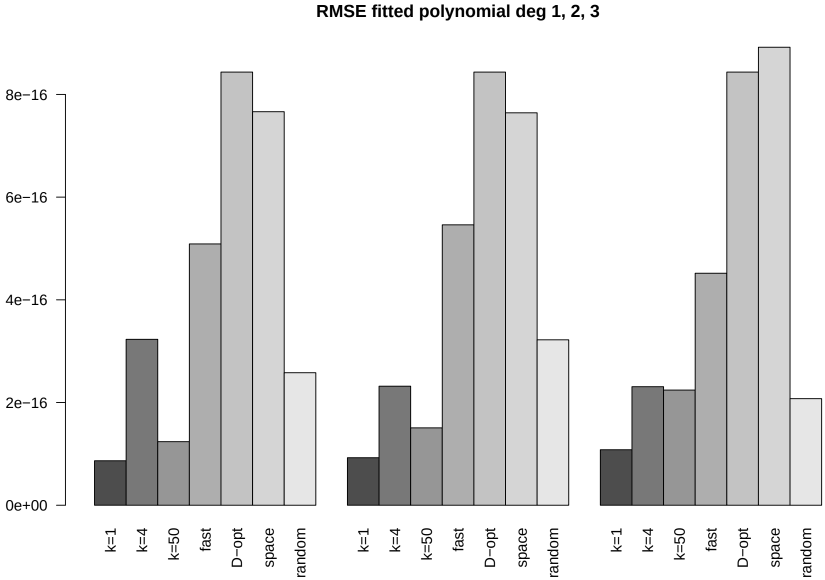
Example 2 Evaluations, N = 100

	1atT,k=1	1atT,k=4	1atT,k=50	Fast,S=5	D-Opt	Space	Random
TPEx10e-3	65.037	58.482	61.175	61.159	Inf	Inf	168.96
Fast Crit	1323.7	719.67	619.29	488	Inf	Inf	20725
1atT Crit (k=4)	1585.5	815.9	692.09	655.64	Inf	Inf	20746
E[P(H0|Y,D)|H0,D]	1	1	1	1	1	1	1
E[P(H1|Y,D)|H0,D]	9.04e-34	2.78e-27	1.29e-28	1.75e-27	1.68e-40	4.65e-28	1.21e-23
E[BF01 | H0,D]	3.23e+55	6.91e+51	5.49e+49	1.74e+50	1.45e+62	3.79e+50	1.13e+44
E[P(H0|Y,D)|H1,D]	9.68e-29	2.73e-25	3.79e-25	1.42e-27	1.17e-31	8.96e-23	4.94e-18
E[P(H1|Y,D)|H1,D]	1	1	1	1	1	1	1
E[BF01|H1,D]	9.68e-29	2.73e-25	3.79e-25	1.42e-27	1.17e-31	8.96e-23	4.94e-18
V[B0|Y,X]	0.000723	0.000788	0.000847	0.000838	0.000588	0.000884	0.00106
V[B1|Y,X]	0.0014	0.00159	0.00169	0.00164	0.000803	0.00153	0.00189
V[B2|Y,X]	0.0014	0.00162	0.00162	0.00156	0.000803	0.00153	0.00186

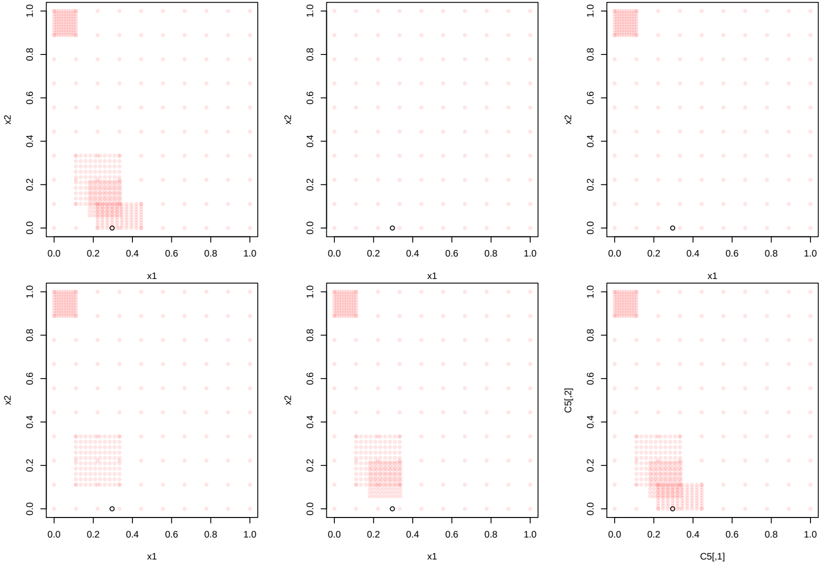
Scaled Prediction Variance (SPV)



Empirical RMSE

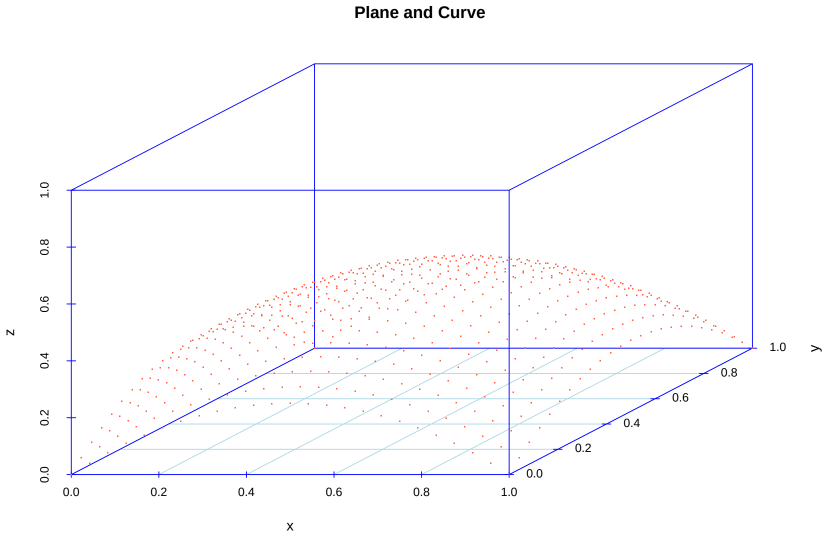


Candidates for Design Point indexed at 10

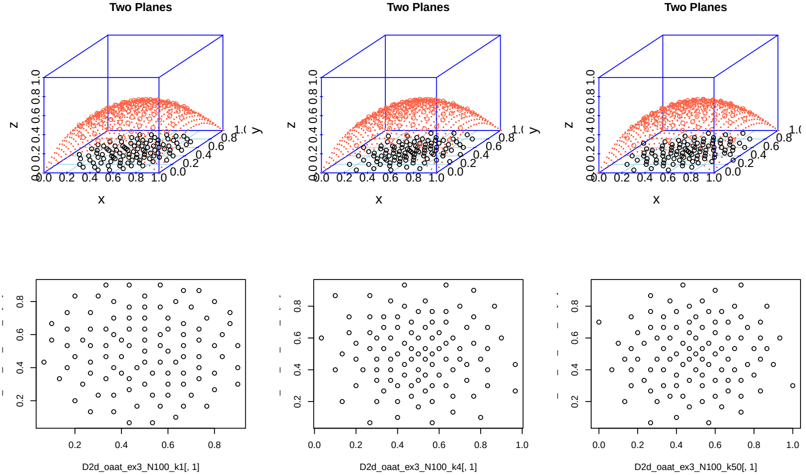


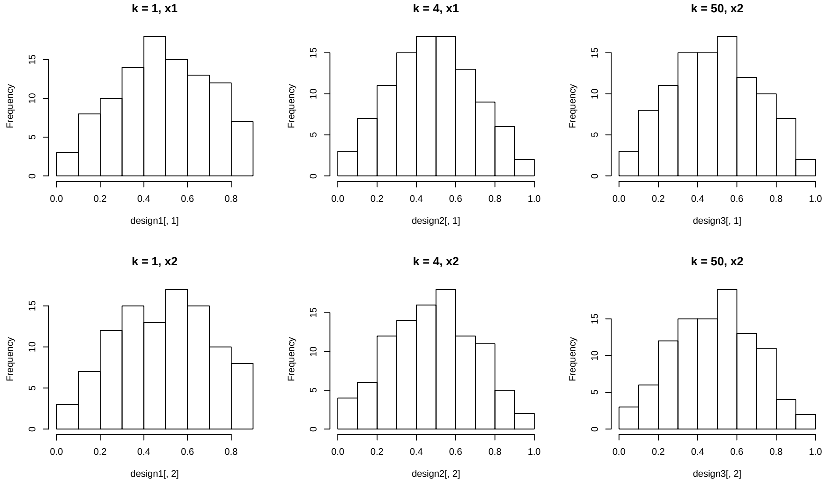
Example 3

Example 3

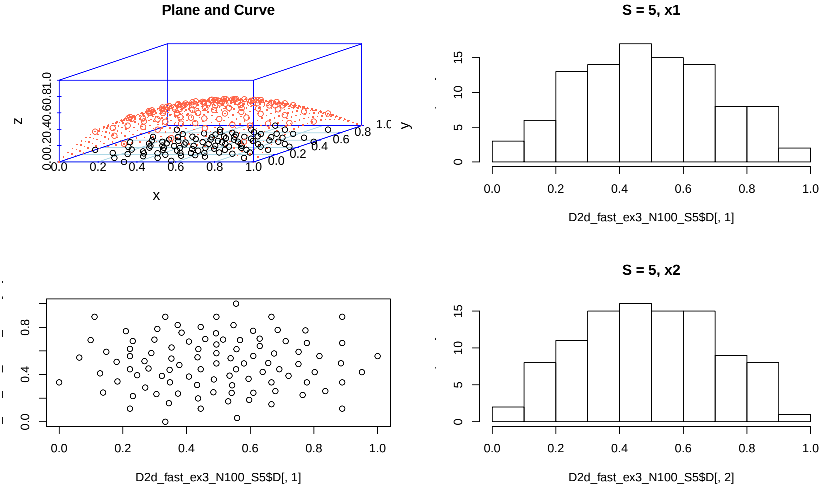

Plane and Curve
z
0.0
0.2
0.4
0.6
0.8
1.0
x
0.0
0.2
0.4
0.6
0.8
1.0
y
0.0
0.2
0.4
0.6
0.8
1.0

One-at-a-Time Algorithm, $k = 1, 4, 50$ and $N = 100$




k = 1, x1
k = 4, x1
k = 50, x2
k = 1, x2
k = 4, x2
k = 50, x2
Frequency
design1[, 1]
design2[, 1]
design3[, 1]
design1[, 2]
design2[, 2]
design3[, 2]
0
5
10
15
0.0
0.2
0.4
0.6
0.8
1.0

Fast Algorithm, S = 5, N = 100



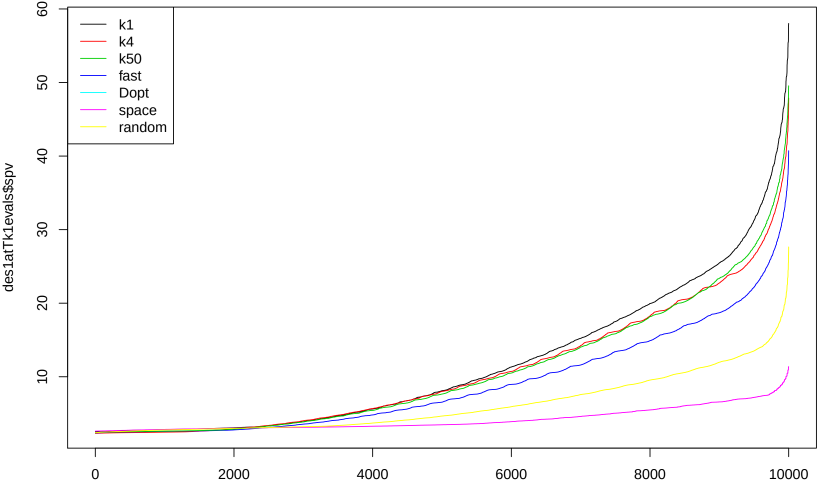
Example 3 Evaluations, N = 100

- D-optimal design tends to be worst i.t.o. $E[P(H_\ell|Y, D)|H_\ell, D], \ell = \{0, 1\}$

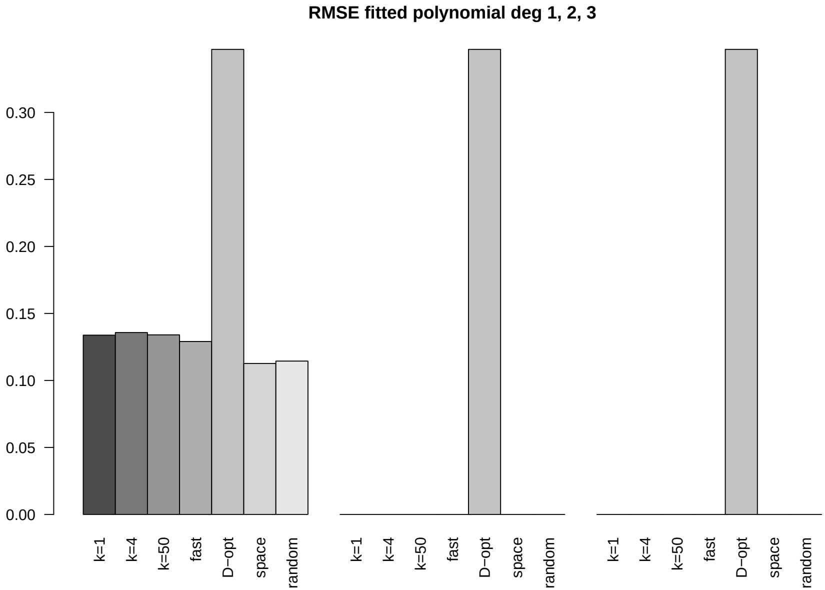
	1atT,k=1	1atT,k=4	1atT,k=50	Fast,S=5	D-Opt	Space	Random
TPEx10e-3	103.81	105.5	104.81	105.92	Inf	Inf	150.6
Fast Crit	142.74	110.2	103.75	109.06	Inf	Inf	6021
1atT Crit (k=4)	323.56	306.98	310.49	313.78	Inf	Inf	6029.9
E[P(H0|Y,D)|H0,D]	1	1	0.995	1	0.529	1	1
E[P(H1|Y,D)|H0,D]	2.82e-05	0.000345	0.00541	1.7e-05	0.471	3.74e-10	0.000138
E[BF01 | H0,D]	7.11e+13	3.25e+15	2.81e+15	5.7e+14	1.23	8.73e+20	5.94e+18
E[P(H0|Y,D)|H1,D]	6.86e-05	1.75e-06	1.81e-05	1.02e-05	0.457	1.48e-09	6.87e-07
E[P(H1|Y,D)|H1,D]	1	1	1	1	0.543	1	1
E[BF01|H1,D]	6.89e-05	1.75e-06	1.81e-05	1.02e-05	1	1.48e-09	6.87e-07
V[B0|Y,X]	0.00121	0.00123	0.0012	0.00114	0.000618	0.000885	0.00106
V[B1|Y,X]	0.00314	0.00316	0.00312	0.0031	0.00272	0.00277	0.00295
V[B2|Y,X]	0.0033	0.00326	0.00323	0.00318	0.00272	0.00273	0.00297
V[B3|Y,X]	0.00313	0.00315	0.00317	0.00309	0.00272	0.00277	0.00294
V[B4|Y,X]	0.00328	0.00329	0.00331	0.00323	0.00272	0.00273	0.0029

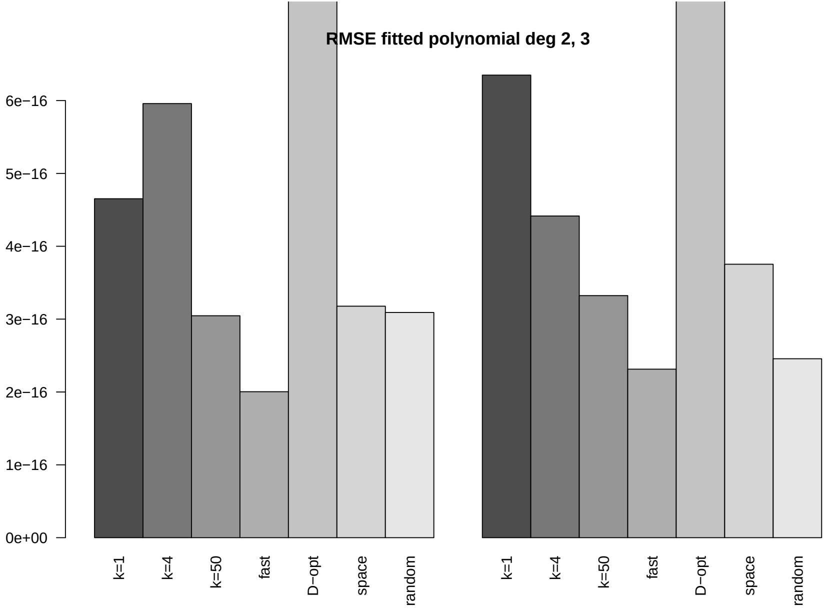
Scaled Prediction Variance (SPV)

Note: For the D-optimal design, repeating columns in the second order model causes $X'X$ to be singular, hence SPV $=$ NA. This is an example of when replication in the D-optimal design can cause isssues.



Empirical RMSE



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## [1] "RMSE for D-opt deg2 and deg3 resp: 0.347043064717696 ,  0.347043064717696"
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Candidates for Design Point indexed at 10