Meeting : 14 May 2019

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5/3/2019

Last Time

Today

Fast Algorithm

One-at-a-Time Algorithm

Random Design

Space-Filling Design

D-Optimal Design

...

Last Time

Evaluating Model Ideas

Tried to evaluate the model based on:

1. Robustness
   - what happens when the power $k = 0:1$ in one-at-a-time algorithm
   - what happens when the number of designs K gets large (how it affects γ_k) in fast algorithm
2. Objective Improvement
   - Total Potential Energy

Today

The Plan

1. Fix optimization thing in first step
2. Make a table!

- Methods:
  - One-at-a-Time Algorithm
  - Fast Algorithm
  - Random design
  - Space-Filling design
  - D-Optimal design (is there one for model selection? e.g. one for H_0 and one for H_1? criterion doesn't seem to incorporate that.)
  - etc.
- Evaluations:
  - Expected Posterior Probabilities of H_0, H_1 & Bayes Factors of data generated from each H_0, H_1 model
  - Regression variance on coefficient (slope here)
  - Total Potential Energy criterion
  - One-at-a-Time Algorithm criterion
  - Fast Algorithm criterion

Regression Variance

- In the case where $y_i = x_i\beta + \varepsilon_i$ (with a fixed β) with ε_i $N(0, \sigma_\varepsilon^2)$, we have:

$$\hat{\beta} \sim N\left(\beta, \frac{\sigma_\varepsilon^2}{\sum_{i=1}^N (x_i - \bar{x})^2}\right)$$

Since $\hat{\beta} = \frac{\sum_i (y_i - \bar{y})(x_i - \bar{x})}{\sum_i (x_i - \bar{x})} = \sum_i w_i y_i$, where $w_i = \frac{(x_i - \bar{x})}{\sum_j (x_j - \bar{x})^2}$, and so $Var[\hat{\beta}] = Var[\sum_i w_i y_i] = Var[\sum_i w_i(x_i\beta + \varepsilon_i)] = \sum_i w_i^2 Var[\varepsilon_i] = \sigma_\varepsilon^2 \sum w_i^2$.

- It is similar when $\beta \sim N(\tilde{\beta}, \sigma_\beta^2)$:
- After marginalizing out β, $y_i \sim N(x_i\tilde{\beta}, \sigma_\varepsilon^2 + x_i^2\sigma_\beta^2)$. Hence:

$Var[\hat{\beta}] = Var[\sum_i w_i y_i] = \sum_i w_i^2 Var[y_i] = \sum_i w_i^2(\sigma_\varepsilon^2 + x_i^2\sigma_\beta^2)$

Criterions

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 criterion tries to minimize:

$$\left\{ \sum_{i \neq j} \left(\frac{q(\mathbf{x}_i)q(\mathbf{x}_j)}{d(\mathbf{x}_i, \mathbf{x}_j)} \right)^k \right\}^{1/k}$$

3. Fast Algorithm tries to minimize:

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

Parameters

- Parameters

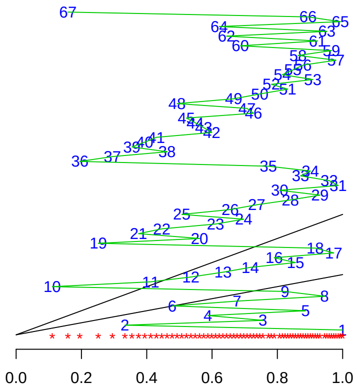
```
mean_beta0 = 1 # slope of null model
mean_beta1 = 1 / 2 # slope of alternative model
var_mean = 0.001 # variance on beta
var_e = 0.01 # variance on error
```

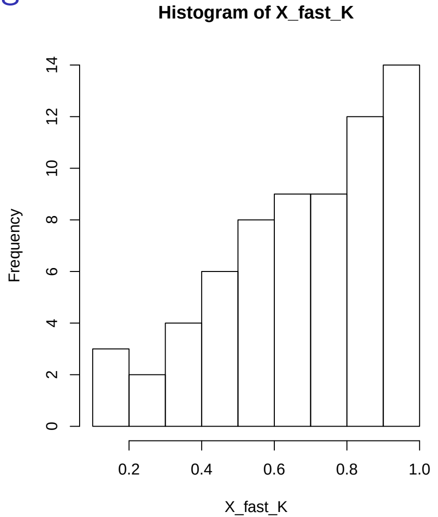
- Settings for Fast and One-at-a-Time algorithms

```
N = 67
# for fast algorithm:
K = 20 # ceiling(4* sqrt(p))
numParameters = 1 # number of parameters (just slope!)
p = numParameters * 2
# for one-at-a-time algorithm:
numCandidates = 10^5 # suggested 10^5
k = 4
```

Fast Algorithm

Design generated by Fast Algorithm






```
mean(X_fast_K)
```

```
## [1] 0.6836593
```

```
sd(X_fast_K)
```

```
## [1] 0.2296987
```

Evaluations

```
# Expected Post Probs and BF01 : Y | H0 Sims
c(expect_post_H0_YH0fast, expect_post_H1_YH0fast, BF01_YH0f
```

```
## [1] 0.874464 0.125536 6.965844
```

```
# Expected Post Probs and BF01 : Y | H1 Sims
c(expect_post_H0_YH1fast, expect_post_H1_YH1fast, BF01_YH1f
```

```
## [1] 0.1232342 0.8767658 0.1405555
```

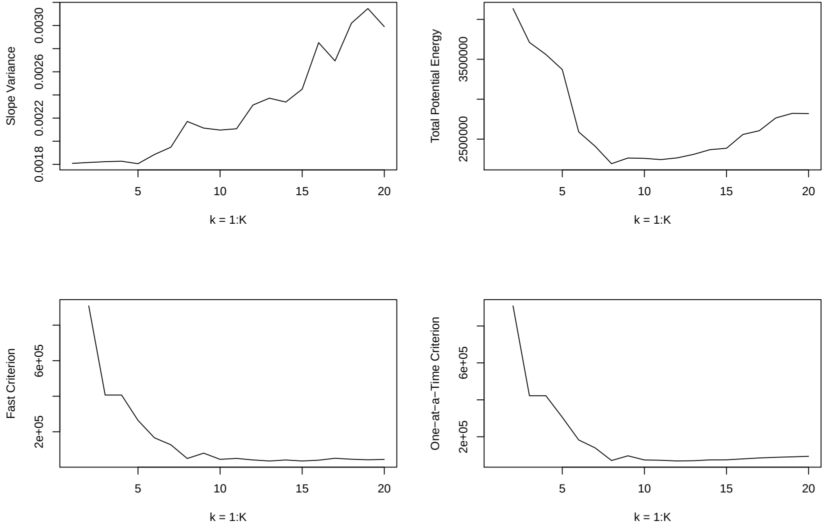
```
# Slope Variance
v_fast
```

```
## [1] 0.002990201
```

```
# Total PE, Fast Alg Crit, One-at-a-Time Alg Crit
c(TPE_fast, c1_fast, c2_fast)
```

```
## [1] 2820354.53   44460.74   94059.71
```

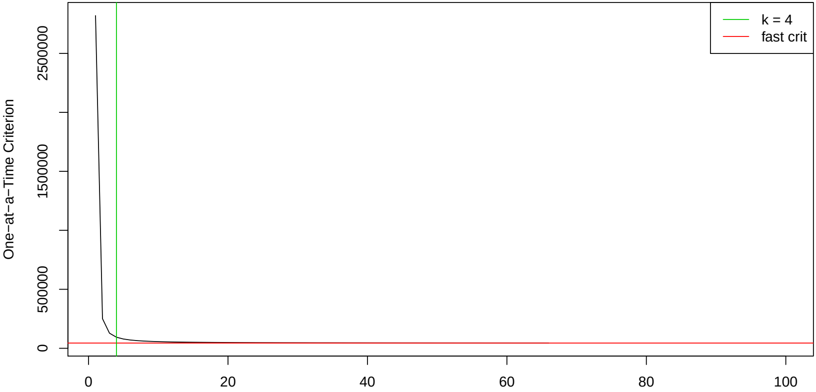
Over the K Designs



- Total Potential Energy criterion starts to increase as the design approaches `K = 20`. It could be that `K = 20` is too large
- Variance on Slope ($\hat{\beta}$) also increases. However, this makes sense since it is mainly a function of the differences between design points and their mean.

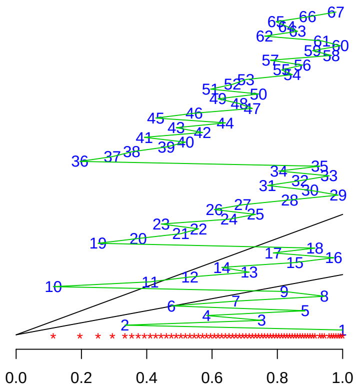
One-at-a-Time Criterion, Different k Powers

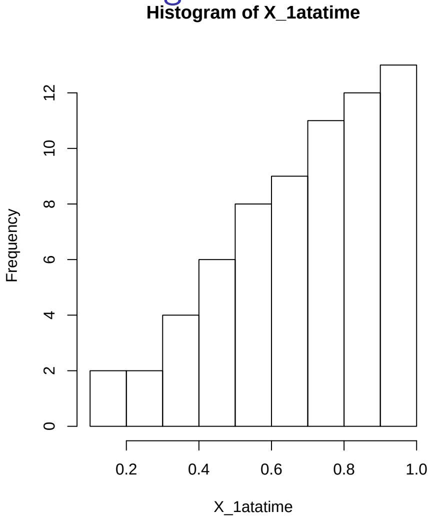
- To see if it decreases as $k \to \infty$, since this algorithm is supposed to be the asymptotic result of the one-at-a-time algorithm, here are the results for $k = 1:100$.
- For the fast algorithm's design, the one-at-a-time algorithm's criterion approaches the fast algorithm's criterion as k gets large (until it becomes `infty`. Compuational issue, probably.)



One-at-a-Time Algorithm

Design generated by One-at-a-Time Algorithm






```r
mean(X_1atatime)
```

```
## [1] 0.6886419
```

```r
sd(X_1atatime)
```

```
## [1] 0.2187448
```

Evaluations

```r
# Expected Post Probs and BF01 : Y | H0 Sims
c(expect_post_H0_YH0oneattime, expect_post_H1_YH0oneattime,
```

```
## [1] 0.8834295 0.1165705 7.5785023
```

```r
# Expected Post Probs and BF01 : Y | H1 Sims
c(expect_post_H0_YH1oneattime, expect_post_H1_YH1oneattime,
```

```
## [1] 0.1148289 0.8851711 0.1297251
```

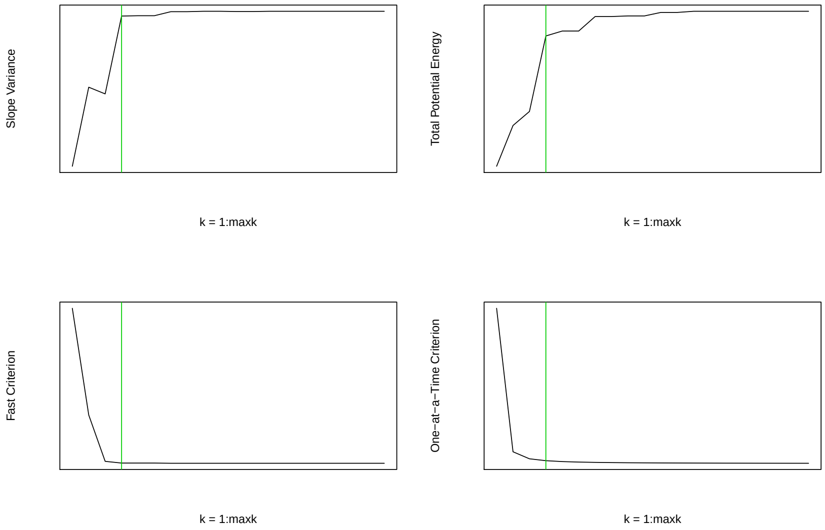
```r
# Slope Variance
v_oneattime
```

```
## [1] 0.003300413
```

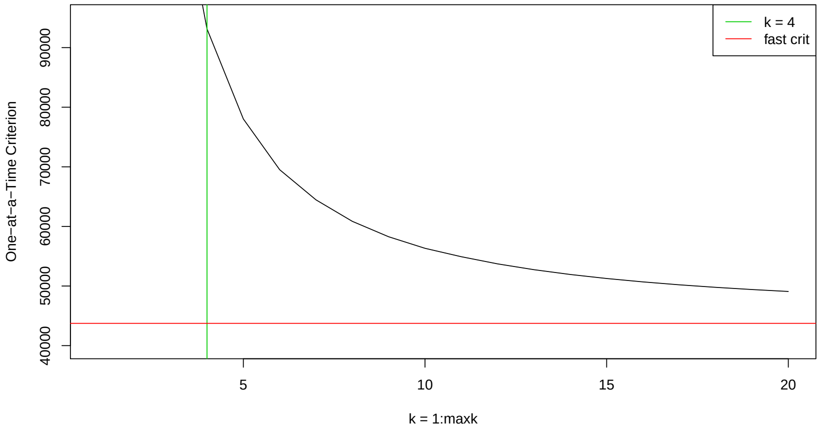
```r
# Total PE, Fast Alg Crit, One-at-a-Time Alg Crit
c(TPE_oneattime, c1_oneattime, c2_oneattime)
```

```
## [1] 2867630.36   43737.03   92199.06
```

Robustness Across k Power



Comparing Evaluations for Criterion



Random Design

Random Designs

10 simulated random designs ($\mathbf{x} \sim U([0,1]^p)$, $\forall \mathbf{x} \in \mathbf{D}_{\text{random}}$).

```r
# Mean Expected Post Probs and BF01 : Y | H0 Sims
c(expect_post_H0_YH0rand, expect_post_H1_YH0rand, BF01_YH0rand)
```

```
## [1] 0.7301598 0.2698402 2.7301864
```

```r
# Mean Expected Post Probs and BF01 : Y | H1 Sims
c(expect_post_H0_YH1rand, expect_post_H1_YH1rand, BF01_YH1rand)
```

```
## [1] 0.2694990 0.7305010 0.3700613
```

```r
# Mean Slope Variance
v_rand
```

```
## [1] 0.001841713
```

```r
# Mean Total PE, Fast Alg Crit, One-at-a-Time Alg Crit
c(TPE_rand, crit1_rand, crit2_rand)
```

```
## [1] 955312216 767617960 770812994
```

```r
# SD Slope Variance
v_rand_sd
```

```
## [1] 0.0001323766
```

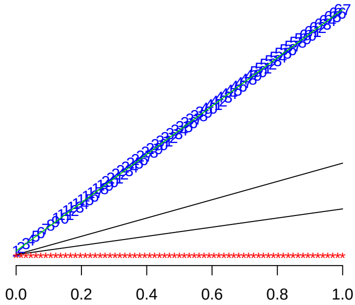
```r
# SD Total PE, Fast Alg Crit, One-at-a-Time Alg Crit
c(TPE_rand_sd, crit1_rand_sd, crit2_rand_sd)
```

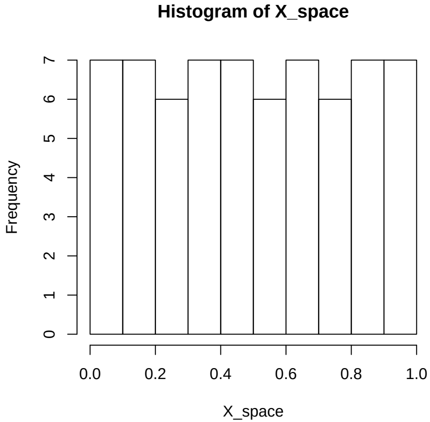
```
## [1] 1575304574 1496514486 1495025103
```

Space-Filling Design

The Design Points

Where the points are in no particular order.






```r
mean(X_space)
```

```
## [1] 0.5
```

```r
sd(X_space)
```

```
## [1] 0.2952278
```

Evaluations

```
# Expected Post Probs and BF01 : Y | H0 Sims
c(expect_post_H0_YH0space, expect_post_H1_YH0space, BF01_YH
```

```
## [1] 0.7370318 0.2629682 2.8027405
```

```
# Expected Post Probs and BF01 : Y | H1 Sims
c(expect_post_H0_YH1space, expect_post_H1_YH1space, BF01_YH
```

```
## [1] 0.2618302 0.7381698 0.3547019
```

```
# Slope Variance
v_space
```

```
## [1] 0.001808684
```

```
# Total PE, Fast Alg Crit, One-at-a-Time Alg Crit
c(TPE_space, c1_space, c2_space)
```

```
## [1] Inf Inf Inf
```

D-Optimal Design

D-Optimal Criterion

Seeks to minimize:

$$|(X^T X)^{-1}|$$

i.e. maximize:

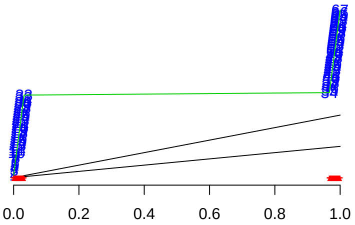
$$|X^T X|$$

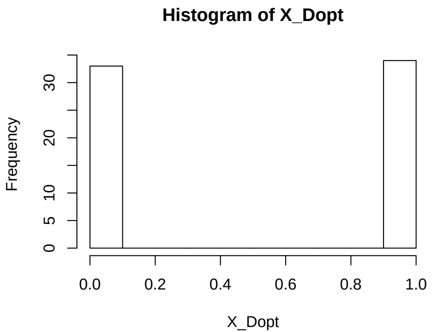
where X is the design.

Design generated by D-Optimal Criterion

Using `AlgDesign` package (using Federov's exchange algorithm),

where the points are in no particular order... assumed to be random order?






```
mean(X_Dopt)
```

```
## [1] 0.5069697
```

```
sd(X_Dopt)
```

```
## [1] 0.4874279
```

Evaluations

```r
# Expected Post Probs and BF01 : Y | H0 Sims
c(expect_post_H0_YH0dopt, expect_post_H1_YH0dopt, BF01_YH0c
```

```
## [1] 0.6703381 0.3296619 2.0334113
```

```r
# Expected Post Probs and BF01 : Y | H1 Sims
c(expect_post_H0_YH1dopt, expect_post_H1_YH1dopt, BF01_YH1c
```

```
## [1] 0.3296886 0.6703114 0.4918439
```

```r
# Slope Variance
v_dopt
```

```
## [1] 0.0006681488
```

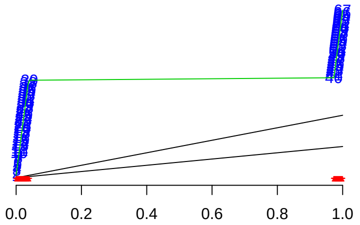
```r
# Total PE, Fast Alg Crit, One-at-a-Time Alg Crit
c(TPE_dopt, c1_dopt, c2_dopt)
```

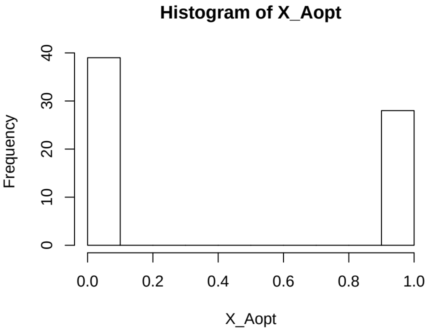
```
## [1] Inf Inf Inf
```

. . .

Design generated by A-Optimal Criterion

Using `AlgDesign` package (using Federov's exchange algorithm),






```r
mean(X_Aopt)
```

```
## [1] 0.4233935
```

```r
sd(X_Aopt)
```

```
## [1] 0.4808294
```

Evaluations

```
# Expected Post Probs and BF01 : Y | H0 Sims
c(expect_post_H0_YH0aopt, expect_post_H1_YH0aopt, BF01_YH0a
```

```
## [1] 0.6327927 0.3672073 1.7232576
```

```
# Expected Post Probs and BF01 : Y | H1 Sims
c(expect_post_H0_YH1aopt, expect_post_H1_YH1aopt, BF01_YH1a
```

```
## [1] 0.3670183 0.6329817 0.5798245
```

```
# Slope Variance
v_aopt
```

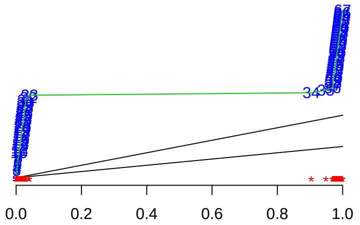
```
## [1] 0.000692498
```

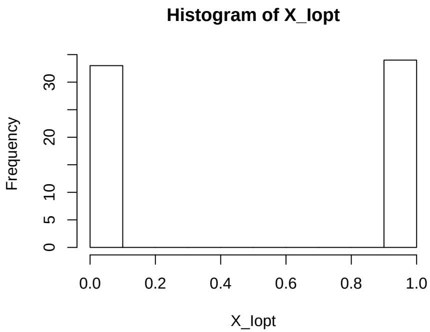
```
# Total PE, Fast Alg Crit, One-at-a-Time Alg Crit
c(TPE_aopt, c1_aopt, c2_aopt)
```

```
## [1] Inf Inf Inf
```

Design generated by I-Optimal Criterion

Using `AlgDesign` package (using Federov's exchange algorithm),






```r
mean(X_Iopt)
```

```
## [1] 0.5059836
```

```r
sd(X_Iopt)
```

```
## [1] 0.4860835
```

Evaluations

```
# Expected Post Probs and BF01 : Y | H0 Sims
c(expect_post_H0_YH0iopt, expect_post_H1_YH0iopt, BF01_YH0:
```

```
## [1] 0.6703644 0.3296356 2.0336530
```

```
# Expected Post Probs and BF01 : Y | H1 Sims
c(expect_post_H0_YH1iopt, expect_post_H1_YH1iopt, BF01_YH1:
```

```
## [1] 0.3296856 0.6703144 0.4918372
```

```
# Slope Variance
v_iopt
```

```
## [1] 0.0006717665
```

```
# Total PE, Fast Alg Crit, One-at-a-Time Alg Crit
c(TPE_iopt, c1_iopt, c2_iopt)
```

```
## [1] Inf Inf Inf
```

The Table

Results!

	Fast	1atTime	Random	Space	D-opt	A-opt	I-opt
H0 | Y, H0	0.8745	0.8834	0.7302	0.737	0.6703	0.6328	0.6704
H1 | Y, H0	0.1255	0.1166	0.2698	0.263	0.3297	0.3672	0.3296
BF01 | Y, H0	6.966	7.579	2.73	2.803	2.033	1.723	2.034
H0 | Y, H1	0.1232	0.1148	0.2695	0.2618	0.3297	0.367	0.3297
H1 | Y, H1	0.8768	0.8852	0.7305	0.7382	0.6703	0.633	0.6703
BF01 | Y, H1	0.1406	0.1297	0.3701	0.3547	0.4918	0.5798	0.4918
Var Slope	0.00299	0.0033	0.001842	0.001809	0.0006681	0.0006925	0.0006718
TPE	2820000	2868000	955300000	Inf	Inf	Inf	Inf
Fast Crit	44460	43740	767600000	Inf	Inf	Inf	Inf
1atTime Crit	94060	92200	770800000	Inf	Inf	Inf	Inf
Mean(D)	0.6837	0.6886	NA	0.5	0.507	0.4234	0.506
sd(D)	0.2297	0.2187	NA	0.2952	0.4874	0.4808	0.4861

- Fast & One-at-a-Time Algorithms have highest expected Bayes Factors (when the H_0 is true, lowest when H_A is true), and hence are better for testing.
- They also have higher variance on $\hat{\beta}$, though, which means they are not as accurate in estimating β. As expected, the D-optimal design is best for estimation.
- Also noticed values of `Inf` for the space-filling and D-optimal designs in the evaluations of each of the 3 criteria. This is to be expected in the D-optimal designs, since they include `0` which has gives as Wasserstein distance of 0 (in the denominator). Underestimated these by using maximum evaluation for q over i, j, instead. D-optimal design - though best for estimating, is worst in criteria evaluations, as a consequence.