MED for Model Selection

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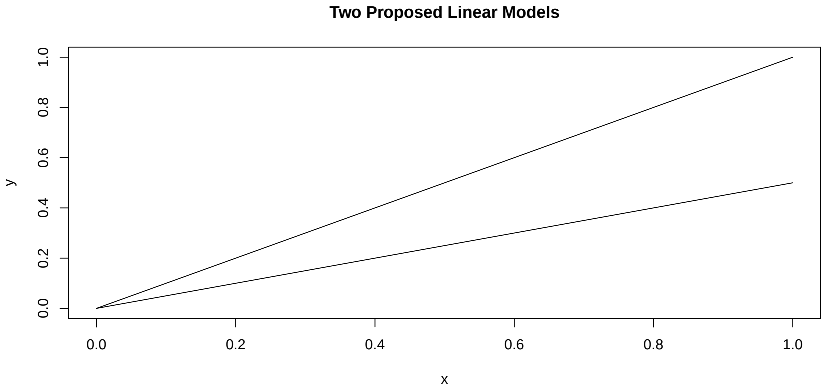
Simple Linear Regression: Unknown Slope

Design an Experiment that Estimates Slope



- Goal: Choose design $\mathbf{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ to gather data that will
  1. help distinguish these two slopes
  2. allow adequate estimation of β.
- Idea: Minimum Energy Design!

Minimum Energy Design

Minimum energy design (MED) is a deterministic sampling method which makes use of evaluations of the target distribution f to obtain a weighted space-filling design.

Definition:

Design $\mathbf{D} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$ is a MED if it minimizes the total potential energy, given by:

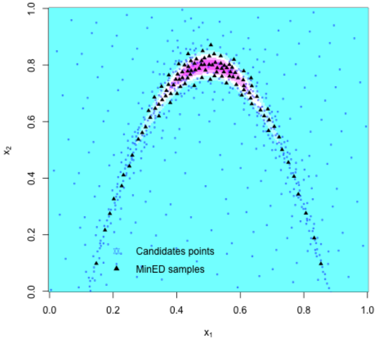
$$\sum_{i \neq j} \frac{q(\mathbf{x}_i) q(\mathbf{x}_j)}{d(\mathbf{x}_i, \mathbf{x}_j)}$$

Choose the charge function, $q = \frac{1}{f^{1/2p}}$ so that the limiting distribution of the design points is target distribution, f.

Advantages of MED

Sampling the "Banana" Function

- $N = 109$
- $K = 6$
- $NK = 654$ evaluations of f



Compared to other sampling methods, MED

- has fewer points and hence (unlike MCMC)
- requires fewer evaluations of f (unlike MCMC)
- is not prone to missing high-density regions (unlike QMC)

Simple Linear Regression without Intercept

- Assume $y_i = x_i\beta + \varepsilon_i$ with $\varepsilon_i \sim N(0, \sigma^2)$ and $\beta \sim N(\mu, \nu^2)$.
- $y|\beta, X \sim N(X\beta, \sigma^2 I)$
- $y|X \sim N(X\mu, \sigma^2 I + \nu^2 XX^T)$ after marginalizing out β

Hypotheses

Suppose we suspect $\beta = \mu_0$ or $\beta = \mu_1$, i.e.

$$H_0 : \beta \sim N(\mu_0, \nu_0^2)$$
$$H_1 : \beta \sim N(\mu_1, \nu_1^2)$$

MED design may distinguish these two hypotheses and allow for adequate estimation of β.

Evaluating the Designs

Evaluating Methods

- Posterior Variance, i.e. $Var[\beta|y, X]$
- Expected Posterior Probabilities of Hypotheses & Bayes Factor
- Design Criteria:
  - Total Potential Energy
  - Criterion for One-at-a-Time Algorithm
  - Criterion for Fast Algorithm

Interpretations

- A design that is better for estimating β may have smaller posterior variance.
- A design that is better for hypothesis testing may give a larger expected posterior probability to the true model from simulated responses.

Posterior Variance

In the Bayesian linear regression framework,

$$y|\beta, X \sim N(X\beta + \sigma^2 I)$$
$$\beta \sim N(\mu, V)$$

with $X \in \mathbb{R}^{N \times p}, \beta \in \mathbb{R}^p, V \in \mathbb{R}^{p \times p}$,

- $\hat{\beta} = \frac{1}{\sigma^2}\Sigma_B(X^T y + \sigma^2 V^{-1}\mu)$ with posterior distribution

$$\beta|y, X \sim N\left(m_B, \Sigma_B\right)$$

  where

$$\Sigma_B = \sigma^2(X^T X + \sigma^2 V^{-1} I)^{-1}$$
$$m_B = \frac{1}{\sigma^2}\Sigma_B(X^T y + \sigma^2 V^{-1}\mu)$$

- Σ_B can be used to evaluate a design **D**'s ability to estimate β

Posterior Probabilities of Hypotheses

- Posterior Probability of model $H_\ell, \ell \in 1, ..., M$:

$$P(H_\ell|y, X) = \frac{\pi_\ell L(y|H_\ell, X)}{\sum_{m=1}^{M} \pi_m L(y|H_m, X)}$$

  where π_m is the prior on H_m (typically $\pi_m = \frac{1}{M}$), and $L(y|H_m, X)$ is the model evidence.
- $P(H_\ell|y, X)$ tells which hypothesis is more likely to give the correct model.
- $E[P(H_\ell|y, X)|H_r]$ may be estimated using MC approximation from simulated responses y under a chosen hypothesis H_r.
- $E[P(H_\ell|y, \mathbf{D})|H_r]$ can be used to evaluate a design $\mathbf{D}$'s ability to distinguish hypotheses

Estimate Expected Posterior Probability of a Hypothesis

Estimate the expected posterior probability of hypothesis H_ℓ for J simulations of Y under H_r, given design $\mathbf{D} = \{x_1, ..., x_N\}$:

1. For $j = 1, \ldots, J$:
   1.1 Draw $\beta \sim N(\mu_r, \nu_r^2)$
   1.2 Draw $y_i^{(j)} | \mathbf{D} \sim N(\mathbf{x}_i \beta, \sigma_r^2)$, $\forall \mathbf{x}_i \in \mathbf{D}$
   1.3 $\forall m \in \{1, ..., M\}$, calculate model evidences $L(y^{(j)} | H_m, \mathbf{D})$
      - model evidence $L(y | H_m, \mathbf{D})$ is the marginal likelihood $N(\mathbf{D}\mu_m, \sigma^2 I + \nu^2 \mathbf{D}\mathbf{D}^T)$ evaluated at y and $\mathbf{D}$.

   1.4 Calculate the posterior probability of H_ℓ, $P(H_\ell | y^{(j)}, \mathbf{D})$, from simulation j

$$P(H_\ell | y^{(j)}, \mathbf{D}) = \frac{\pi_\ell P(y^{(j)} | H_\ell, \mathbf{D})}{\sum_{m=1}^{M} \pi_m P(y^{(j)} | H_m, \mathbf{D})}$$

2. Average the estimated posterior probabilities of H_ℓ over $\forall j$ to obtain MC estimate of $E[P(H_\ell | y, \mathbf{D}) | H_r]$

MED Criteria

1. The Total Potential Energy, which both algorithms aim to minimize:
$$\sum_{i \neq j} \frac{q(\mathbf{x}_i)q(\mathbf{x}_j)}{d(\mathbf{x}_i, \mathbf{x}_j)}$$

2. One-at-a-Time Algorithm: minimize
$$\left\{ \sum_{i \neq j} \left(\frac{q(\mathbf{x}_i)q(\mathbf{x}_j)}{d(\mathbf{x}_i, \mathbf{x}_j)} \right)^k \right\}^{1/k}$$
which gives the Total Potential Energy criterion when $k = 1$.

3. Fast Algorithm: minimize
$$\max_{i \neq j} \frac{q(\mathbf{x}_i)q(\mathbf{x}_j)}{d(\mathbf{x}_i, \mathbf{x}_j)}$$

MED-generating Algorithms

One-at-a-Time Algorithm (2015)

Steps to obtain MED using One-at-a-Time algorithm:

1. Obtain *numCandidates* candidate points, $\mathbf{x}$, in $[0,1]$.
2. Initialize D_N by choosing $\mathbf{x}_j$ to be the candidate $\mathbf{x}$ which optimizes f, where $f(\mathbf{x}) = \text{Wasserstein}(\phi_{0,\mathbf{x}}, \phi_{1,\mathbf{x}})$ and

$$\phi_{0,\mathbf{x}} = N(\mu_0 \mathbf{x}, \sigma_0^2 + \mathbf{x}^2 \nu_0^2),$$
$$\phi_{1,\mathbf{x}} = N(\mu_1 \mathbf{x}, \sigma_1^2 + \mathbf{x}^2 \nu_1^2)$$

3. Choose the next point $\mathbf{x}_{j+1}$ by:

$$\mathbf{x}_{j+1} = \arg\min_{\mathbf{x}} \sum_{i=1}^{j} \left(\frac{q(\mathbf{x}_i) q(\mathbf{x})}{d(\mathbf{x}_i, \mathbf{x})} \right)^k$$

where $q = 1/f^{(1/2p)}$, $d(x,y)$ is Euclidean distance and $k = 4p$.

- This is a greedy algorithm for choosing points one at a time

Fast Algorithm (2018)

In each of S stages, create a new design to iteratively minimize

$$\max_{i \neq j} \frac{q(\mathbf{x}_i)q(\mathbf{x}_j)}{d(\mathbf{x}_i, \mathbf{x}_j)}$$

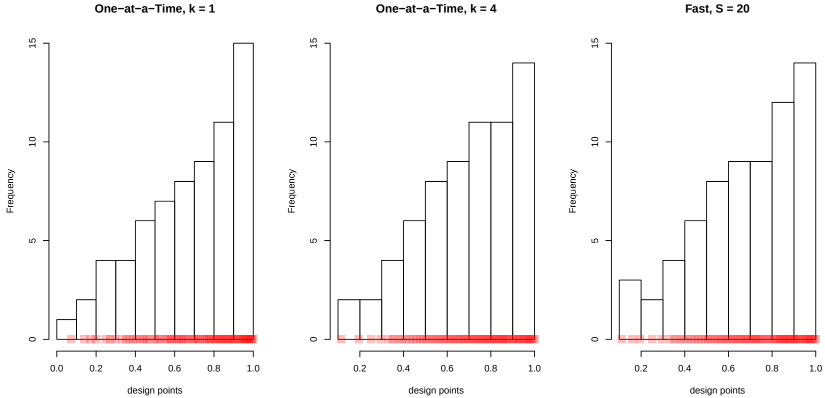
1. Initialize space-filling design $\mathbf{D}_1 = \{\mathbf{x}_1^{(1)} \ldots \mathbf{x}_N^{(1)}\}$
2. For $s = 1, \ldots, S-1$ steps, obtain each design point $\mathbf{x}_j^{(s+1)} \in \mathbf{D}_{s+1}$ by:

$$\begin{aligned} \mathbf{x}_j^{s+1} &= \operatorname*{arg\,min}_{\mathbf{x} \in \mathbf{C}_j^{s+1}} \max_{i=1:(j-1)} \frac{1}{f^{\gamma_s}(\mathbf{x}_i) f^{\gamma_s}(\mathbf{x}) d^{(2p)}(\mathbf{x}_i, \mathbf{x})} \\ &= \operatorname*{arg\,min}_{\mathbf{x} \in \mathbf{C}_j^{s+1}} \max_{i=1:(j-1)} \frac{q^{\gamma_s}(\mathbf{x}_i) q^{\gamma_s}(\mathbf{x})}{d(\mathbf{x}_i, \mathbf{x})} \end{aligned}$$

where $\gamma_s = s/(S-1)$ and $\mathbf{C}_j^{s+1}$ is the candidate set for $\mathbf{x}_j^{(s+1)}$

- Points migrate to more optimal locations in each stage

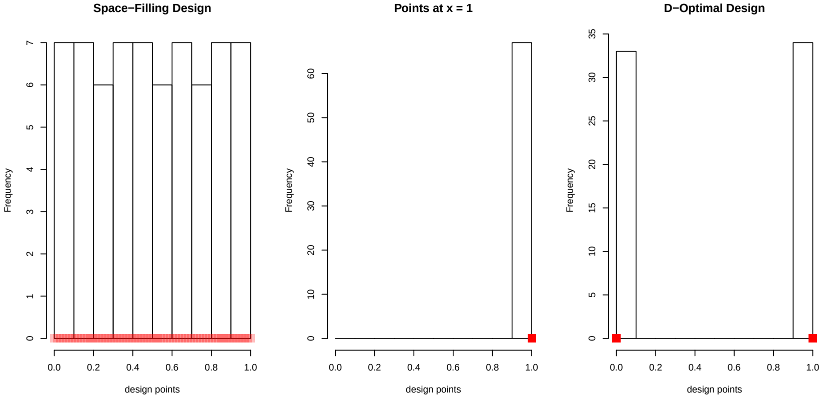
Designs from MED-Generating Algorithms



Other Designs

Other Designs

- Random designs: 50 random designs ($\mathbf{x} \sim U([0,1]^p)$, $\forall \mathbf{x} \in \mathbf{D}$).
- Space-Filling Design: evenly spaced points over $[0,1]$
- $\mathbf{D} = \mathbf{1}$: $\forall \mathbf{x} \in \mathbf{D}, \mathbf{x} = 1$.
- D-optimal Design: seeks to minimize the variance of the estimated regression coefficients.
  - generated by `AlgDesign` (using Federov's exchange algorithm).


Space−Filling Design
Frequency
design points
0.0 0.2 0.4 0.6 0.8 1.0
0 1 2 3 4 5 6 7
Points at x = 1
Frequency
design points
0.0 0.2 0.4 0.6 0.8 1.0
0 10 20 30 40 50 60
D−Optimal Design
Frequency
design points
0.0 0.2 0.4 0.6 0.8 1.0
0 5 10 15 20 25 30 35

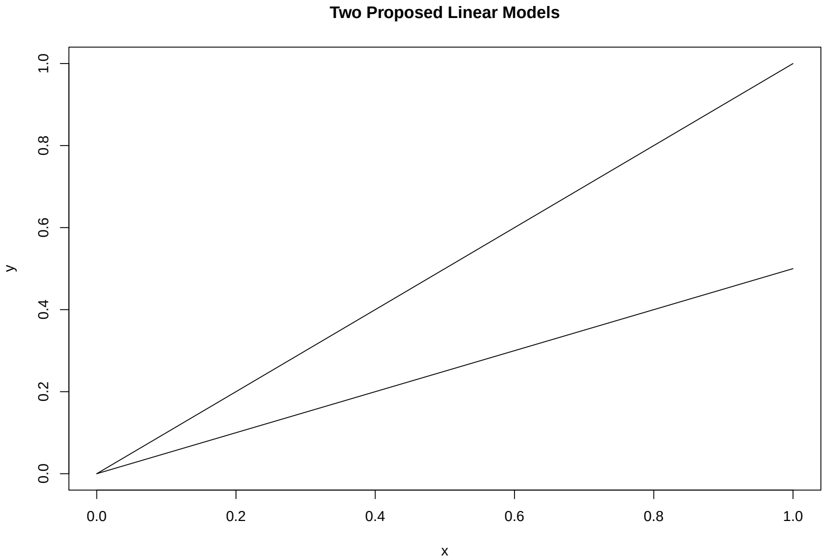
Results

Results!

	1atT,k=1	1atT,k=4	Fast	Random	Space	D = 1	D-opt
E[P(H0|Y,D)|H0]	0.999	0.999	0.999	0.999	0.999	0.999	0.999
E[BF01 | H0]	3.67e+15	3.55e+16	5.21e+16	6.53e+15	5.3e+14	6.63e+16	6.3e+15
E[P(H1|Y,D)|H1]	0.999	0.999	0.999	0.999	0.999	0.999	0.999
E[BF01|H1]	0.0108	0.00142	0.000913	0.0522	0.00318	0.00104	0.000738
PostVar b x10e-4	6.33	6.25	6.28	9.15	9.09	3.47	6.41
TPE x10e3	2810	2870	2820	8050000	Inf	Inf	Inf
Fast x10e3	97.5	43.7	44.5	7810000	Inf	Inf	Inf
1atT(k=4) x10e3	120	92.5	94.1	7810000	Inf	Inf	Inf
Mean(D)	0.674	0.689	0.684	NA	0.5	1	0.507
sd(D)	0.247	0.219	0.23	NA	0.295	0	0.504

Simple Linear Regression: Unknown Slope and Intercept

Design an Experiment that Estimates Slope and Intercept



SetUp

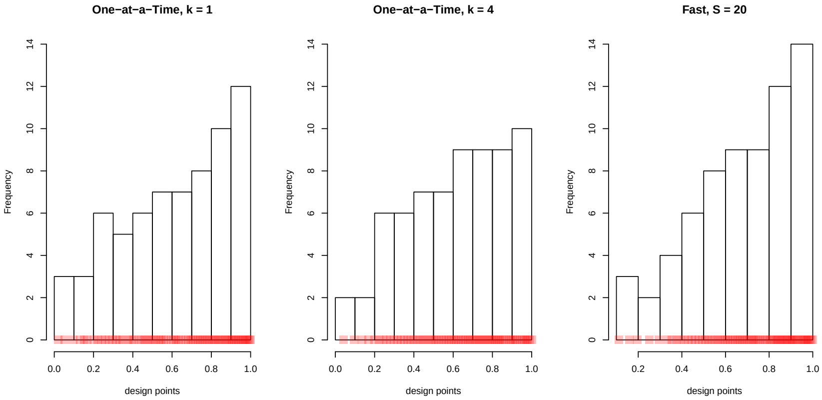
Similar to the unknown slope case,

- Assume $y_i = \beta_0 + x_i\beta_1 + \varepsilon_i$, where $\varepsilon_i \sim N(0, \sigma^2)$ and $\beta \sim N(\mu, V), \mu = (\mu_0, \mu_1)^T, V = \text{diag}(\nu_0^2, \nu_1^2)$.
- $y|\beta, X \sim N(X\beta, \sigma^2 I)$
- $y|X \sim N(X\mu, \sigma^2 I + XVX^T)$

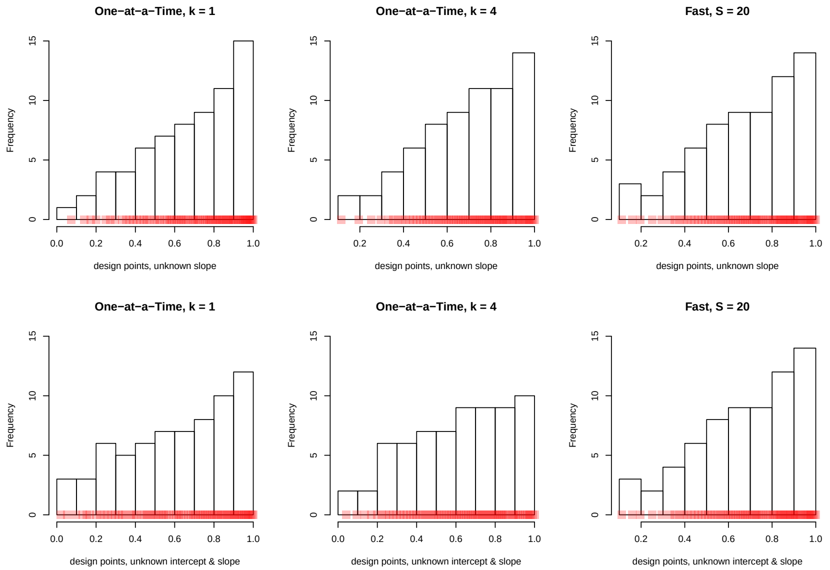
Hypotheses

Suppose we suspect $\beta = \mu_0$ or $\beta = \mu_1$, i.e.

$$
\begin{aligned}
H_0 : \beta &\sim N\left(\mu_0, V_0\right), \\
\mu_0 &= \left(\mu_{00}, \mu_{01}\right)^T, \\
V_0 &= \text{diag}(\nu_{00}^2, \nu_{01}^2) \\
H_1 : \beta &\sim N\left(\mu_1, V_1\right), \\
\mu_1 &= \left(\mu_{10}, \mu_{11}\right)^T, \\
V_1 &= \text{diag}(\nu_{10}^2, \nu_{11}^2)
\end{aligned}
$$


One−at−a−Time, k = 1
One−at−a−Time, k = 4
Fast, S = 20
Frequency
design points

Compare Unknown Slope to Unknown Intercept & Slope



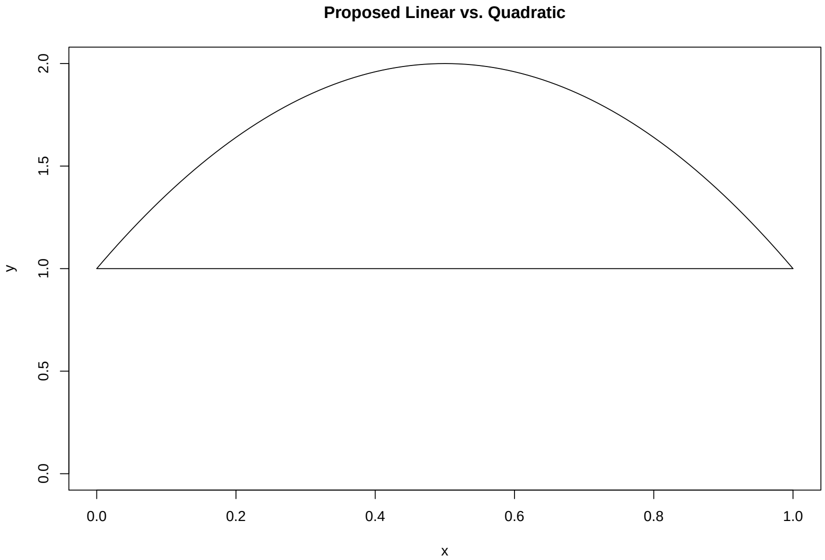
Table

	1atT,k=1	1atT,k=4	Fast	Space	D = 1	D-opt
E[P(H0|Y,D)|H0]	0.997	0.995	0.994	0.994	0.991	0.998
E[BF01 | H0]	3.99e+10	3.66e+09	1.87e+10	4.32e+10	5.72e+09	1.84e+14
E[P(H1|Y,D)|H1]	0.992	0.993	0.994	0.994	0.986	0.997
E[BF01|H1]	0.0925	0.0427	0.0919	1.03	0.144	0.0417
PostVar b0 x10e-4	10.3	10.8	13	8.01	25.9	5.9
PostVar b1 x10e-4	21.2	22.6	23.5	21	25.9	10.9
TPE x10e3	2270	2190	2820	Inf	Inf	Inf
Fast x10e3	56.2	24.1	44.5	Inf	Inf	Inf
1atT(k=4) x10e3	80.1	62.1	94.1	Inf	Inf	Inf
Mean(D)	6.66e+09	0.611	0.684	0.5	1	0.507
sd(D)	1.63e+10	0.255	0.23	0.295	0	0.504

- Compared to the alphabet-optimal designs, the MED methods allow the experimenter to determine how similar the intercepts and slopes are and determines the design points accordingly.

Linear vs Quadratic

Linear Model vs. Quadratic Model



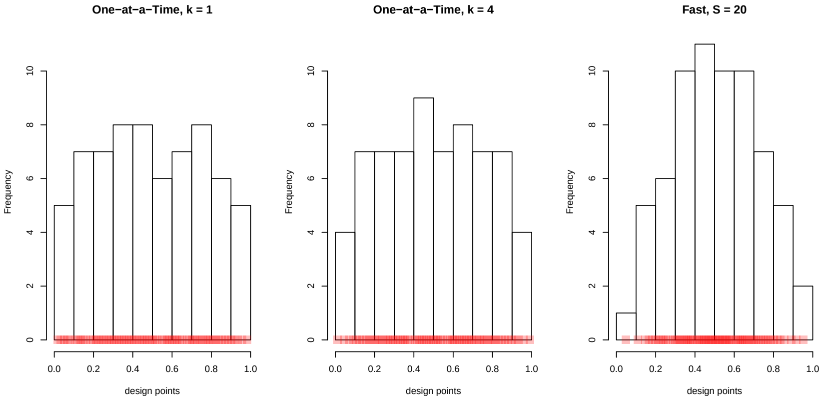
SetUp

We compare the linear model $y_i = \beta_0 + x_i\beta_1 + \varepsilon_i$ with the quadratic model $y_i = \beta_0 + x_i\beta_1 + +x_i^2\beta_2 + \varepsilon_i$

- $y|\beta, X \sim N(X\beta, \sigma^2 I)$
- $y|X \sim N(X\mu, \sigma_m^2 I + XVX^T)$

Hypotheses

$$
\begin{aligned}
H_0 : \beta \sim N\left(\mu_0, V_0\right), \\
\mu_0 = \left(\mu_{00}, \mu_{01}\right)^T, \\
V_0 = \mathrm{diag}(\nu_{00}^2, \nu_{01}^2) \\
H_1 : \beta \sim N\left(\mu_1, V_1\right), \\
\mu_0 = \left(\mu_{10}, \mu_{11}, \mu_{12}\right)^T, \\
V_1 = \mathrm{diag}(\nu_{10}^2, \nu_{11}^2, \nu_{12}^2)
\end{aligned}
$$


One−at−a−Time, k = 1
One−at−a−Time, k = 4
Fast, S = 20
Frequency
0
2
4
6
8
10
0.0
0.2
0.4
0.6
0.8
1.0
design points

Table

	1atT,k=1	1atT,k=4	Fast	Space	D = 0.5	D = 1	D-opt
E[P(H0|Y,D)|H0]	1	1	1	1	1	0.511	0.52
E[BF01 | H0]	5.66e+77	3e+75	5.69e+68	7.33e+88	1.83e+47	1.06	1.12
E[P(H1|Y,D)|H1]	1	1	1	1	1	0.51	0.516
E[BF01|H1]	1.18e-38	1.73e-40	1.09e-30	2.17e-50	1e-19	0.997	1.01
PostVar b0 x10e-4	8.39	8.67	9.77	8.12	14	33.7	6.2
PostVar b1 x10e-4	30.9	31.2	32.9	30.3	41	33.7	28.1
PostVar b2 x10e-4	32.2	32.4	34.7	30.9	47.7	33.7	28.1
TPE x10e3	872	786	973	Inf	Inf	Inf	Inf
Fast x10e3	40.2	11.7	12.9	Inf	Inf	Inf	Inf
1atT(k=4) x10e3	43.6	22.3	30	Inf	Inf	Inf	Inf
Mean(D)	0.494	0.501	0.51	0.5	0.5	1	0.507
sd(D)	0.272	0.263	0.217	0.295	0	0	0.504